Active

Project #: E-20-X79 Cost share #: E-20-361 Rev #: 3
Center # : 10/24-6-R7945-1A0 Center shr #: 10/22-1-F7945-1A0 OCA file #:
Work type : RES
Contract#: U50/ATU499828-01 Mod #: CARRY FORWARD Document : COOP AG
Prime #: Contract entity: GTRC

Subprojects ? : N CFDA: 93.161
Main project #: PE #:

Project unit: CIVIL ENGR Unit code: 02.010.116
Project director(s):
ARAL M M CIVIL ENGR (404)894-2243

Sponsor/division names: DHHS/PHS/OSHA-ATLANTA / ATLANTA, GA
Sponsor/division codes: 108 / 011

Award period: 930930 to 950929 (performance) 951229 (reports) //

Sponsor amount	New this change	Total to date
Contract value	(11,216.00)	443,609.00
Funded	(11,216.00)	443,609.00
Cost sharing amount		23,933.00

Does subcontracting plan apply ?: N

Title: RESEARCH PROGRAM ON EXPOSURE DOSE RECONSTRUCTION & MULTIMEDIA SIMULATION TOOL

PROJECT ADMINISTRATION DATA

OCA contact: E. Faith Gleason 894-4820

Sponsor technical contact

CINDY WILLIAMS, MAILSTOP E-32
(404)639-0649

AGENCY FOR TOXIC SUBSTANCES AND
DISEASE REGISTRY
DIVISION OF HEALTH ASSESSMENT
16000 CLIFTON ROAD, N.E.
ATLANTA, GA 30333

Sponsor issuing office

HENRY CASSELL, III, MAGGIE SLAY
(404)842-6797

PROCUREMENT AND GRANTS OFFICE
CENTERS FOR DISEASE CONTROL
255 E. PACES FERRY ROAD, NE
ROOM 300, MAILSTOP E-13
ATLANTA, GA 30305

Security class (U,C,S,TS) : U
ONR resident rep. is ACO (Y/N): N
Defense priority rating :
supplemental sheet
Equipment title vests with: Sponsor X GIT
PROVIDE A COPY OF TITLE TO THE SPONSOR (ATSDR)
Administrative comments -
CARRY FORWARD FROM 01 YEAR BUDGET TO 03 (E-20-W89). PROJECT END DATE CHANGED TO 9/29/95. EACH YR MUST BE ACCOUNTED FOR SEPARATELY AND WILL HAVE A NEW #.

GEORGIA INSTITUTE OF TECHNOLOGY
OFFICE OF CONTRACT ADMINISTRATION

NOTICE OF PROJECT CLOSEOUT

Closeout Notice Date 10/03/95

Project No. E-20-X79 Center No. 10/24-6-R7945-1A0

Project Director ARAL M M School/Lab CIVIL ENGR

Sponsor DHHS/PHS/OSHA-ATLANTA/ATLANTA, GA

Contract/Grant No. U50/ATU499828-01 Contract Entity GTRC

Prime Contract No.

Title RESEARCH PROGRAM ON EXPOSURE DOSE RECONSTRUCTION & MULTIMEDIA SIMULATION

Effective Completion Date 950929 (Performance) 951229 (Reports)

Closeout Actions Required:	Y/N	Date Submitted
Final Invoice or Copy of Final Invoice	N	
Final Report of Inventions and/or Subcontracts	N	
Government Property Inventory & Related Certificate	N	
Classified Material Certificate	N	
Release and Assignment	N	
Other	N	

Comments
CONTINUED BY E-20-W89.

Subproject Under Main Project No.

Continues Project No.

Distribution Required:

Project Director	Y
Administrative Network Representative	Y
GTRI Accounting/Grants and Contracts	Y
Procurement/Supply Services	Y
Research Property Managment	Y
Research Security Services	N
Reports Coordinator (OCA)	Y
GTRC	Y
Project File	Y
Other	N
	N

E-20-X79

Georgia Tech

School of Civil and Environmental Engineering

Georgia Institute of Technology
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MEMORANDUM

To : **Mr. Henry S. Cassell, III**
Grants Management Officer, Grants Management Branch
Centers for Disease Control and Prevention
Ms. Maggie Slay
Project Specialist, Grants Management Branch
Centers for Disease Control and Prevention

From : **Dr. M. M. Aral**
Project Director, School of Civil Engineering, Georgia Tech

Copy : **Dr. Allen Susten**, Project Director, ATSDR - DHHS
Mr. Morris Maslia, Technical Project Officer, ATSDR - DHHS
Ms. Janis Goddard, Office of Contract Administration, Ga. Tech.

Date : **April 17, 1995**

Subject : Annual Progress Report and other Technical Reports Submitted to ATSDR
Award No. U61/ATU499828-02

The purpose of this memorandum is to provide CDC&P Grants Management Office a response to their letter dated 4/12/95 regarding the annual and other technical reports submitted to ATSDR for the above referenced project. Our contract reporting requirements indicate that an "Annual Performance" report is due no later than 90 days after the end of each budged period.

During 1993-1994 contract period the following technical reports, software packages and annual progress report were submitted to ATSDR.

i) **Annual Progress Report and Application for Extension, RESEARCH PROGRAM FOR EXPOSURE-DOSE RECONSTRUCTION,** June 27, 1994, Submitted to CDC&P Grants Management Branch.

ii) **SOFTWARE TOOLS SUBMITTED TO ATSDR, USDHHS**

(a) Site **R**anking **S**ystem	(SRS Version 1.10)
(b) **A**nalytical **C**ontaminant **T**ransport analysis **S**ystem	(ACTS Version 1.10)
(c) **HAZ**ardous Substance **D**atabase **A**nalysis **T**ool	(HAZDAT Version 1.10)
(d) **GIS** Interphase **SYS**tem	(GIS-SYS Version 1.10)

iii) **TECHNICAL REPORTS SUBMITTED DIRECTLY TO ATSDR AND PUBLISHED JOINTLY WITH ATSDR TECHNICAL PERSONNEL**

a) **Aral, M. M.**, Maslia, M. and Williams, R., "Integration of GIS and Environmental Transport Models for Exposure Assessment of Populations," *Water Resources Bulletin*, Vol. 30, No. 6, pp. 1025-1041, 1994.

b) Maslia, M., **Aral, M. M.**, Williams, R., Williams, S., Hayes, L. and Wilder, L., "Use of Computational Models to Determine Human Exposure Resulting from Remediation Activities at Hazardous Waste Sites," Proceedings of the Water Environment Federation Specialty Conference *How Clean is Clean*, 85p, January 10-13, 1993.

c) Maslia, M., **Aral, M. M.**, Williams, R., Williams, S., Hayes, L. and Wilder, L., "Use of Computational Models to Reconstruct and Predict Trichloroethylene Exposure," Proceedings of the International Congress on the Health Effects of Hazardous Waste, 22p, 1993.

d) **Aral, M. M.**, Maslia, M., and Williams, R., "Ground-Water Remediation Using Smart Pump-and Treat," *Ground Water Journal*, Discussion, Vol. 31, No. 4, pp. 680-681, 1993.

e) Maslia, M. L. and **Aral, M. M.**, "Health Implications Associated with Hazardous Waste Site Clean-Up Goals: A Case Study of Trichloroethylene (TCE) Contamination", <u>Proceedings of the Annual Meeting of the Geological Society of America</u>, Boston, 1993.

f) Maslia, M. L. and **Aral, M. M.**, "Analysis of Populations Exposed to Groundwater Contaminated with Trichloroethylene (TCE) at the Gratuity Road Site, Groton, Massachusetts", Submitted to ATSDR, July 12, 1993.

g) Maslia, M. L. and **Aral, M. M.**, "Conducting Exposure Assessment of Populations by Integrating Environmental Transport Models, Demographic Analysis, and Geographic Information Systems", <u>Proceedings of the International Symposium on Assessing and Managing Health Risks from Drinking Water Contamination: Approaches and Applications</u>, Rome, Italy, September 1994.

Among the submittals listed above, the software tools were directly submitted to ATSDR technical project officer since they were technical application packages to be reviewed and implemented by technical project personnel at ATSDR.

The annual progress report was submitted to CDC&P, Grants Management Branch on June 27, 1994. A copy of this report is enclosed to this letter.

The other technical publications which are the outcome of the Exposure-Dose Reconstruction project efforts were directly submitted to ATSDR project personnel since they are technical contributions to be reviewed by the technical project personnel of ATSDR. A copy of these technical reports are also enclosed to this letter.

Similar submittals are being made for the project period 1994-1995. An annual progress report will be submitted to CDC&P, Grants Management Branch during June 1995. I hope the information provided in this letter answers the questions posed in your letter dated 4/12/95. If you have any further questions please do not hesitate to contact me at the above telephone numbers and address.

Progress Report and Application for Extension

RESEARCH PROGRAM FOR EXPOSURE-DOSE RECONSTRUCTION

Submitted to:

Agency for Toxic Substances and Disease Registry (ATSDR)

Project Officer: Allan S. Susten, Ph.D. (DHAC, MS E-32)
Technical Project Officer: Morris L. Maslia, P.E. (DHAC, MS E-32)

Submitted by:

Mustafa M. Aral, Ph.D.

Principal Investigator
School of Civil Engineering
Georgia Institute of Technology
Atlanta, Georgia 30332

Project Year: 2

June 27, 1994

TABLE OF CONTENTS

REVIEW OF RESEARCH ACTIVITIES FOR PROJECT YEAR 1

The cooperative agreement on Exposure-Dose Reconstruction Project (EDRP) was awarded towards the end of September 1993. Since then our efforts focused on several tasks of the research program in order to start the project in a most efficient and cost effective manner. A description of these activities and the progress made in each activity are given below.

- **Purchase of the computational equipment and establishing an ethernet communication line between ATSDR and Ga. Tech:**

  The initial phase of the purchase of the computer equipment necessary for the project has been completed. We anticipate that we will be adding to this equipment throughout the duration of the project as future needs arise. The equipment purchased for the Exposure Dose Reconstruction Research program is compatible with the present standards and other computational equipment used by ATSDR. Utilizing this equipment direct communication between ATSDR and Ga. Tech has been established through ethernet communication platform. It is anticipated that this communication line will accelerate the data exchange requirements of the research program in the future.

- **Development of the analytical framework for the prediction of contaminant migration scenarios in multiple exposure pathways:**

  It is anticipated that the contaminant migration analysis (the forward pathway calculation environment) will include several analytical tools to evaluate the contaminant concentration levels in multiple and interactive pathways. These pathways, at a minimum, will include the following:

  (i) air pathway;
  (ii) ground-water pathway;
  (iii) surface water pathway; and,
  (iv) soil pathway.

  According to the proposed schedule of the research program, the analytic tools for these pathways will be developed throughout the duration of the project. However, during the first project year, it was extremely important to conceptualize the overall system and develop a unified analytical structure and a user friendly framework for this computational environment. As parts of the overall system are developed, and several analytical tools are put together, this unified structure will provide the framework necessary for a user friendly computational environment. This approach will also minimize the revisions that will be necessary during the later stages of the research program. This task, although may not be in its final form, is completed and initial computational tools developed for the ground-water pathway is submitted to ATSDR within this framework.

- **Development of the preliminary structure of a unified user friendly environment for a "forward" calculation productivity tool:**

In the next stage of the computational tool development, the conceptualization developed above needs to be integrated in a practical and user friendly analytical computational tool. This can only be accomplished if the complex analytical exposure pathway analysis methods can be integrated in a seamless computational environment. This environment should also provide tools for graphical presentation of results, for immediate interpretation of the analytical solutions. The preliminary computational software tool submitted to ATSDR for the ground-water pathway, during the first period of the research program, may describe our line of thought in this effort. In this tool several analytic solutions for the ground-water pathway was developed along with a graphical and text output format interphase which may be used to interpret the results. This software will be updated throughout the project period to include analytical tools for other pathways as well as other revisions that may be recommended by ATSDR. In its present form the computational tool submitted to ATSDR can be used to evaluate concentration distributions in site specific cases for the ground-water pathway. The software developed can be installed in ATSDR's network system for immediate access by all health professionals. At the present this computational tool is tested and used successfully in several site specific applications by ATSDR professionals.

- **Development of user friendly GIS interface programs:**

It is our understanding that ATSDR's needs for computational tools in the area of health assessment is multilevel. The range of complexity of these tools may vary between screening tools, similar to the analytical computational environment described above, to the sophisticated GIS integrated multimedia modeling tools which may be used to analyze more complex cases. Given the number of sites that needs to be analyzed by ATSDR periodically and given the variability in complexity of the contaminant migration pathways in these sites, there would be a need for sophisticated approaches as well as the screening tools. Thus, in addition to the analytical tool development phase of the project, we are also in the process of developing user friendly GIS interface programs to simplify the analysis steps necessary in these complex cases. Our initial efforts in this phase of the study was concentrated towards the development of a shell structure for the GISPlus software which is presently used by ATSDR. This shell program will simplify the manipulation of data structures within a GIS integrated computation and the interaction of the complex simulation tools with the GIS system. The preliminary shell structure submitted to ATSDR during the first period of the project may describe our line of thought in this effort. Although this shell program will be updated throughout the project period, in its present form it is being tested and used to evaluate site specific conditions for the ground-water pathway at ATSDR and Ga. Tech. In this effort, in addition to the general shell structure submitted to ATSDR, certain coordinate transformation routines and data base generation routines, compatible with the existing ground-water flow and contaminant transport models, has been developed and submitted to

ATSDR for beta testing. These codes were tested and used successfully in six site specific applications by ATSDR professionals during the first year of the research program.

- **Development of a GISPlus integrated automatic mesh generation routine for numerical idealization of solution domains**:

The most important and also the most time consuming component of application of the finite element method to site specific case studies is the development of a suitable mesh to idealize the analysis region. To accomplish this task in a most efficient way, a GIS integrated mesh generation routine was developed and submitted to ATSDR during the first phase of the research program. This mesh generation routine is now in use by professionals at ATSDR to analyze ground-water pathway problems.

- **Adaptation of existing ground-water flow models to GISPlus software**:

The PC-based GIS system in use at ATSDR is the GISPlus system. The implementation of existing ground-water pathway analysis tools required substantial revision of these codes to make them compatible with the GISPlus system. Although this is an ongoing task, our initial efforts provided ATSDR with these tools which are now in use in predicting ground-water flow patterns in several sites of interest to ATSDR. These codes were tested and used in six site specific applications by ATSDR professionals during the first period of the research program and the results are shared with several federal and state agencies involved in the program.

- **Development of Hazardous Substance Data Base Analysis Tool**:

The Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), as amended by the Superfund Amendments and Reauthorization Act (SARA), establishes certain Requirements for ATSDR and EPA with regard to hazardous substances which are most commonly found at facilities on the CERCLA National Priorities List (NPL). Section 104(i)(2) of CERCLA, as amended (42 U.S.C. 9604(i)(2), required that the two agencies prepare a list, in order of priority, of at least 100 hazardous substances that are most commonly found at facilities on the NPL and which, in their sole discretion, are determined to pose the most significant potential threat to human health. CERCLA also required the agencies to revise the priority list to include 100 or more additional hazardous substances, and to include at least 25 additional hazardous substances in each of the three successive years following the 1988 revision. The computational procedures used in this analysis is described in the document "Support Document for the CERCLA 104 Priority List of Hazardous Substances that will be the Subject of Toxicological Profiles," [ATSDR, 1992]. In the computational tool prepared and submitted to ATSDR on January 1993, this process is automated in a user friendly environment. Using this tool new chemicals can be added to the list, prioritized and ordered with relative ease.

SOFTWARE TOOLS SUBMITTED TO ATSDR, USDHHS

During the first year of the cooperative agreement the following computational software were submitted to ATSDR for their evaluation and beta testing. Some of this software are still in the development stage and should not be considered to be a final product. All of these products are presently used by ATSDR health assessors in evaluating health consequences of contaminants released to subsurface pathways.

(i)	**S**ite **R**anking **S**ystem	(SRS Version 1.10)
(ii)	**A**nalytical **C**ontaminant **T**ransport analysis **S**ystem	(ACTS Version 1.10)
(iii)	**HAZ**ardous Substance **D**atabase **A**nalysis **T**ool	(HAZDAT Version 1.10)
(iv)	**GIS** Interphase **SYS**tem	(GIS-SYS Version 1.10)

RESEARCH ACTIVITIES FOR PROJECT YEAR 2

As the first year effort, the progress made in all of the activities summarized above are substantial. Our ongoing efforts will be directed towards the completion of these task and improving the tools we are developing for ATSDR during the next three years of the project period. In this effort, additional pathways described above will be incorporated into the computational environment. These tools will be periodically submitted to ATSDR for their evaluation and beta testing.

The primary pathway that will be analyzed during the second project period is selected to be the air pathway. Analytical tools that will be developed to evaluate exposure in this pathway will include, vapor emission models and both Box and Gaussian dispersion models. Details of this computational processes were described in the original proposal submitted to ATSDR which will not be repeated here.

More importantly, during the second project year, we will concentrate on evaluating uncertainties involved in these computations and the effect of these uncertainties on the numerical results generated. Implementation of analytical tools in all pathways requires a number of input parameters including source-specific, media-specific, and chemical-specific variables. Typically, the values of these parameters are not known exactly due to measurement errors and/or inherent spatial and temporal variability. Therefore, it is often more appropriate to express these parameter values in terms of a probability distribution rather than a single deterministic value and use an uncertainty propagation model to assess the effect of the variability on the output of the models. Most suitable method that can be employed for this purpose is the Monte Carlo method. Based on the principles of this approach, the following procedure will be incorporated to the computational method developed for ATSDR.

Whatever the source of the parameter uncertainty, the uncertainty can be quantified using a cumulative probability distribution. Thus, for each parameter to be analyzed as an uncertain variable, the user may select and assign a probability distribution (normal, log normal, uniform, exponential, triangular) for the variable and specify the parameters that describe the distribution. In Monte Carlo simulations, data sets randomly generated from these distributions form the basis of the data sets that will be used in deterministic models which in turn will generate a population of model outputs. This series of outputs can than be analyzed to yield a cumulative probability distribution of expected model results. This distribution quantitatively describes the uncertainty in the model output and can be used in decision making.

Thus, during the second project year, our goal is to introduce Monte Carlo simulation tools into the overall computational framework developed in the first project year. With this component added to the system, users will have the choice to select between direct calculations (deterministic mode computations) and Monte Carlo simulations in all pathway analysis exercises based on the confidence they have on the parameters they are using in their applications. With the addition of Monte Carlo methods, the flexibility and reliability of the computational system will be improved and the applicability of the overall system will be enhanced.

TECHNICAL PUBLICATIONS

Based on the progress made during the first year of the research program, several technical publications were published or submitted for publication. The following technical publications were accepted for publication in refereed journals or were accepted for inclusion in the proceedings of the conferences listed below.

1. **Aral, M. M.**, Maslia, M. and Williams, R., "Integration of GIS and Environmental Transport Models for Exposure Assessment of Populations," *Water Resources Bulletin*, (submitted for publication), 1993.

2. Maslia, M., **Aral, M. M.**, Williams, R., Williams, S., Hayes, L. and Wilder, L., "Use of Computational Models to Determine Human Exposure Resulting from Remediation Activities at Hazardous Waste Sites," Proceedings of the Water Environment Federation Specialty Conference *How Clean is Clean*, 85p, January 10-13, 1993.

3. Maslia, M., **Aral, M. M.**, Williams, R., Williams, S., Hayes, L. and Wilder, L., "Use of Computational Models to Reconstruct and Predict Trichloroethylene Exposure," Proceedings of the International Congress on the Health Effects of Hazardous Waste, 22p, 1993.

4. **Aral, M. M.**, Maslia, M., and Williams, R., "Ground-Water Remediation Using Smart Pump-and Treat," *Ground Water Journal*, Discussion, Vol. 31, No. 4, pp. 680-681, 1993.

5. Maslia, M. L. and **Aral, M. M.**, "Health Implications Associated with Hazardous Waste Site Clean-Up

Goals: A Case Study of Trichloroethylene (TCE) Contamination", Proceedings of the Annual Meeting of the Geological Society of America, Boston, 1993.

6. Maslia, M. L. and **Aral, M. M.**, "Conducting Exposure Assessment of Populations by Integrating Environmental Transport Models, Demographic Analysis, and Geographic Information Systems", Proceedings of the International Symposium on Assessing and Managing Health Risks from Drinking Water Contamination: Approaches and Applications, Rome, Italy, September 1994.

PROPOSED BUDGET AND JUSTIFICATION

With this proposal continuation of the cooperative agreement between ATSDR USDHHS and Georgia Institute of Technology is proposed. The second year budget for the services of the personnel and other resources are itemized below.

Budget summary for second year :

	ATSDR Funds Allocated to the Project	Matching Funds Source GA.TECH
a. Salaries and Wages :		
Principal Investigator	$ 30,000.00	$ 9,000.00
Research Faculty	$ 10,000.00	--
Research Engineer	$ 30,000.00	--
Five full time Ph.D. students	$ 75,000.00	--
Two full time M.S. students	$ 14,000.00	--
Secretarial Support	$ 2,500.00	--
Total (excluding students)	$ 72,500.00	$ 9,000.00
Total (including students)	$161,500.00	
b. Fringe Benefits :		
25.1 % of salaries (excluding students)	$ 18,198.00	$ 2,259.00
c. Supplies :	$ 6,000.00	--
d. Publication costs :	$ 0.00	--
e. Travel :	$ 4,000.00	--
f. Equipment (computer/hardware):	$ 30,000.00	--
g. Total direct costs :	$219,698.00	$ 11,259.00
h. Indirect costs :		
37 % of Direct Costs (excluding equipment)	$ 70,188.00	$ 4,166.00
i. Total amount proposed :	$289,886.00	$ 15,425.00
j. GA.TECH share for the second year :	--	$ 15,425.00
k. ATSDR share for the second year:	$ 289,886.00	--

Justification of Budget :

The proposed budged will be primarily used to underwrite graduate and post-graduate student research funds, and secondarily to support release time for the research faculty. This approach will foster the training of professionals specialized in this much needed area of research and increase the awareness of engineering and science students on health related issues. This trained resource pool will be of vital importance to ATSDR's and also to other federal and state health organization's needs in the future. Part of the research funds requested will be used to purchase certain computer equipment and software. The main purpose of this purchase is to develop the proposed simulation tools on computational platforms which are similar to the computational and data processing environment available at ATSDR and utilize the most recent and advanced software available in the literature. The compatibility between the computational systems at ATSDR and Ga. Tech is essential and will definitely simplify the technology transfer phase of the proposed study. These dedicated computational equipment will only be used by the graduate students and research scientists for the exclusive purposes of the proposed study.

Budget Breakdown:

Personnel	Annual Salary	Percentage of effort	No. of Months	Amount Requested(Federal Funds)
Principal Inv.	$ 70,000	50 %	6	$ 30,000.00
Research Fac.	$ 70,000	15 %	2	$ 10,000.00
Research Eng.	$ 30,000	100 %	12	$ 30,000.00
1 PhD Student	$ 15,000	33 %	12	
Total PhD Students (5)				$ 75,000.00
1 MS Student	$ 7,000	33 %	9	
Total MS Students (2)				$ 14,000.00
Secretary	$ 25,000	10 %	1.5	$ 2,500.00

Principal Investigator : Dr. M. M. Aral is the principal investigator of the Exposure Dose Reconstruction Research program. He is the main contributor and the coordinator for all research activities in the proposed program. His contribution and time will form the nucleus of all research activities proposed in this program.

Research Faculty: On an as needed basis services of several other faculty members will be requested under this category.

Research Engineer: Our first year research efforts clearly indicate there is a need for a full time programmer in this research programs. A research engineer will be hired to fill this position.

PhD Students (5 students) Contribution of several PhD students are an essential element of this research program. At the present there are three PhD students working in the program. It is anticipated that this number will increase to five during the second project year.

MS Students (2 students) Contribution of several MS students are an essential element of this research program. At the present there are two MS students working in the program. We do not anticipate an increase in this number.

Fringe Benefits:

Fringe benefits are applicable to direct salaries and wages of all personnel excluding students. The present fringe benefit rate is 25.1 %. This rate may change during the academic year 1994-95. However, this change will not effect the total amount requested from federal funds for the second year of the cooperative agreement.

Travel:

It is expected that the principal investigator will participate in at least two conferences during the academic year 1994-95 related to the research program topic. The funds in this category will be only used by the principal investigator for this purpose. The details of these conferences, their location and travel costs will be itemized and submitted to ATSDR towards the end of August 1994. The total cost of this category will be within the limits allocated for the program ($ 4,000.00).

Equipment:

We anticipate that we will be adding to the initial equipment purchased throughout the duration of the project as future needs arise. The equipment purchased for the Exposure Dose Reconstruction Research program is compatible with the present standards and other computational equipment which is used by ATSDR and will remain the property of ATSDR. We anticipate to purchase four more computers, a scanner and a printer for the research program. The total cost of this equipment will be within the limits allocated for the program ($ 30,000.00).

Supplies:

The computational tools developed for the program requires special software as utility tools. We anticipate to purchase these tools and use them in or research efforts. The total cost of this supplies purchase will be within the limits allocated for the program ($ 6,000.00).

Contractual: None

Consultant: None

Other: None

Indirect Costs:

Overhead rates are applicable to direct salaries and wages of all personnel and other expenses excluding equipment purchases. The present overhead rate is 37 %. This rate may change during the academic year 1994-95. However, this change will not effect the total amount requested from federal funds for the second year of the cooperative agreement.

Biographical Sketch

Dr. Mustafa M. Aral

Personal Data Summary

Born	: February 26, 1945, Ankara, Turkey
Citizenship	: U.S.A.
Home Address	: 2974 Cravey Dr. NE., Atlanta, GA. 30345

Business Address

School of Civil Engineering
Georgia Institute of Technology
Atlanta, Georgia 30332
Buss. Phone : (404) 894-2243 / (404) 894-5111

Professional Registration

Professional Engineer : GA : 15254
Professional Ground Water Hydrologist, National Registration : No.: 649

Educational Background

School of Civil Engineering, Georgia Institute of Technology, Ph.D. in Water Resources Engineering with minor in Numerical Analysis and Applied Mathematics, September 1971.

School of Civil Engineering, Georgia Institute of Technology, M.S. in Civil Engineering with major in Environmental and Water Resources Engineering, June 1969.

Department of Civil Engineering, Middle East Technical University (Ankara, Turkey), B.S. in Civil Engineering, June 1967.

Professional Experience

1983-Present	Associate Professor	School of Civil Engineering, Georgia Institute of Technology.
1978-1983	Visiting Professor	School of Civil Engineering, Georgia Institute of Technology.
1974-1983	Adjunct Professor	At Marine Sciences Department, Civil Engineering Department, Engineering Science Department, Middle East Technical University.
1977-1983	Associate Professor	Mathematics Department, Middle East Technical University.

Professional Experience (cont.)

1975-1978	Assistant Chairman	Mathematics Department, Middle East Technical University.
1971-1977	Assistant Professor	Mathematics Department, Middle East Technical University.

Publications

42. **Aral, M.M.**, Ground Water Modeling in Multilayer Aquifers - Steady Flow, *Lewis Publishers Inc.*, February, 1990 (Book).

43. **Aral, M.M.**, Ground Water Modeling in Multilayer Aquifers - Unsteady Flow, *Lewis Publishers Inc.*, March, 1990 (Book).

44. Tang, Y., and **Aral, M. M.**, Contaminant Transport in Layered Porous Media: A. General Solution, *Water Resources Research*, Vol. 28, No. 5, pp. 1389-1397, 1992.

45. Tang, Y., and **Aral, M. M.**, Contaminant Transport in Layered Porous Media: B. Applications, *Water Resources Research*, Vol. 28, No. 5, pp. 1399-1406, 1992.

46. Ratzlaff, S., **Aral, M. M.**, and Alkhayyal, F., Optimal Capture Zone Design Using Segmental Velocity Direction Constraints, *Groundwater Journal*, Vol. 30, No. 4, pp. 607-612, 1992.

47. **Aral, M. M.**, and Tang, Y. Flow Against Dispersion in Two Dimensional Aquifers, *Journal of Hydrology*, Vol. 140, pp. 261-277, 1992.

48. Maslia, M., **Aral, M. M.**, and Houlihan, M., "Evaluation of Ground-Water Flow Regime at a Landfill with Liner System," *Journal of Environmental Science and Health*, Vol. A27, No. 7, pp. 1793-1816, 1992.

49. Maslia, M., **Aral, M. M.**, and Gill, H. E., "The Importance of Hydrogeologic Controls on Remedial Action Alternatives," *Geophysical Society of America*, Southeastern Section Meeting, Contaminant Hydrogeology Session, Vol. 24, No. 2, pp. 53, 1992.

50. Maslia, M., **Aral, M. M.**, Williams, R., Williams, S., Hayes, L. and Wilder, L., "Use of Computational Models to Determine Health Implications of Human Exposure Resulting from Remediation Activities at Hazardous Waste Sites," Report for: *Division of Health Assessment and Consultation, DHHS-ATSDR*, 20p, November 5, 1992.

51. **Aral, M. M.**, Maslia, M. and Williams, R., "Integration of GIS and Environmental Transport Models for Exposure Assessment of Populations," *Water Resources Bulletin*, (submitted for publication), 1993.

52. Maslia, M., **Aral, M. M.**, Williams, R., Williams, S., Hayes, L. and Wilder, L., "Use of Computational Models to Determine Human Exposure Resulting from Remediation Activities at Hazardous Waste

Sites," Proceedings of the Water Environment Federation Specialty Conference *How Clean is Clean*, 85p, January 10-13, 1993.

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Expertise Areas

Research, teaching and engineering experience in the following specific areas :

- Fluid mechanics, Hydraulics Engineering
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- Evaluation of ground water and surface water monitoring data
- Ground water flow and contaminant transport modeling in aquifers
- Ground water resources evaluation and management
- Disposal and ground water quality effects of hazardous substances, aquifer remediation
- Saturated and unsaturated ground water flow analysis
- Miscible and immiscible ground water flow analysis
- GIS applications in environmental systems

USE OF COMPUTATIONAL MODELS TO RECONSTRUCT AND PREDICT TRICHLOROETHYLENE EXPOSURE

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INTRODUCTION

In this paper, we present a case study of the type frequently encountered by the Agency for Toxic Substances and Disease Registry (ATSDR), a Public Health Service agency of the U.S. Department of Health and Human Services. ATSDR is mandated by Congress to evaluate the public health threat of hazardous waste sites using environmental and health outcome data and community concerns. Results of this public health assessment process are published and disseminated to interested parties. For this study, we used the Gratuity Road site, located in the town of Groton, Massachusetts (Figure 1). Ground-water and surface-water contamination have occurred near Gratuity Road in the town of Groton. A petitioned public health assessment for the Gratuity Road site identified the primary contaminants as trichloroethylene (TCE), 1,1,1-trichloroethane (TCA), hexavalent chromium (Cr^{+6}), chromium (Cr), and lead (Pb) [ATSDR, 1992]. The health assessment also indicated that off-site residential ground-water wells had been contaminated with TCE and TCA. For the present study, therefore, we analyzed exposure through one environmental medium, ground water, for a single contaminant, TCE (dissolved in ground water).

Because direct measures of historical exposure to TCE are unavailable for the Gratuity Road site, computational models were used to reconstruct and predict exposure to TCE. A critical database needed to estimate exposure is the temporal and spatial distribution of TCE contamination referenced to a geographical location. To obtain this data, we applied environmental transport models (ground-water flow and contaminant transport) to the Gratuity Road site. Using the output from these models, we then estimated human inhalation exposure to TCE during showering by use of empirical formulae developed from results of laboratory studies and compared these results with estimates of exposure by ingestion.

ENVIRONMENTAL TRANSPORT MODELS

In this study, the mathematical models used to describe ground-water flow and contaminant transport are solved by using finite element Galerkin procedures. Because this procedure is well established in the ground-water literature, only a brief review of the development of the governing equations is provided here. A more detailed description of the methodology can be found in a number of texts, including Pinder and Gray [1977].

The governing equation for two-dimensional, vertically averaged, steady-state flow in an unconfined aquifer is shown next:

$$\frac{\partial}{\partial x_i}\left(K_{ij} h \frac{\partial h}{\partial x_j}\right) - \sum_{m=1}^{w} Q_m \delta(x_m, y_m) - I = 0 \qquad (1)$$

where convention for tensor notation applies to indices i and j (i,j = 1,2 designate x, y, respectively), K_{ij} represents the hydraulic conductivity tensor of the unconfined aquifer, h is the piezometric head in the aquifer, w is the number of wells, Q_m is the pumping rate for well m, $\delta(x_m, y_m)$ is the Dirac delta function evaluated at (x_m, y_m), and I is the infiltration or leakage flux into or out of the aquifer, which is a function of piezometric head distribution in adjacent aquifers. The governing equation for an unconfined aquifer is nonlinear because the location of the position of the water table is unknown; this location must be determined as a part of the solution through an iterative process. The associated boundary conditions for the ground-water flow problem can be given in terms of Dirichlet, Neuman, and Cauchy conditions, which are shown below for an unconfined aquifer:

$$\begin{aligned} h &= h_c && (x, y) \in \Gamma_1{}^h \\ n_i\left(h K_{ij} \frac{\partial h}{\partial x_j}\right) &= f_h && (x, y) \in \Gamma_2{}^h \\ n_i\left(h K_{ij} \frac{\partial h}{\partial x_j}\right) &= F_1 + F_2 h && (x, y) \in \Gamma_3{}^h \end{aligned} \qquad (2)$$

where n_i is the component of the outward normal to the boundary of the solution domain, and f_h, F_h, and h_c are functions defined on the boundary.

The governing equation for the two dimensional, vertically averaged, convective-dispersive transport of a miscible contaminant can be given as follows:

$$R\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - V_i \frac{\partial C}{\partial x_i} + \sum_{m=1}^{w} \frac{Q_m (C - C_p)}{B n} \delta(x_m, y_m) - \lambda C \qquad (3)$$

where C is the contaminant concentration, R is the retardation factor, D_{ij} is the hydrodynamic dispersion tensor, V_i are the pore velocities in x and y directions, C_p is the concentration of the pumped water, B is the aquifer thickness, n is the aquifer porosity, λ is the first order decay constant, and Q_m, w, and $\delta(x_m, y_m)$ are as defined in Equation (1). Boundary and initial conditions for a contaminant transport problem can be defined as follows:

$$\begin{aligned} &C=C_o \quad (x,y)\in\Omega \quad ; \quad t=t_o \\ &C=C_c \quad (x,y,)\in\Gamma_1 \quad ; \quad t\geq t_o \\ &n_i\left[nB\left(V_i-D_{ij}\frac{\partial C}{\partial x_j}\right)\right]=f_c \quad (x,y)\in\Gamma_2 \quad ; \quad t\geq t_o \end{aligned} \tag{4}$$

The retardation factor, R, is equal to $(1 + K_s)$, where K_s is the adsorption solubility rate constant defined in terms of the bulk density and porosity of the soil and the partition coefficient, which is a function of organic carbon content of soil and octanol water partition coefficient of the chemical constituent. The pore velocities are defined using Darcy's Law:

$$\begin{aligned} V_x &= -\frac{K_{xx}}{n}\frac{\partial h}{\partial x} \\ V_Y &= -\frac{K_{yy}}{n}\frac{\partial h}{\partial y} \end{aligned} \tag{5}$$

where K_{xx} and K_{yy} are the hydraulic conductivities in the x and y directions as defined in Equation (1).

The diffusion tensor terms may be defined using the identities of Schiedegger [1961]:

$$\begin{aligned} D_{xx} &= \frac{\alpha_L V_x^2 + \alpha_T V_y^2}{|V|} \\ D_{yy} &= \frac{\alpha_L V_y^2 + \alpha_T V_x^2}{|V|} \\ D_{xy} = D_{yx} &= \frac{(\alpha_L - \alpha_T)\, V_x V_y}{|V|} \end{aligned} \tag{6}$$

where α_L and α_T are the longitudinal and transverse dispersivities of the porous media, and $|V|$ is the magnitude of the velocity vector.

Groundwater flow as described by Equations (1) and (2) is subject to the assumptions of two-dimensional, vertically averaged, steady-state (non-time varying) flow, recharge and discharge to and from streams and surface-water bodies, infiltration due to precipitation, and pumping and injection of water. The transport of contaminants described by Equations (3), (4) and (5) is subject to the assumptions of single species transport, variation of contaminant concentration with time, retardation, diffusion, and advection, contribution of contaminant concentration variation due to pumping, and injection, no volatilization or biodegradation of TCE, and no dynamic surface-water and groundwater transport interaction. A more detailed discussion of the limitations and assumptions of the equations of groundwater flow and contaminant transport can be found in a number of texts including Bear [1979], Freeze and Cherry [1979], and Pinder and Gray [1977].

In finite element analysis the solution domain is idealized by a network of elements. It is then assumed that the differential equation can be approximated by a series of independent basis functions defined in terms of the nodal values of the unknown function in each element. For example, when solving Equation (1), the piezometric head can be approximated as follows:

$$h \approx \sum_{i=1}^{n} N_i h_i \tag{7}$$

where N_i is the basis function at node i, n is the total number of nodes for an element, and h_i is the approximate value of the piezometric head at node i.

When Equation (7) is substituted in Equation (1) a residual will be generated. The best approximation is then achieved when the residuals are minimized by using a process known as the method of weighted residuals. The Galerkin method, a typical weighed residual method, minimizes residuals using the basis functions as the weighting functions. This residual or orthogonality condition can be defined as follows:

$$\sum_{e}^{N} \int_{A_e} N_k L(h) \, dA^e = 0 \tag{8}$$

where L is the differential operator defined as Equations (1) or (3), and N_k are the weighting functions. The integration is performed over an element, and the summation indicates the assembly of all elemental integral evaluations.

Using this process, Equation (1) can be written as follows for a typical element:

$$\iint_{A^e} N_l \left[\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right) - \sum_{m=1}^{w} Q_m \delta(x_m, y_m) - I\right] dA = 0 \quad ; \quad l = i, j, k \tag{9}$$

where i, j, and k refer to the nodal numbers of the element. The minimization of the residual over each element, the assembly of all elemental matrices, and the introduction of boundary conditions yield the following global matrix system:

$$[\,S\,]\{h\} = \{F\} \tag{10}$$

Equation (10) may now be solved for the piezometric head at each node after the introduction of appropriate boundary conditions.

The contaminant transport equation may also be analyzed using a similar process. In this case the contaminant transport solution is tied to the ground-water flow solution through Darcy velocity terms. Thus, in this sequential solution process Equation (1) is solved first followed by the solution of Equation (3). The weighed integral residual of the convective transport equation can be given as follows:

$$\begin{aligned} \iint_{A^e} N_l \Bigg[& R\frac{\partial C}{\partial t} - \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial C}{\partial x} + D_{xy}\frac{\partial C}{\partial y}\right) - \frac{\partial}{\partial y}\left(D_{yy}\frac{\partial C}{\partial y} + D_{yx}\frac{\partial C}{\partial x}\right) + V_x\frac{\partial C}{\partial x} \\ & + V_y\frac{\partial C}{\partial y} + \sum_{i=1}^{w} \frac{Q_m(C-C_p)}{Bn}\delta(x_m, y_m) + \lambda C \Bigg] dA = 0 \quad ; \quad l = i, j, k \end{aligned} \tag{11}$$

Minimization of the residual over each element and the assembly of all elemental matrices yield the following resultant matrix equations:

$$[M]\left[\frac{\partial C}{\partial t}\right]+[S][C]=[F] \tag{12}$$

After the introduction of boundary conditions, finite difference techniques are used in the solution of the above equation to determine the concentration for each node at each time step. This sequential solution process yields spatial and temporal distribution of contaminants at each node over the solution domain. This equation may be given as:

$$([M]+(1-\alpha)\Delta t[S])[C]^{t+\Delta t}=([M]-\alpha\Delta t[S])[C]^{t}+\left(F^{t}\right)+\left(F^{t+\Delta t}\right) \tag{13}$$

where Δt is the time step, α is a weighting factor that may vary from zero to one, and the superscripts identify the time at which matrices or vectors in Equation (13) are defined. Selecting $\alpha = 1$ corresponds to forward differencing. Central differencing is achieved by selecting $\alpha = 0.5$, and $\alpha = 0$ results in backward differencing [Aral, 1990a, b].

APPLICATION OF ENVIRONMENTAL TRANSPORT MODELS TO STUDY AREA

The environmental transport models described previously were used to evaluate the transport of the contaminant TCE at the Gratuity Road site. The site is underlain by a stratified glacial drift water-table aquifer that varies in thickness from a few feet to more than 50 feet. Historical data indicate that TCE contamination of ground water from the Conductorlab area (Figure 1) began during the mid-1960s [HMM Associates, Inc., 1988, 1990]. A 1985 environmental investigation revealed significant TCE contamination of ground water. By the summer of 1987 all Gratuity Road residences were connected to the Groton municipal water supply system. Thus, ongoing contamination of ground water with TCE and exposure of the population to the contaminated ground water occurred for approximately 20 years.

Our analysis began with a steady-state ground-water flow calibration using November 1989 water levels to determine flow field characteristics. The SLAM (<u>S</u>teady <u>L</u>ayered <u>A</u>quifer <u>M</u>odel) code [Aral, 1990a] was used to simulate the ground-water flow field. The finite element idealization (or mesh) using three-nodal triangular elements is shown in Figure 2. For this study, the mesh consisted of 3,828 elements and 2,010 nodes. The selected model boundary and calibrated water levels, based on November 1989 field data, are shown in Figure 3. The boundary adjacent to the Nashua River was simulated as a Dirichlet boundary and assigned a value of 200 ft (referenced to sea level datum), the stage of the river. The eastern boundary was simulated as a Neuman boundary and assigned a value of 0.002 ft/d (feet per day). The top and bottom boundaries also were simulated as Neuman boundaries and assigned a value of zero (no-flow). The calibrated infiltration rate due to precipitation was assumed to be constant over the model area and was assigned a value of 8.5 inches per year. Calibrated hydraulic conductivity values ranged from 0.5 to 22 ft/d, which were consistent with and within the range of field and laboratory derived values [HMM Associates, Inc., 1988, 1990]. As shown in Figure 3, the flow field is characterized by ground-water and surface-water interaction as indicated by the curvature of water-level contours near Tuity and Unamed Brooks. Graphical display of the calibrated velocity field and simulation of alternative flow-field scenarios are not presented here because of space limitations.

Aquifer contamination and proposed remediation were simulated by investigating two contaminant transport scenarios using the CLAM (Contaminant transport in Layered Aquifer Media) code [Tang and Aral, 1992]. In all simulations, we assumed a constant porosity of 0.35, a retardation factor of 3 for the dissolved TCE (HMM Associates, 1990) with no volatilization or biodegradation, and longitudinal and transverse dispersivities (α_L, α_T) of 64 and 8 ft, respectively. In the first scenario, we conducted a 40-year simulation with a maximum source concentration of 50,000 parts per billion (ppb) located at the assumed point of contamination in the Conductorlab area. Results of this simulation are shown in Figure 4 as temporal distributions of TCE. The contour lines represent the U.S. Environmental Protection Agency's (USEPA) maximum contaminant level (MCL) for TCE of 5 ppb for times of 5, 10, 15, 20, 30, and 40 years. Model results indicate, that after 20 years, ground water contaminated with TCE has migrated into the Gratuity Road and Anthony Drive areas and has encroached into nearby surface-water streams (Tuity Brook and Unamed Brook).

In the second scenario, we simulated a proposed pump-and-treat remediation plan by conducting a 20-year simulation with a maximum source concentration of 50,000 ppb and then removing the source from the site and pumping and injecting 20 gallons per minute (gpm) of water for another 20 years. Figure 5 shows the location of the 500 and 5 ppb TCE contours after 40 years (20 years of contamination and 20 years of pump-and-treat technology). Results indicate that, after 40 years, TCE concentrations in part of the source area have been reduced to less than 50 ppb. Downgradient of the site near Gratuity Road and Anthony Drive, however, an area of TCE contamination of more than 500 ppb, which represents the historical TCE contamination that has escaped the pump-and-treat remediation process, now exists [Aral et al., 1993]. Figure 6, a three-dimensional surface plot of the change in TCE concentration in the aquifer after 20 years of remediation, clearly illustrates the effect of remediation at the site (depression) and the downgradient migration of the noncaptured historical contamination (mound). The darker area surrounding the mound represents an increase in TCE concentration of 5 to 50 ppb after 20 years of remediation in areas of the aquifer previously uncontaminated .

Results of the contaminant transport simulations indicate that, after 20 years of contamination, some people living in the Gratuity Road area and using ground water were probably exposed to TCE that exceeds the MCL (5 ppb). Additionally, the simulations suggest that although the pump-and-treat technology may clean up the site and source area (Figure 6, depression area), populations downgradient from the site may still be at risk of exposure from TCE that exceeds the MCL (Figure 6, mound area).

VARIATION OF HYDRAULIC AND TRANSPORT PARAMETERS

Because measured values of hydraulic and transport parameters are unknown at every location within the modeling domain (Figure 2), it is important to understand and recognize the effect of possible variation in the parameter values on modeling results. For example, the use of November 1989 water levels was justified by comparing long-term (1951-1980) monthly mean precipitation (3.99 inches) from the Ashburn, Massachusetts weather station with monthly precipitation for November 1989 (4.1 inches). Because there is no large-scale regional pumping near Groton, groundwater levels are influenced by increases and decreases in precipitation which result in increased or decreased infiltration to the aquifer. Thus, to simulate a period of higher groundwater levels (for example, May 1989), infiltration input to the model would have to be increased.

Although the variation of any parameter valuable may result in some change in simulation results, by far the most significant changes occur (with respect to the movement of TCE) when transport parameters such as retardation (R), porosity (n), and dispersivity (α_L, α_T) are changed in value. A sensitivity analysis was conducted by varying the values of retardation, porosity, and longitudinal and transverse dispersivity from the values previously described. A series of simulations were conducted and the values of the parameters are listed in Table 1 for each simulation. Results of the simulations are displayed as a series of line graphs of time in years on the abscissa and TCE concentration on the ordinate (Figure 7). With simulation number "RUN00" being the original parameter values previously described, the most sensitive parameter to variation is retardation. The change in this parameter value has the effect of reducing or increasing the movement of the contaminant with respect to the mean velocity of groundwater. The value of the porosity of the aquifer is also sensitive to change as it results in the an increase or decrease of the fluid (pore) velocity, thereby advecting more or less contaminant. Thus, in order to improve the simulation, more refined estimates (based on field observations and measurements) of retardation and porosity would be necessary.

Table 1. Variation of transport parameter values.

RUN NUMBER	RETARDATION	POROSITY	DISPERSIVITY (FEET)	
			LONGITUDINAL	TRANSVERSE
RUN00*	3	0.35	64	8
RET1	1	0.35	64	8
RET10	10	0.35	64	8
RET15	15	0.35	64	8
POR15	3	0.15	64	8
POR25	3	0.25	64	8
POR45	3	0.45	64	8
DIS805	3	0.35	80	5
DIS4010	3	0.35	40	10

*Simulation using aquifer and transport parameters described above in section on "Application of Environmental Transport Models to Study Area"

EXPOSURE MODEL

Exposure models attempt to quantify a person's contact with a contaminant at a specific concentration for a specified duration of time. Total human exposure is composed of contributions from all environmental media (water, soil, air, and plants) that contain the contaminant, and all routes of entry to the human body (dermal contact, ingestion, and inhalation). From a mathematical perspective, total human exposure may be defined by the following equation:

$$E = \int_{t_1}^{t_2} C(t)\, dt \qquad \textbf{(14)}$$

where E is the exposure, $C(t)$ is the time-varying concentration of a contaminant, and dt is the time increment from t_1 to t_2.

Although total human exposure is described by Equation (14), data are usually insufficient to account for exposure from all environmental media and by every route of entry. Consequently, researchers and regulators have, in the past, focused their attention on exposure to hazardous substances from potable water supplies by the ingestion route. However, when contaminants (such as TCE) belonging to the class of compounds known as volatile organic chemicals (VOCs) are considered, evidence is mounting that entry by the route of inhalation may be as important as ingestion. For example, laboratory experiments using standard shower conditions have indicated that an average of 80% to 85% of TCE contained in the water supply for the shower volatilized into air [Wilder, 1986]. Therefore, exposure by the route of inhalation should be accounted for in exposure assessment studies involving VOCs.

For the present study, we will be using empirical equations that were derived from results of laboratory shower experiments in which TCE was added to the shower water supply to determine volatilization and inhalation characteristics. Because of space limitations, details of the laboratory experiments will not be provided herein, but can be found in Andelman [1990] and Wilder [1986]. The maximum contaminant concentration in the air during the shower can be described by the following equation:

$$C_{a_{max}} = k\,t\,C_w / V_a \qquad (15)$$

where Ca_{max} is the maximum contaminant concentration in the shower air in milligrams per liter (mg/L), k is the volatilization mass transfer coefficient in liters per minute (L/min), t is time in the shower in hours (h), C_w is the contaminant concentration in the shower water supply (mg/L), and V_a is the volume of the shower room (L). Assumptions used for the laboratory shower experiments are listed below in Table 2.

Using these standard assumptions, Equation (15) reduces to the following equation:

$$C_{a_{max}} = 4.5x10^{-3}\,C_w \qquad (16)$$

It can also be shown that for the given shower assumptions used in the laboratory experiments, after the shower period of time t, the average TCE concentration in the air C_a that an individual is exposed to is equal to Ca_{max} at time t (at the end of the shower) [Andelman, 1990].

Table 2. Assumptions used for laboratory shower experiments [Wilder, 1986].

SHOWER	CONTAMINANT	HUMAN
Flow rate in the shower: 8 L/min.	Fraction volatilization rate of TCE from shower water: 0.90.	Adult body weight: 70 kg.
Air exchange rate in the shower and shower room: 0.53/hr.	Rate of volatilization during the shower is constant.	Ingestion: 1.3 L of domestic water per day.
Volume of shower and shower room: 10,000 L.	Rate of decay of TCE in the shower room after shower is constant.	Inhalation rate at rest: 1,000 L of air per hour.
	Shower and shower room treated as a one-compartment model.	Takes one 6-minute shower per day, 365 days per year.
		Remains in shower room for 15 minutes after showering.

Inhalation exposures in the shower can be defined as the product of the concentration of the contaminant in the air, the breathing rate (for an adult), and the exposure time, such that:

$$E_i = C_a B t \tag{17}$$

where E_i is the exposure (mg), B is the breathing rate (L/h), and C_a and t are as previously defined. Assuming a human adult takes one shower per day (Table 2), using results of the laboratory experiments, inhalation exposure to TCE during showering can be defined by the following equation:

$$E_i = 1.35 C_w \tag{18}$$

where E_i is now defined as the exposure from inhalation of TCE in mg/d.

APPLICATION OF EXPOSURE MODEL TO STUDY AREA

As a result of the environmental transport simulations, the temporal and spatial distribution of TCE contamination for the study area was known. Thus, if the domestic water supply was obtained from ground water, the concentration of TCE in the water supply, C_w, for a specific point in time at a specific location would be known. Equation (14) can be solved using the concentration data derived from the environmental transport model to compute exposure to TCE. However, for illustrative purposes, we will compute exposure for only one point in time. After 20 years of remediation the concentration of TCE in ground water at a certain location in the study area is 250 ppb or 0.25 mg/L. Letting C_w = 0.25 mg/L, and inserting this value into Equation (15), the exposure an adult receives by the route of inhalation during and after a shower is computed as follows:

$$1.35 \text{ L/d} \times 0.25 \text{ mg/L} = 0.34 \text{ mg/d} .$$

Alternatively, if an adult ingests 1.3 liters of water per day, then the exposure by the route of ingestion can be computed as follows:

$$0.25 \text{ mg/L} \times 1.3 \text{ L/d} = 0.33 \text{ mg/d}.$$

Therefore, using concentration data from the study area in conjunction with laboratory determined inhalation parameters indicates that an adult would receive nearly the same exposure by the route of inhalation during and after showering as from ingestion of ground water contaminated with TCE.

SUMMARY AND CONCLUSIONS

In this paper, we presented a study of the type frequently encountered by ATSDR. Ground-water and surface-water contamination have occurred near the Gratuity Road site in the town of Groton, Massachusetts. A petitioned public health assessment for the Gratuity Road site identified the primary contaminants as trichloroethylene (TCE), 1,1,1-trichloroethane (TCA), hexavalent chromium (Cr^{+6}), chromium (Cr), and lead (Pb) [ATSDR, 1992]. The health assessment also indicated that off-site residential ground-water wells had been contaminated with TCE and TCA. Because direct measures of historical exposure to TCE are unavailable for the Gratuity Road site, computational models were used to reconstruct and predict exposure to TCE. These computational models included environmental transport and exposure models. For the environmental transport models, numerical methods were used to approximate the equations of ground-water flow and contaminant transport.

Results of using the environmental transport models provided us with the spatial and temporal database necessary to conduct an exposure analysis. This database indicated that ground-water concentrations of TCE typically exceeded the USEPA's MCL of 5 ppb for TCE. The study demonstrated that although a hazardous waste site can be remediated, nearby populations may experience significant exposure because of historical contamination, which will not be captured by remediation activities.

The exposure analysis used the simulated concentrations of TCE predicted by the environmental transport models. .These concentrations were used to compare exposure to TCE from inhalation in a one-compartment model shower with exposure from ingestion of domestic water contaminated by TCE. The exposure model indicated that exposure to TCE by the inhalation route during showering is nearly identical to exposure by ingestion of domestic water supplies contaminated with TCE. As a result, entry by route of inhalation is as important as entry by route of ingestion when conducting exposure analyses due to contamination from volatile organic chemicals such as TCE.

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ABSTRACT

A case study is presented in which computational models were used to evaluate environmental conditions at a hazardous waste site to determine potential health consequences of the release of trichloroethylene (TCE) into a stratified glacial drift aquifer. Historical levels of TCE concentration were predicted for populations residing upgradient and downgradient from the source of contamination. In this analysis, numerical methods were used to approximate the equations of groundwater flow and contaminant transport.

Analysis of potential health consequences resulting from remediation activities indicated that under the proposed cleanup plan, the population may experience significant TCE exposure. This exposure is due to historical contamination, which will not be captured by remediation activities. In the remediation scenario evaluated, ground-water concentrations of TCE typically exceeded the Environmental Protection Agency's maximum contaminant level of 5 parts per billion. Additional analyses were conducted to quantify human exposure of persons whose household water was contaminated with TCE. The analyses were conducted by using the TCE concentration predicted by the computational models for a typical location within the study area.

Results of the study demonstrate the effective use of computational models to reconstruct historical contaminant levels, assess present contaminant levels, and predict future contaminant levels in a subsurface environment. This spatial and temporal contaminant distribution is the preliminary database necessary to conduct exposure analyses. Additionally, this study has demonstrated that although the hazardous waste site can be remediated, nearby populations may experience significant exposure because of historical contamination, which will not be captured by remediation activities.

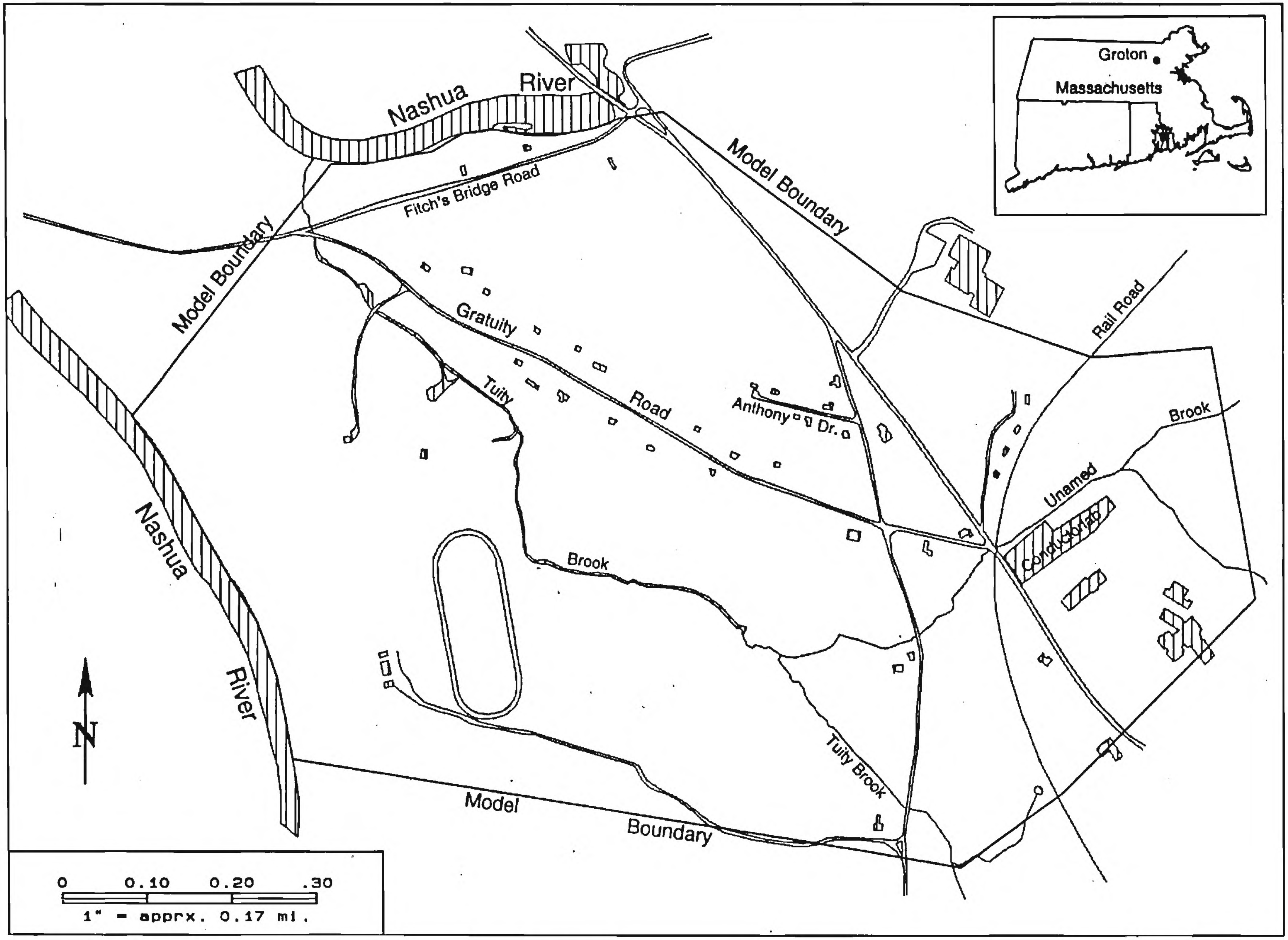

Figure 1. Site location, Groton, Massachusetts

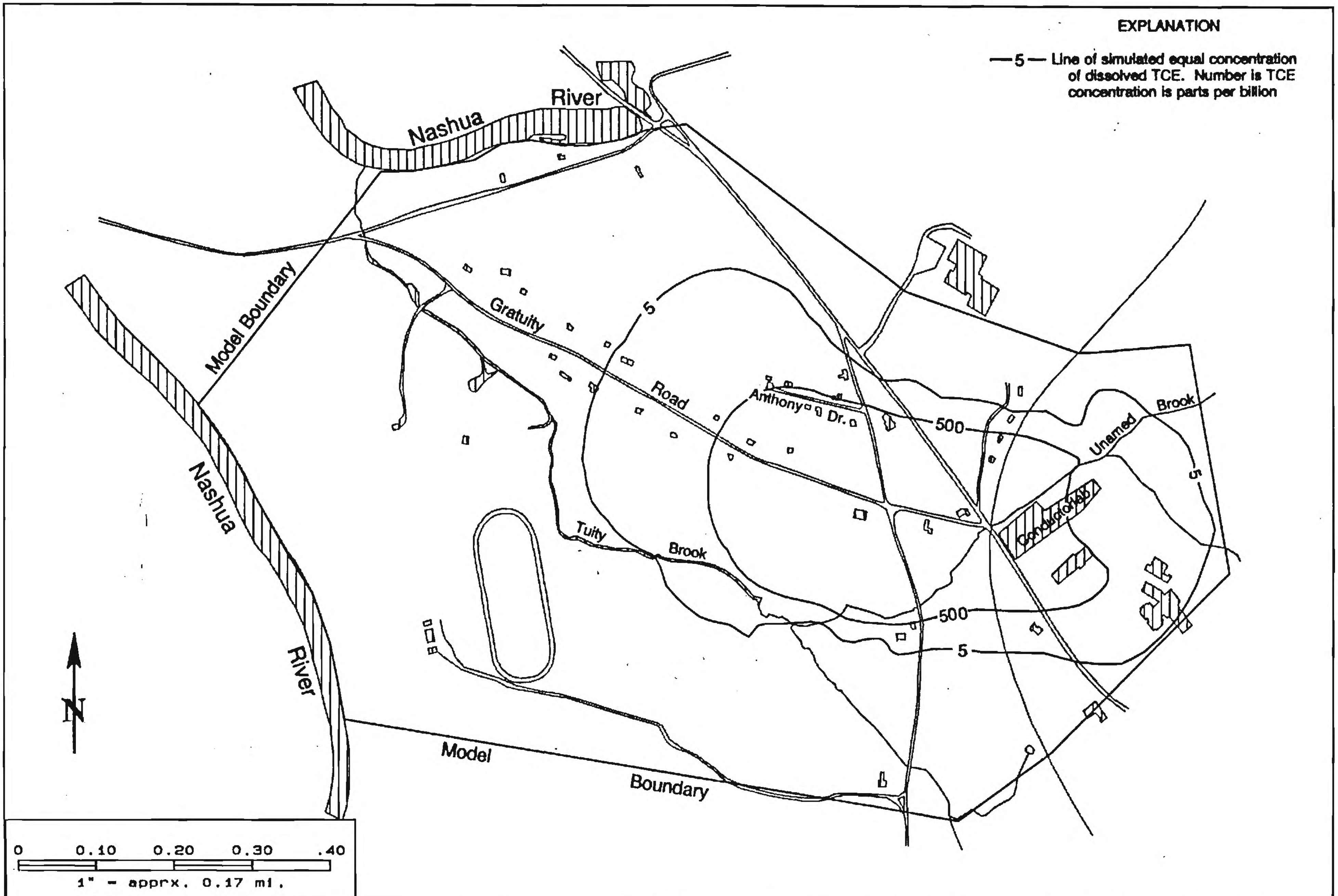

Figure 5. Location of the 5 and 500 ppb TCE concentration contours after 20 years of remediation

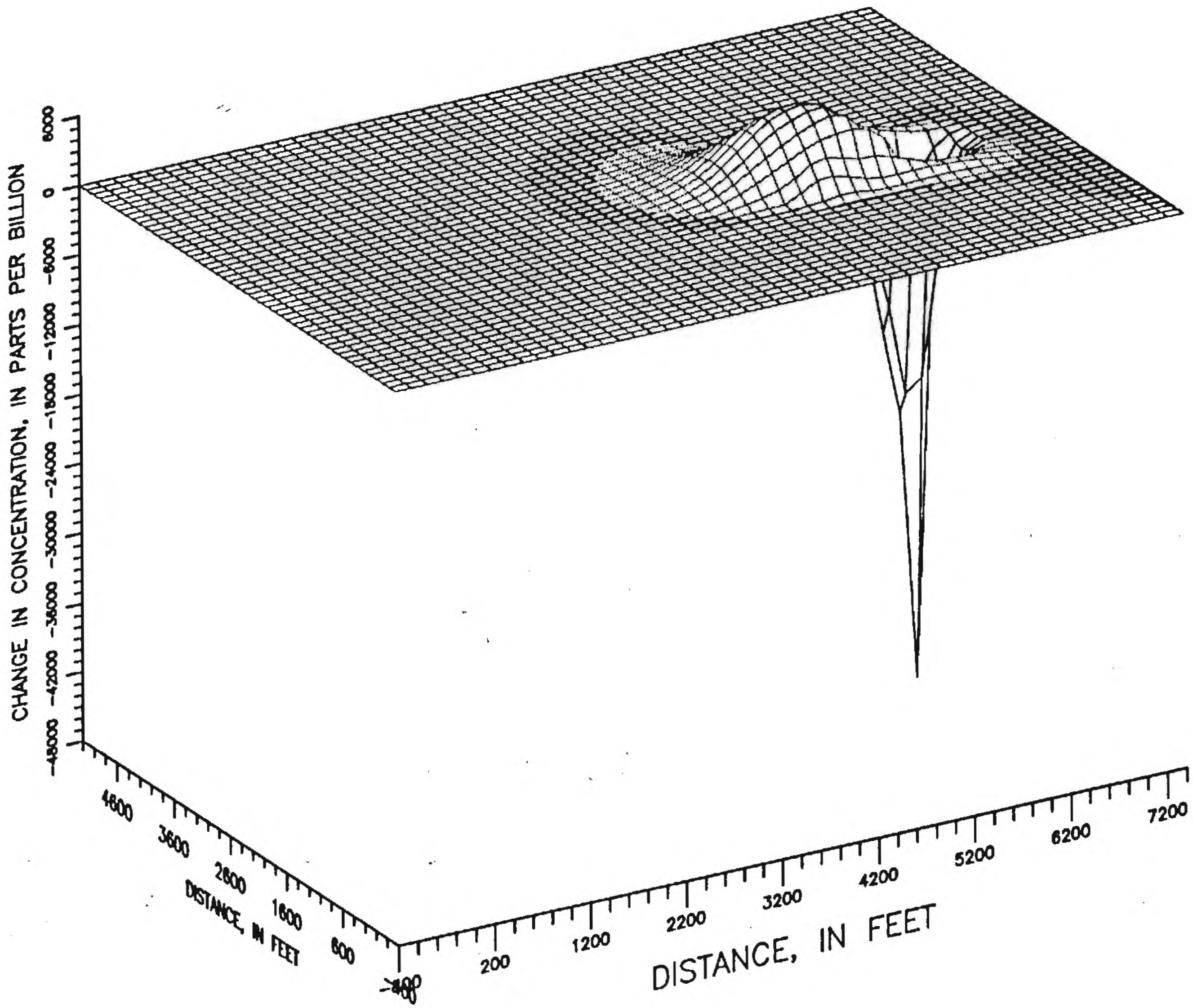

Figure 6. Change in TCE concentration after 20 years of remediation showing effect of site remediation (depression area) and downgradient migration of non-captured historical contamination (mound area)

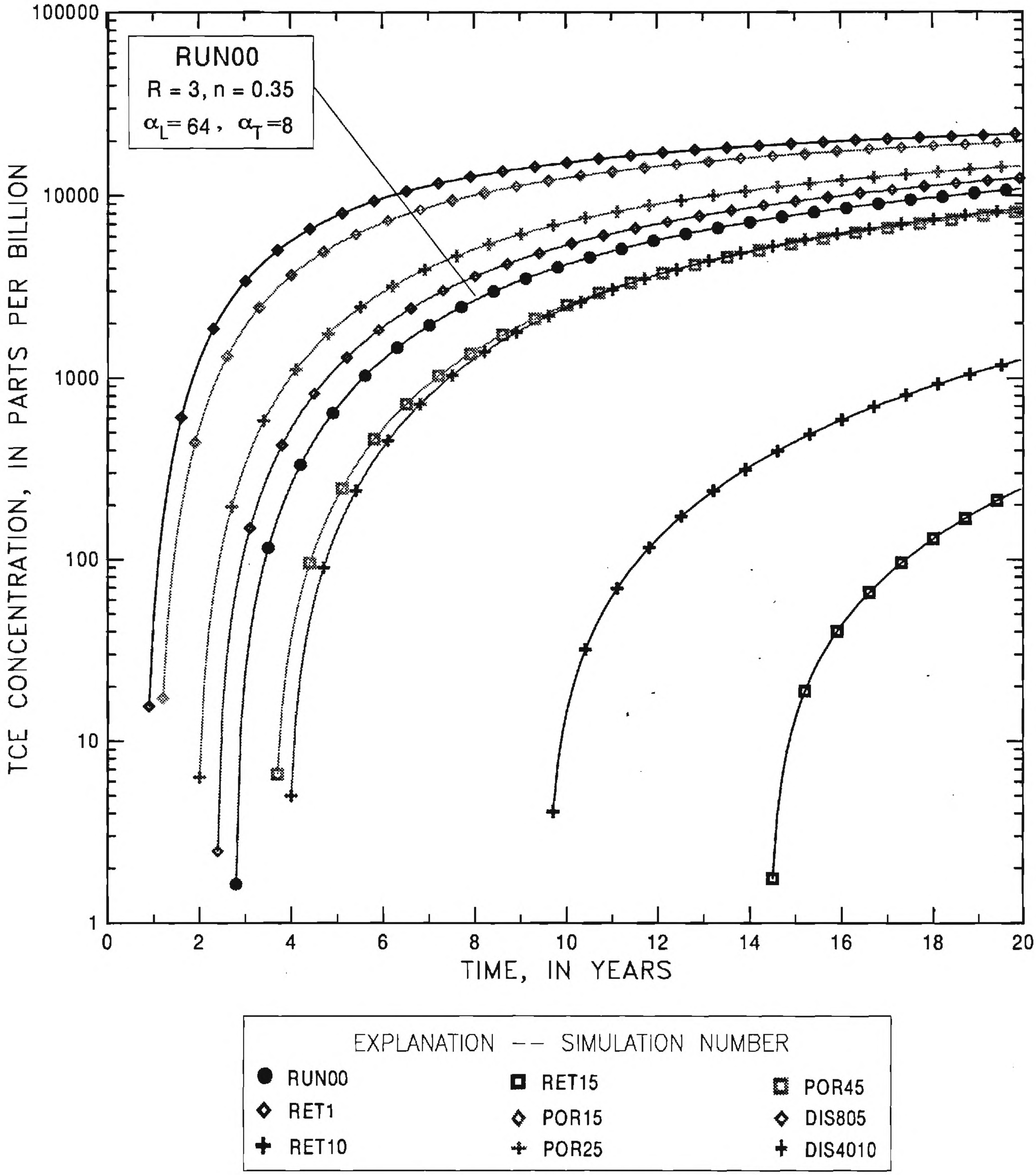

Figure 7. Response of TCE concentration to variation in transport parameters

(See Table 1 for explanation of simulation number.)

EXPOSURE-DOSE RECONSTRUCTION PROJECT

ANALYSIS OF POPULATIONS EXPOSED TO GROUNDWATER CONTAMINATED WITH TRICHLOROETHYLENE (TCE) AT THE GRATUITY ROAD SITE, GROTON, MASSACHUSETTS

BY:

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DIVISION OF HEALTH ASSESSMENT AND CONSULTATION
AGENCY FOR TOXIC SUBSTANCES AND DISEASE REGISTRY

July 12, 1993

FOREWORD

At a meeting held on June 21, 1993, the Division of Health Studies (DHS), Health Investigations Branch (HIB) requested the assistance of the Division of Health Assessment and Consultation (DHAC) in assessing populations potentially exposed to groundwater contaminated with trichloroethylene (TCE) at the Gratuity Road site, Groton, Massachusetts. To address this issue, DHAC used the resources of its Exposure-Dose Reconstruction Project (EDRP). The following report is a summary of the methodologies used to assess the potentially exposed populations at the Gratuity Road site. The analyses described herein are based solely on data available to the EDRP staff at the time of the analysis. For this study, no resources were expended to obtain additional data. At the conclusion of the report, methods by which the current analysis might be extended and enhanced to encompass additional data needs and refined analysis techniques are discussed.

CONTENTS

LIST OF ILLUSTRATIONS

LIST OF TABLES

Analysis of Populations Exposed to Groundwater Contaminated with Trichloroethylene (TCE) at the Gratuity Road Site, Groton, Massachusetts

Introduction

Groundwater and surface-water contamination have occurred near Gratuity Road in the Town of Groton, Massachusetts (Figure 1). A petitioned public health assessment for the Gratuity Road site [ATSDR, 1992] identified the primary contaminants as trichloroethylene (TCE), 1,1,1-trichloroethane (TCA), hexavalent chromium (Cr^{+6}), chromium (Cr), and lead (Pb). It also indicated that off-site residential groundwater wells had been contaminated with TCE and TCA. The petitioned public health assessment recommended the evaluation of environmental data to help identify the duration of exposure and the past, present, and future extent of groundwater contamination. For the purpose of the present study, exposure along **one** pathway, **groundwater**, for a single contaminant, **TCE** (dissolved in groundwater), is being analyzed.

Approach

Because direct measures of historical exposure to TCE are unavailable for the Gratuity Road site, computational models integrated with spatial analysis of demographic data were used to reconstruct and estimate the population's past exposure. The Agency for Toxic Substances and Disease Registry (ATSDR) defines exposure-dose reconstruction as an approach that uses computational models and other approximation techniques to estimate cumulative amounts of hazardous substances internalized by persons at presumed or actual risk from contact with substances associated with hazardous waste sites [ATSDR, 1993]. For this study, therefore, the approach that was used to approximate the number of people potentially exposed to groundwater contaminated with TCE at the Gratuity Road site consisted of the following steps:

1. Determining the direction of groundwater flow by use of a numerical groundwater flow model (described in section on Environmental Transport);

2. Determining the spatial and temporal distributions of TCE contamination of groundwater by use of a numerical contaminant and fate transport model (described in section on Environmental Transport);

3. Determining the spatial distribution of population for Groton, Massachusetts

by use of digital census data and a geographic information system (GIS) software package (described in section on Demographic Analysis); and

4. Integrating steps 1 and 2 with step 3 by use of a GIS to determine the spatial and temporal distribution of populations exposed to groundwater contaminated with TCE (described in section on Exposure Analysis).

Environmental Transport

To determine the spatial and temporal distribution of TCE concentration in groundwater, two numerical models were used. The first model computed the spatial distribution of groundwater levels and flow velocities throughout the Gratuity Road area. For this study the SLAM[1] code [Aral, 1990] was used to compute these values. The assumptions and limitations of the groundwater model are:

(a) steady-state (non-time varying) flow,
(b) recharge and discharge to and from streams and surface-water bodies,
(c) infiltration due to precipitation, and
(d) pumping and injection.

Details of this model and illustrations showing measured and simulated groundwater levels and the computed velocity field are described in Maslia [1992].

Using the groundwater velocities computed above, the spatial and temporal distribution of TCE was computed by use of the contaminant and fate transport model CLAM [Aral, 1992]. The assumptions and limitations of this model are:

(a) single specie transport,
(b) change of contamination with time and space,
(c) retardation, diffusion, and advection,
(d) contribution of contaminant concentration variation due to pumping and/or injection,
(e) no volatilization or biodegradation of TCE, and
(f) no dynamic surface-water and groundwater transport interaction.

In order to apply this type of model to a site, information regarding the source (or sources) of contamination must be known. Based on historical data [HMM Associates, Inc., 1988; 1990] and results of the public health assessment [ATSDR, 1992], the Conductorlab area (Figure 1) was

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[1]Use of brand or trade names in this report is for identification purposes only and does not constitute endorsement by ATSDR.

identified as the primary source of the TCE contamination. Details of applying the CLAM code to the site and illustrations showing the temporal and spatial distributions of TCE in groundwater are described in Maslia [1992].

Historical data indicates that TCE contamination of groundwater from the Conductorlab area began during the mid-1960's. A 1985 environmental investigation revealed significant TCE contamination of groundwater. By the Summer of 1987 all Gratuity Road residences were connected to the Groton municipal water supply system. Thus, on-going contamination of groundwater with TCE and exposure of the population to the contaminated groundwater occurred for approximately 20 years. Figure 2 shows the model simulated spatial distribution of groundwater contaminated with TCE after 20 years of contamination (approximately 1965 - 1985). The hatchured area in Figure 2 represents concentrations of TCE (dissolved in groundwater) that are equal to or greater than the U.S. Environmental Protection Agency's (USEPA) maximum contaminant level (MCL) of 5 parts per billion (ppb). The model indicates that after 20 years of contamination, TCE contaminated groundwater has migrated into the Gratuity Road and Anthony Drive areas and has encroached into nearby surface-water streams.

DEMOGRAPHIC ANALYSIS

The smallest subdivision of census data is at the block level. Census data at the block level, however, is only available for the 1990 census. Therefore, the 1990 census data were used to determine the demographics of the Groton area because:

(1) data were available at the block level, and
(2) previous census data (prior to 1990) were not available at the time of the analysis.

The 1990 census data comes in a CD-ROM (compact disc, read-only-memory) format. For the Gratuity Road site, the Summary Tape File 1B Extract (STF1BX) was used [Census of Population and Housing, 1991]. In order to visualize the distribution of the census blocks and data, a method of graphically displaying the location of the census blocks relative to the Gratuity Road site was required. This was accomplished in a two-step process by using a geographic information system (GIS) software package, GisPlus [Caliper Corporation, 1992], that runs on a personal computer (PC) platform.

The first step in the process was to determine the location of the census block level areas and boundaries for the Groton area. This was accomplished through the use and translation of the 1990 TIGER/Line census files for Middlesex County, Massachusetts [TIGER/Line Census Files, 1991]. GisPlus contains an internal translator for the TIGER/Line census files. Thus, once the block level areas and boundaries were translated, they were graphically displayed. Figure 3 shows the block level areas and boundaries for the Groton area (for state, county, and tract code 250173261). Note, Gratuity Road is classified as a block level boundary that divides blocks 602 and 603.

Table 1. Population and housing statistics for Groton, Massachusetts[a]

Statistic	Census Block Number[b]						
	119	121	135	506	507	602	603
Area[c]	0.22985	0.01487	0.29954	0.04261	0.10842	0.14087	0.39453
People	62	6	66	33	39	106	62
White	58	6	66	33	37	106	62
Other[d]	4	0	0	0	2	0	0
Less than 18 years	16	2	12	6	5	33	13
65 years or more	6	0	14	18	6	9	2
Total housing units	25	2	30	14	14	37	20
Single units	21	1	22	13	13	37	19
Owner occupied	18	1	20	11	12	33	20
Renter occupied	6	1	8	2	2	3	0
Mean house value[e]	177,500	0	290,500	179,500	251,300	137,900	176,900
Mean rent value[e]	475	675	359	875	675	550	0
Population density[f]	269.74	403.40	254.29	774.47	359.71	752.45	157.15

[a]Data for 1990 [Census of Population and Housing, 1991].
[b]State, county, and tract code 250173261
[c]Units are square miles
[d]Other includes Black; American Indian, Eskimo, or Aleut; Asian or Pacific Islander; and Other
[e]Value in U.S. dollars
[f]Units are people per square mile

The second step in the process is to relate data from the STF1BX to the appropriate census block. Again, this was accomplished through the use of the GIS software. Population and housing statistics for each of the Groton area census blocks are listed in Table 1. As part of this process, the area of each census block (in square miles) is also obtained. Thus, the statistic for population density was computed by using the equation entry capability of GisPlus and computing population density according to the formula:

$$\textit{Population Density} = \textit{People} \, / \, \textit{Area}$$

where population density is defined as the number of people per square mile of census block area.

EXPOSURE ANALYSIS

The exposure analysis was conducted by spatially integrating results of the environmental transport (location of the 5 or greater ppb area of TCE contamination) with the demographic analysis for the Groton area. If done manually, this is a complex and time consuming effort. However, when accomplished by using the spatial query capabilities of a GIS, this task becomes a simple operation. Figure 4 shows the relation between TCE contamination after 20 years (environmental transport) with the 1990 census block level areas (demographic analysis) derived by conducting a spatial analysis using the GIS. The resulting parameter is the area of the census blocks that have TCE contamination that equals or exceeds the MCL (5 ppb). Conducting a spatial query on the hatchured areas within each census block (Figure 4) yields the area that has been contaminated. Results of this spatial query are listed in Table 2 for each census block.

Table 2. Population exposed to TCE contaminated groundwater, Groton, Massachusetts

Census Block Number	Population Density	Block Area Contaminated with TCE (square miles)	Exposed Population
119	269.74	0.00761	2.1
121	403.40	0.00914	3.7
135	254.29	0.03859	9.8
506	774.47	0.00232	1.8
507	359.71	0.01688	6.0
602	752.45	0.01035	7.8
603	157.15	0.02826	4.4

The population that has been exposed to the contaminated groundwater for each census block is obtained by multiplying the population density for each block (column 2, Table 2) by the area of contamination within each block (column 3, Table 2). Based on this approach, it was estimated that nearly 36 people have been exposed to groundwater contaminated with TCE that exceeds the MCL (5 ppb).

ENHANCED ANALYSIS CAPABILITIES

The analyses described in the previous sections were based on groundwater flow and environmental transport models with some simplified and limiting assumptions and on limited census data (1990 data only). More refined estimates of exposed populations (down to individual land lots and households) could be attained if these tools were to be refined and additional data were to be obtained. Such additional data and refined tools might include:

(1) Data describing location of individual land lots in the Groton area (see Figure II in the petitioned public health assessment [ATSDR, 1992]),

(2) Historical census data for individual households in the Groton area,

(3) Modifications of the groundwater flow and contaminant transport models to include the following (pending availability of site-specific data):

    (a) time-dependent (unsteady-state) groundwater flow,
    (b) dynamic interaction and simulation of surface-water and groundwater flow,
    (c) dynamic interaction and simulation of surface-water and groundwater transport,
    (d) sensitivity and uncertainty analysis of model hydraulic parameters,
    (e) simulation of multiple specie (TCE, TCA, Cr^{+6}) transport,
    (f) simulation of specie biodegradation and volatilization,
    (g) sensitivity and uncertainty analysis of model transport parameters, and

(4) Multiple pathway analysis.

ATSDR can conduct analyses that include the above described enhancements. In order to do so, however, will require additional funding and time. These funds can be contributed to the Exposure-Dose Reconstruction Project budget as additional funds. A project with the scope designed to develop and apply the enhancements described above would have an estimated duration of 24 months.

CONCLUSIONS

Groundwater and surface-water contamination have occurred near Gratuity Road in the Town of Groton, Massachusetts. For this study, exposure along the groundwater pathway for a single constituent, TCE dissolved in groundwater, has been analyzed. Conducing a spatial analysis using information obtained from environmental transport and demographic analysis by using a geographic information system, indicates that approximately 36 people in the Gratuity Road area may have been exposed to groundwater contaminated with TCE.

ATSDR can conduct additional exposure analyses on the Gratuity Road site that could include multiple pathway exposure, multiple contaminant analysis, and groundwater and surface-water interaction. Such analyses would require additional funds and would require approximately 24 months to complete the study.

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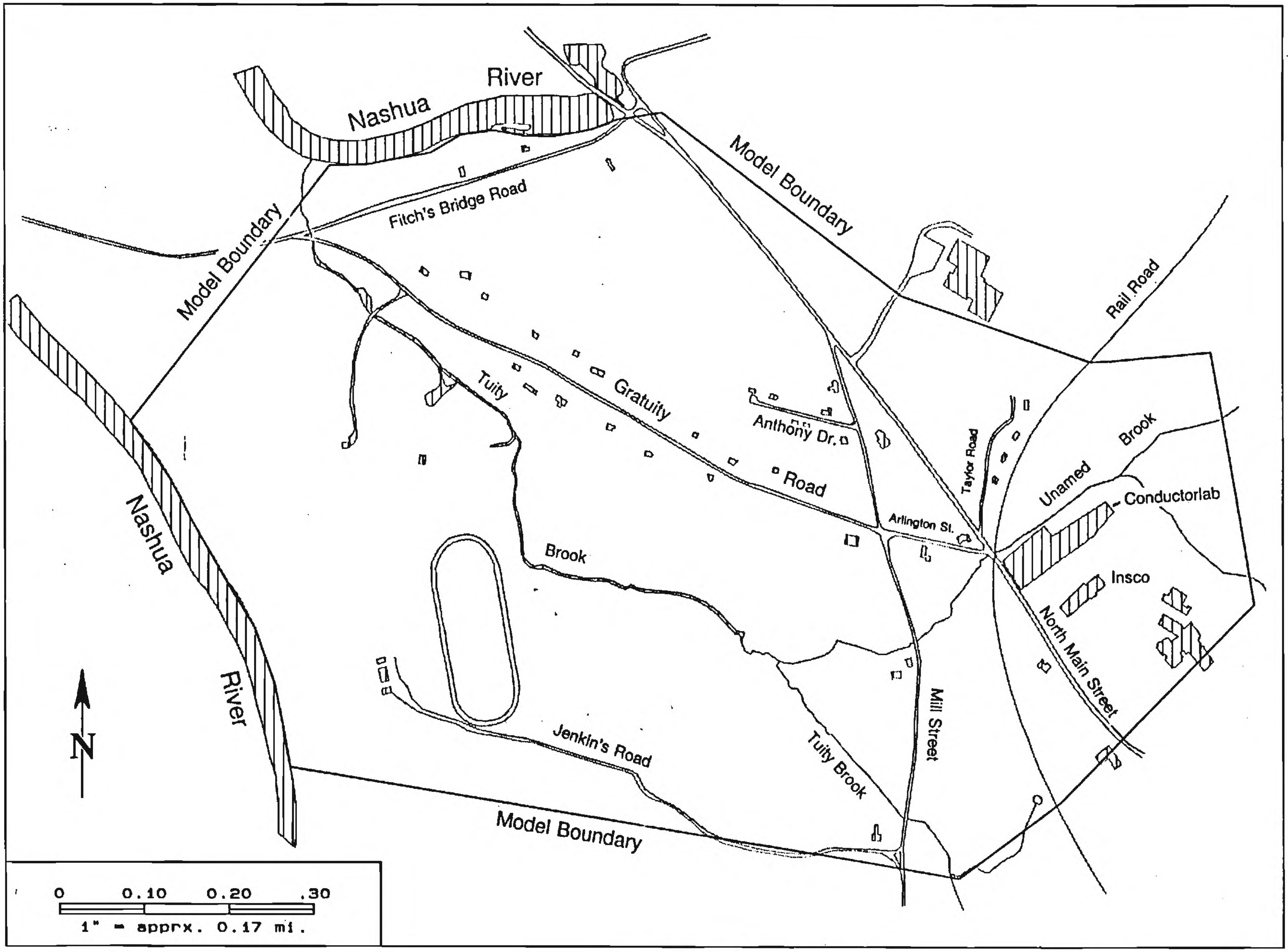

Figure 1. Location of study area, Groton, Massachusetts

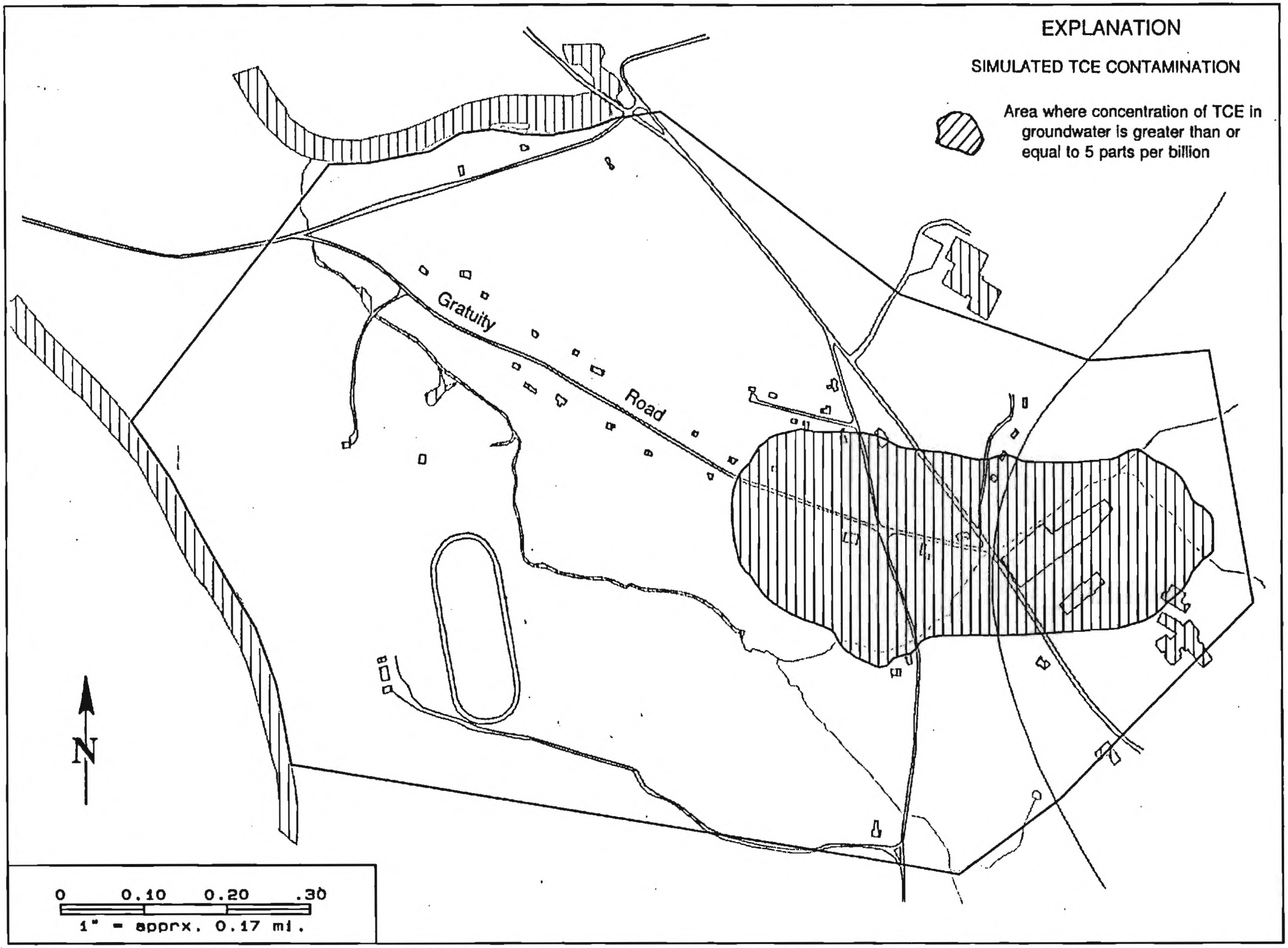

Figure 2. Simulated TCE contamination after 20 years

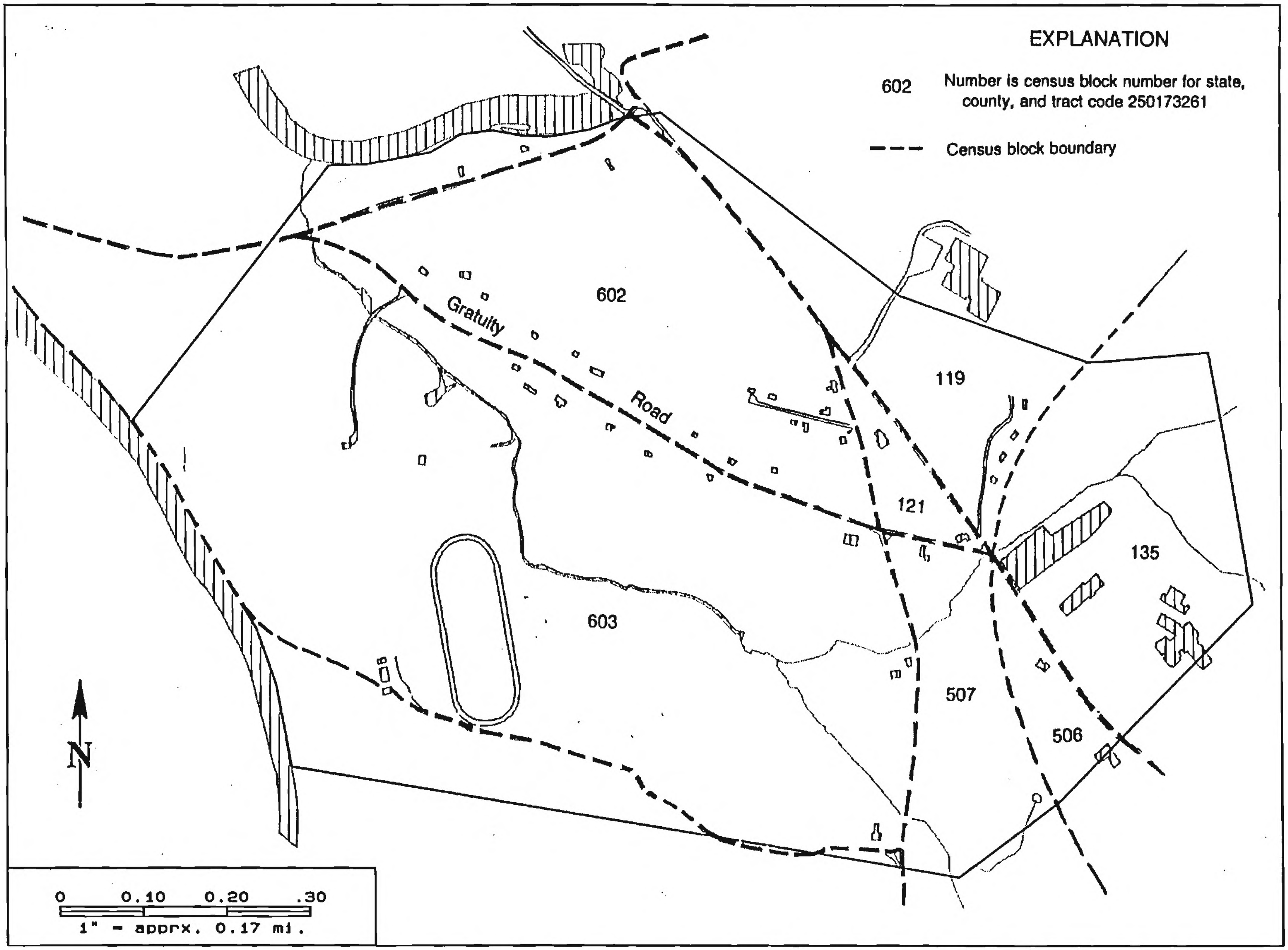

Figure 3. Location of 1990 census blocks

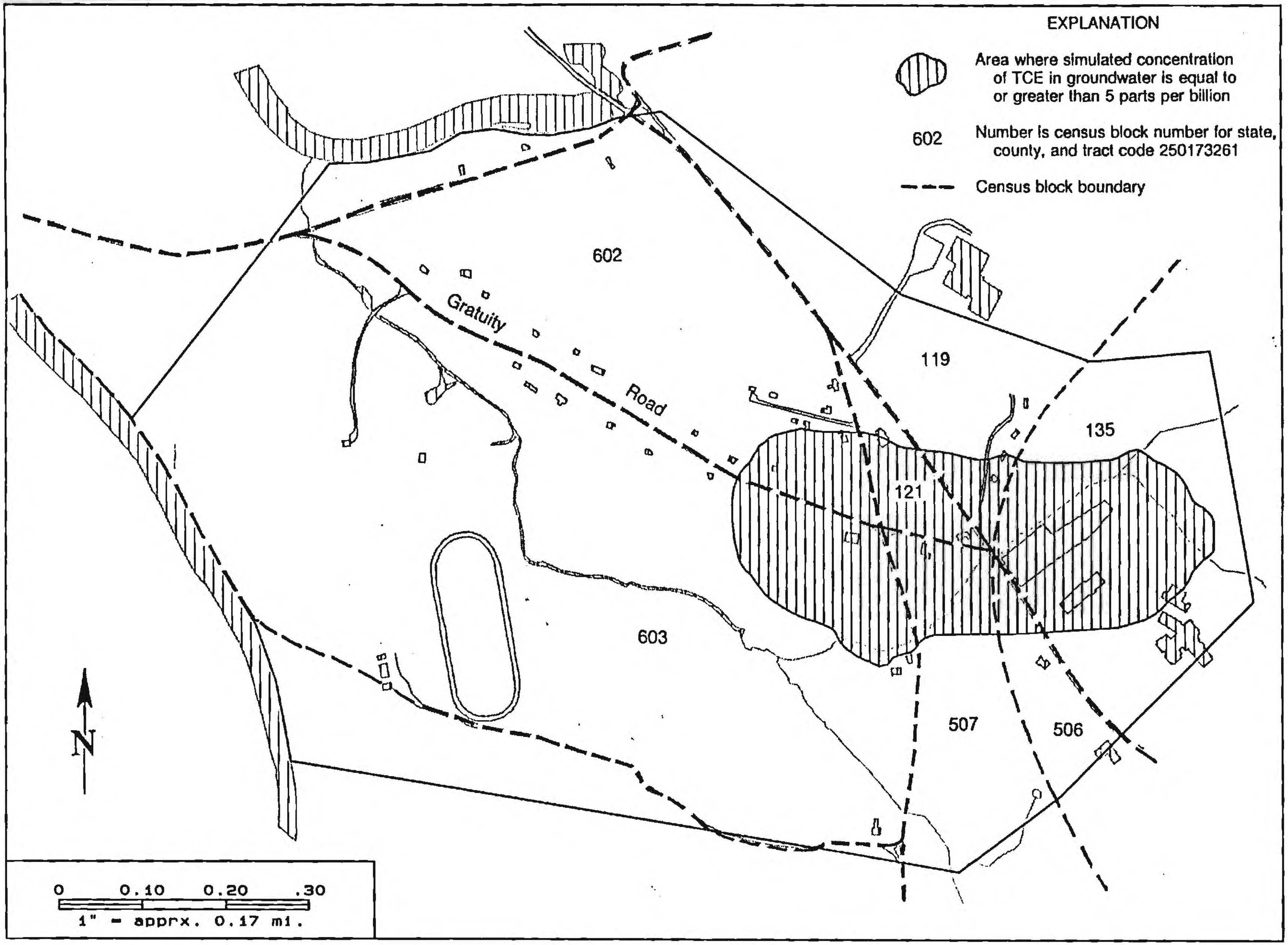

Figure 4. Relation of TCE contamination with census blocks

GROUND WATER

Discussion of Papers

DISCUSSION OF "Ground-Water Remediation Using Smart Pump and Treat," by Fredric Hoffman, January-February 1993 issue, v. 31, no. 1, pp. 98-106

by M. M. Aral, Georgia Tech; and M. L. Maslia and R. C. Williams, ATSDR, U. S. Public Health Service

We read with interest the paper by Fredric Hoffman, in which the author provides an outline of procedures employed in design of a successful pump-and-treat site remediation project. We agree with most of the concepts described in the paper, such as the emphasis on hydrogeologic characterization, the use of computer-aided data interpretation, the importance of source control, and detailed monitoring of the remediation. The organizational structure provided by the author for incorporating the components into a pump-and-treat plan is well-defined. However, we believe that some of the more important and critical issues related to designing a successful pump-and-treat project were not covered in the paper. We also believe that, in evaluating the performance of this particular remediation technology, the author has raised expectations for success too high. In the following discussion, we expand on some of these points.

In our opinion, the most important design defect, or misuse, of the pump-and-treat technology is designing the technology to address *site* cleanup goals rather than *aquifer* cleanup goals. The difference between the two is that the first approach ignores the effects of historical contamination on the aquifer. The environmental effect of historical contamination is particularly important when health issues are of concern. When the site cleanup option is excercised in remediation design, downgradient and upgradient populations near the site may remain at risk of exposure to hazardous substances even if the pump-and-treat remediation design is successful. This voluntary or involuntary bias toward site cleanup is commonly explained in terms of feasibility, economics, accessibility, future land use, or lack of aquifer characterization data, when the most important factor that should be employed in remediation design is the protection of populations at risk. In present-day jargon, the phrase "protection of the environment" is used so often and in so many different contexts that we sometimes forget the main goal of environmental restoration: to protect populations at risk of adverse health effects. Including the evaluation of historical contamination in the decision structure is a necessary criterion in designing a successful aquifer restoration project.

To demonstrate the importance of considering historical contamination, we present a scenario of the type frequently encountered by the Agency for Toxic Substances and Disease Registry (ATSDR), U.S. Public Health Service. ATSDR is mandated by Congress to evaluate the public health threat of hazardous waste sites using environmental and health outcome data and community concerns. Results of this public health assessment process are published and disseminated to interested parties. Site identifiers in the following case history have been changed because space limitations do not allow us to provide specific details of the study; the example could apply to any hazardous waste site.

From historical records, XYZ Inc., a facility that produces electronic circuit boards in the east central part of Anytown,

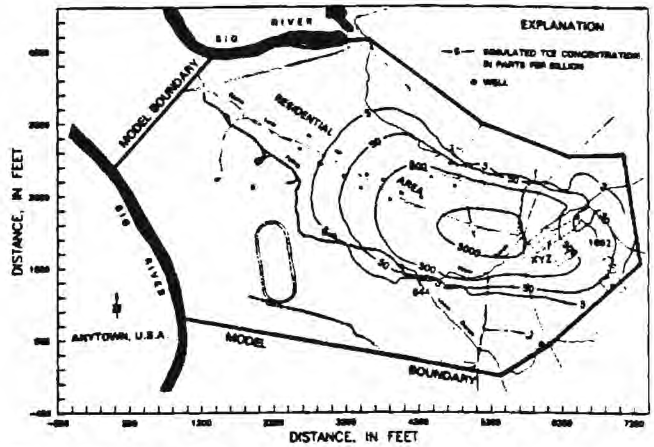

Fig. 1. Simulated TCE concentration after 40 years (20 years of plant operation and 20 years of remediation).

U.S.A. (Figure 1), contaminated the ground water of a stratified glacial drift water-table aquifer with trichloroethylene (TCE), 1,1,1-trichloroethane (TCA), and hexavalent chromium (Cr^{+6}) over a 20-year period. The environmental consultant hired by the current owners designed a pump-and-treat remediation scheme using *site* characterization data and a *site-specific* digital analysis. According to the consultant's analyses, ground-water contamination at the site can be remediated to the U.S. Environmental Protection Agency's (EPA) maximum contaminant level (MCL) of 5 parts per billion (ppb) in three to five years by pumping about 20 gallons per minute of contaminated ground water.

Because of its public health emphasis, ATSDR seeks answers to the following questions: (1) Which residents have been at risk, are now at risk, or will be at risk? and (2) Will remediation clean up the contaminated ground water so that residents will not be at risk? To answer those questions, we conducted an analysis of the aquifer. Our analysis included a steady-state ground-water flow calibration using November 1989 water levels (the only data available) to determine the flow field characteristics. The SLAM-486 code (Aral, 1990) was used to simulate the ground-water flow field. The model boundary selected is shown in Figure 1. We simulated aquifer contamination by conducting a 20-year contaminant transport simulation with a maximum source concentration at the site of 50,000 ppb, using the code CLAM-486. To simulate the pump-and-treat scenario, we removed the 50,000-ppb TCE source from the site and pumped and injected 20 gpm of water in accordance with the remediation design (100% pump and cleanup efficiency is assumed). We conducted this simulation for another 20 years. Figure 1 shows the distribution of TCE after 40 years (20 years of contamination and 20 years of pump-and-treat technology). As can be seen, simulated TCE concentration is less than 50 ppb in some parts of the site after 20 years of remediation. Downgradient of the site, however, an area of TCE contamination of more than 5,000 ppb, which represents the historical TCE contamination that has escaped the pump-and-treat remediation process, now exists.

Figure 2 shows a three-dimensional plot of downgradient population exposure to noncaptured TCE after 20 years of remediation. As shown, at the *site*, more than 90 percent of the TCE that was dissolved in ground water has been removed (indicated by the depression in the surface). However, downgradient of the site, a slug of noncaptured TCE continues to migrate toward a residential area, giving rise to potential exposure. Figure 3 shows the simulated TCE concentration before and during remediation of an on-site hypothetical well (well 1692) and of an off-site hypothetical well (well 644). (See Figure

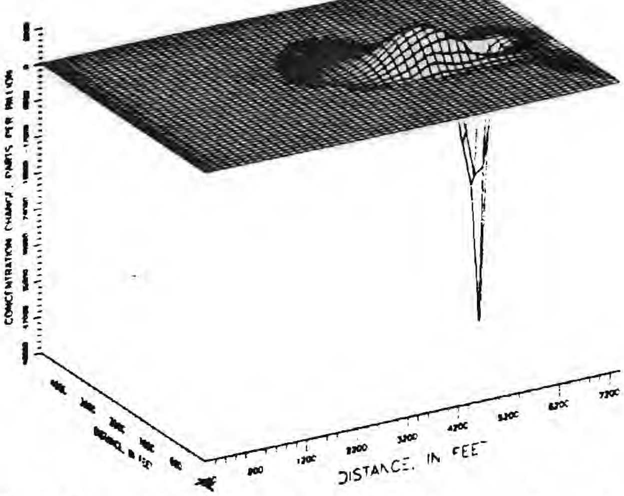

Fig. 2. Change in TCE concentration after 20 years of remediation showing the effect of site remediation (depression) and downgradient migration of noncaptured historical contamination (mound).

1 for well locations.) The simulated TCE concentration at well 1692 indicates a nearly successful remediation; after 20 years of remediation, the maximum concentration at this well is about two times the MCL. However, the effect of not considering or capturing the historical contamination is resulting in off-site contamination, as is shown by the simulated TCE concentration at well 644. During the first 20 years of remediation, that well shows no sign of contamination. However, because of noncaptured historical contamination, well 644 becomes contaminated during the next 20 years and, in fact, the simulated TCE concentration at year 40 far exceeds the MCL for TCE.

In this case study, off-site migration of contaminants after 20 years of plant operation also was verified by field data. This example, therefore, demonstrates that cleanup standards at the *site* can most likely be met, but unless the pump-and-treat system is designed to clean up the *aquifer*, people could be exposed to contaminants during and after remediation. Additionally, this example has demonstrated that the proposed pump-and-treat system may need to be operated for a significantly longer period (more than 20 years) than originally designed in order to achieve the cleanup goals.

The next point we would like to address is the expectation of success raised by the application of the procedures described in the paper. Are we expecting too much from a pump-and-treat remediation project? In the first paragraph (on page 100),

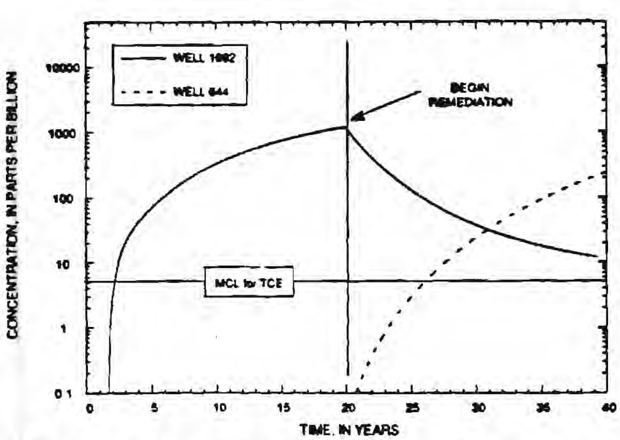

Fig. 3. Simulated TCE concentration before and during remediation for on-site well (1692) and off-site well (644).

the Hoffman article (1993) states: "*In fact, given enough time and a properly designed and operated extraction system, pump-and-treat can clean up ground water to any desired contaminant concentration.*" We disagree with that statement because it exaggerates the performance level of a pump-and-treat operation. Some contaminated sites will never be cleaned to precontaminated or drinking-water supply standards. In those cases, perhaps the only practical approach to protecting human health, by preventing future migration of contaminants and exposure to those contaminants, is long-term management of the aquifer.

Finally, there is the problem of asymptotically approaching cleanup levels in typical pump-and-treat remediation projects. How long is "*enough time*?" If infinite time is implied, is it feasible to continue remediation forever? We must be more realistic in evaluating the performance of remediation technologies. If we raise the expectations of the public to the level described in the aforementioned quote, the reputation of our profession will suffer when the remediation does not live up to the expectations set forth (Bredehoeft, 1992).

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REPLY TO the preceding discussion by M. M. Aral, M. L. Maslia, and R. C. Williams of "Ground-Water Remediation Using Smart Pump and Treat"

by Fredric Hoffman

The thought-provoking discussion by Aral, Maslia, and Williams concentrates on two significant points: (1) the importance of designing our ground-water remediation systems to clean up "*aquifers*" as opposed to "*sites*," and (2) the importance of projecting realistic expectations for success. I am in complete agreement with both of these points and believe that they are both addressed in the original paper.

As for the issue of "*site*" vs. "*aquifer*" remediation, the improved pump-and-treat techniques outlined in the paper are directed at the entire area of the plume of contamination resulting from the activities at the facility in question. At Lawrence Livermore National Laboratory (LLNL), used as an example in the paper, "site" has been defined, in the Federal Facility Agreement, to include the entire area of the plume of contaminated ground water. If such a definition had been applied to the scenario in the discussion, the off-site migration would not have been allowed to proceed unremediated. Perhaps the way to avoid any misunderstandings, resulting from terminology, is to discuss our cleanup efforts in terms of "contaminant plume" remediation.

Regarding the question of raising unwarranted expectations of success: one of the purposes of the paper was to counter what I consider unwarranted "gloom and doom" regarding ground-water cleanup in the literature, examples of which are cited in the paper, and in conversations within the environmental restoration community. The paper acknowledges that there are ground-water contamination situations which are not amenable to any practical remediation techniques known today. However, it also points out that there are a number of techniques which, if applied, can greatly improve the efficacy of ground-water remediation. Contaminant removal rates can be increased, contaminant concentrations can be reduced, and the time to reach cleanup goals can be greatly shortened, thereby reducing real and/or perceived threats to the public health and the environment and reducing the ultimate costs of remediation.

Hazardous Waste and Public Health: International Congress on the Health Effects of Hazardous Waste

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U.S. DEPARTMENT OF HEALTH AND HUMAN SERVICES
Public Health Service
Agency for Toxic Substances and Disease Registry

Use of Computational Models to Reconstruct and Predict Trichloroethylene Exposure

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Introduction

The Agency for Toxic Substances and Disease Registry (ATSDR), a Public Health Service agency of the U.S. Department of Health and Human Services, evaluates the public health threat of hazardous waste sites using environmental and health outcome data and community concerns. Results of this public health assessment process are published and disseminated to interested parties. For the current study, a type frequently encountered by ATSDR, we used the Gratuity Road site, located in the town of Groton, Massachusetts (Figure 1). Groundwater and surface-water contamination have occurred near Gratuity Road. A petitioned public health assessment for the site identified the primary contaminants as trichloroethylene (TCE), 1,1,1-trichloroethane (TCA), hexavalent chromium (Cr^{+6}), chromium (Cr), and lead (Pb) (ATSDR 1992). The health assessment also indicated that off-site residential groundwater wells had been contaminated with TCE and TCA. Therefore, we analyzed exposure through one environmental medium, groundwater, for a single contaminant, TCE (dissolved in groundwater).

Because direct measures of historical exposure to TCE are unavailable for the site, computational models were used to reconstruct and predict exposure to TCE. A critical database needed to estimate exposure is the temporal and spatial distribution of TCE contamination referenced to a geographic location. To obtain these data, we applied environmental transport models (groundwater flow and contaminant transport) to the site. Using the output from these models, we then estimated human inhalation exposure to TCE during showering using empirical formulae developed from results of laboratory studies and compared these results with estimates of exposure by ingestion.

Environmental Transport Models

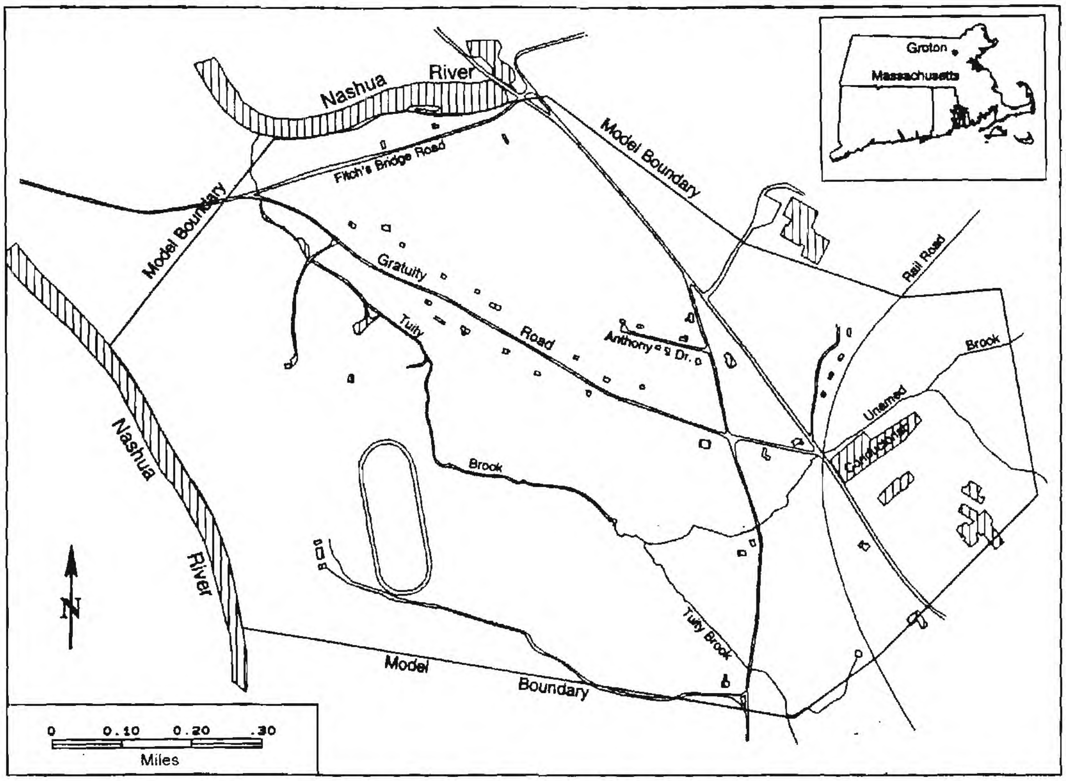
The mathematical models used to describe groundwater flow and contaminant transport were solved using finite element Galerkin procedures. Because these procedures are well established in the groundwater literature, only a brief review of the development of the governing equations is provided here. A more detailed description of the methodology can be found in several texts, including Pinder and Gray (1977).

The governing equation for two-dimensional, vertically averaged, steady-state flow in an unconfined aquifer is

$$\frac{\partial}{\partial x_i}\left(K_{ij}h\frac{\partial}{\partial x_j}\right) - \sum_{m=1}^{w} Q_m \delta(x_m, y_m) - I = 0 \tag{1}$$

where convention for tensor notation applies to indices i and j (i,j = 1,2 designate x, y, respectively), K_{ij} represents the hydraulic conductivity tensor of the unconfined aquifer, h is the piezometric head in the aquifer, w is the number of wells, Q_m is the pumping rate for well m, $\delta(x_m, y_m)$ is the Dirac delta function evaluated at (x_m, y_m), and I is the infiltration

Figure 1. Site location, Groton, Massachusetts, for demonstration of computational models to predict exposure.



or leakage flux into or out of the aquifer, which is a function of piezometric head distribution in adjacent aquifers. The governing equation for an unconfined aquifer is nonlinear because the location of the position of the water table is unknown; this location must be determined as part of the solution through an iterative process. The associated boundary conditions for the groundwater flow problem can be given in terms of Dirichlet, Neuman, and Cauchy conditions, which are shown below for an unconfined aquifer

$$h = h_c \quad (x,y) \in \Gamma_1^h$$

$$n_i \left(hK_{ij} \frac{\partial h}{\partial x_j} \right) = f_h \qquad (x, y) \in \Gamma_2^h$$

$$n_i \left(hK_{ij} \frac{\partial h}{\partial x_j} \right) = F_1 + F_2 h \quad (x, y) \in \Gamma_3^h \tag{2}$$

where n_i is the component of the outward normal to the boundary of the solution domain, and f_h, F_h, and $\bar{h}_c$ are functions defined on the boundary.

The governing equation for the two-dimensional, vertically averaged, convective-dispersive transport of a miscible contaminant can be given as

$$R \frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial C}{\partial x_j} \right) - V_i \frac{\partial C}{\partial x_i} + \sum_{m=1}^{w} \frac{Q_m (C - C_p)}{Bn} \delta (x_m, y_m) - \lambda C \tag{3}$$

where C is the contaminant concentration, R is the retardation factor, D_{ij} is the hydrodynamic dispersion tensor, V_i are the pore velocities in x and y directions, C_p is the concentration of the pumped water, B is the aquifer thickness, n is the aquifer porosity, λ is the first order decay constant, and Q_m, w, and $\delta(x_m, y_m)$ are as defined in Equation (1). Boundary and initial conditions for a contaminant transport problem can be defined as

$$C = C_o \qquad (x,y) \in \Omega \; ; \; t = t_o$$

$$C = C_c \qquad (x,y) \in \Gamma_1 \; ; \; t \geq t_o$$

$$n_i \left[nB \left(V_i - D_{ij} \frac{\partial C}{\partial x_j} \right) \right] = f_c \quad (x,y) \in \Gamma_2 \; ; \; t \geq t_o \tag{4}$$

The retardation factor, R, is equal to $(1 + K_s)$, where K_s is the adsorption solubility rate constant defined in terms of the bulk density and porosity of the soil and the partition coefficient, which is a function of organic carbon content of soil and octanol water partition coefficient of the chemical constituent. The pore velocities are defined using Darcy's Law:

$$V_x = -\frac{K_{xx}}{n} \frac{\partial h}{\partial x}$$

$$V_y = -\frac{K_{yy}}{n} \frac{\partial h}{\partial y} \tag{5}$$

where K_{xx} and K_{yy} are the hydraulic conductivities in the x and y directions as defined in Equation (1).

The diffusion tensor terms may be defined using the identities of Schiedegger (1961).

$$D_{xx} = \frac{\alpha_L V_x^2 + \alpha_T V_y^2}{|V|}$$

$$D_{yy} = \frac{\alpha_L V_y^2 + \alpha_T V_x^2}{|V|}$$

$$D_{xy} = D_{yx} = \frac{(\alpha_L - \alpha_T) V_x V_y}{|V|} \tag{6}$$

where α_L and α_T are the longitudinal and transverse dispersivities of the porous media, and $|V|$ is the magnitude of the velocity vector.

Groundwater flow as described by Equations (1) and (2) is subject to the assumptions of two-dimensional, vertically averaged, steady-state (non-time varying) flow, recharge and discharge to and from streams and surface-water bodies, infiltration due to precipitation, and pumping and injection of water. The transport of contaminants described by Equations (3), (4) and (5) is subject to the assumptions of single species transport, variation of contaminant concentration with time, retardation, diffusion and advection, contribution of contaminant concentration variation due to pumping and injection, no volatilization or biodegradation ofTCE, and no dynamic surface-water and groundwater transport interaction. A more detailed discussion of the limitations and assumptions of the equations of groundwater flow and contaminant transport can be found in several texts including Bear (1979), Freeze and Cherry (1979), and Pinder and Gray (1977).

In finite element analysis, the solution domain is idealized by a network of elements (Figure 2). The differential equation can then be assumed to be approximated by a series of independent basis functions defined in terms of the nodal values of the unknown function in each element. For example, when solving Equation (1), the piezometric head can be approximated as

$$h = \sum_{i=1}^{n} N_i h_i \tag{7}$$

where N_i is the basis function at node i, n is the total number of nodes for an element, and h_i is the approximate value of the piezometric head at node i.

When Equation (7) is substituted in Equation (1), a residual will be generated. The best approximation is then achieved when the residuals are minimized using a process known as the method of weighted residuals. The Galerkin method, a typical weighed residual method, minimizes residuals using the basis functions as the weighting functions. This residual or orthogonality condition can be defined as

$$\sum_{e}^{N} \int_{A_e} N_k L(h)\, dA^e = 0 \qquad (8)$$

where L is the differential operator defined as Equations (1) or (3), and N_k are the weighting functions. The integration is performed over an element, and the summation indicates the assembly of all elemental integral evaluations.

Using this process, Equation (1) can be written as follows for a typical element.

$$\iint_{A^e} N_l \left[\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right) - \sum_{m=1}^{w} Q_m \delta\,(x_m, y_m) - I \right] dA = 0; \quad l = i, j, k \qquad (9)$$

where i, j, and k refer to the nodal numbers of the element. The minimization of the residual over each element, the assembly of all elemental matrices, and the introduction of boundary conditions yield the following global matrix system.

$$[S]\,\{h\} = \{F\} \qquad (10)$$

Equation (10) may then be solved for the piezometric head at each node after the introduction of appropriate boundary conditions.

The contaminant transport equation may also be analyzed using a similar process. In this case, the contaminant transport solution is tied to the groundwater flow solution through Darcy velocity terms. Thus, in this sequential solution process, Equation (1) is solved first, followed by the solution of Equation (3). The weighed integral residual of the convective transport equation can be given as

$$\iint_{A^e} N_l \left[R\frac{\partial C}{\partial t} - \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial C}{\partial x} + D_{xy}\frac{\partial C}{\partial y}\right) - \frac{\partial}{\partial y}\left(D_{yy}\frac{\partial C}{\partial y} + D_{yx}\frac{\partial C}{\partial y}\right) + V_x\frac{\partial C}{\partial y} + V_y\frac{\partial C}{\partial y} + \sum_{i=1}^{w} \frac{Q_m(C-C_p)}{Bn}\,\delta\,(x_m, y_m) + \lambda C \right] dA = 0; \quad l = i, j, k \qquad (11)$$

Minimizing the residual over each element and the assembly of all elemental matrices yields the following resultant matrix equation.

$$[M]\left[\frac{\partial C}{\partial t}\right] + [S]\,[C] = [F] \qquad (12)$$

After introducing boundary conditions, finite difference techniques are used in solving the above equation to determine the concentration for each node at each time step. This sequential solution process yields spatial and temporal distribution of contaminants at each node over the solution domain. This equation may be given as

$$([M] + (1-\alpha)\Delta t[S])\,[C]^{t+\Delta t} = ([M] - \alpha\Delta t[S])\,[C]^t + (F^t) + (F^{t+\Delta t}) \qquad (13)$$

where Δt is the time step, α is a weighting factor that may vary from zero to one, and the superscripts identify the time at which matrices or vectors in Equation (13) are defined. Selecting $\alpha = 1$ corresponds to forward differencing. Central differencing is achieved by selecting $\alpha = 0.5$, and $\alpha = 0$ results in backward differencing (Aral 1990a, b).

Figure 2. Finite element idealization of Groton, Massachusetts, site used for environmental contamination transport models.

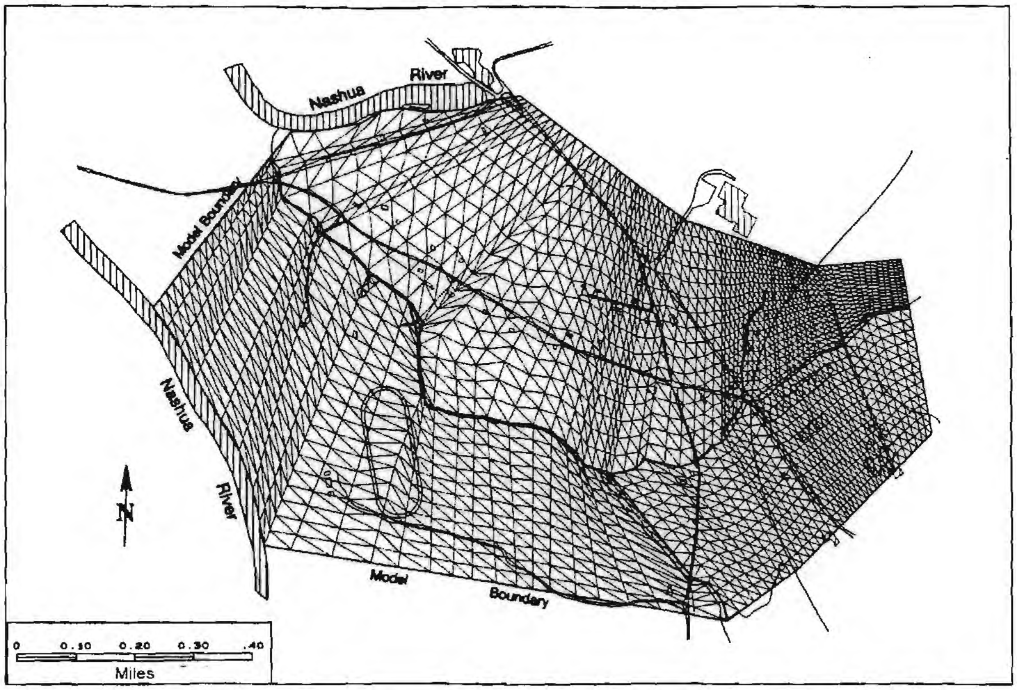
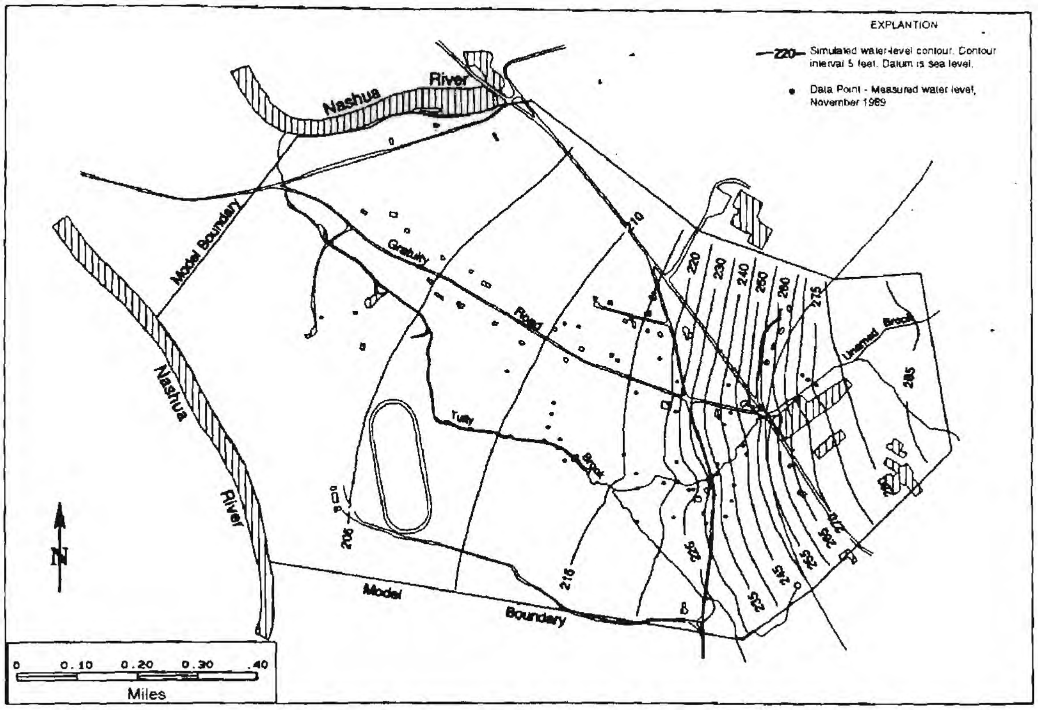


Figure 3. Calibrated water levels at Groton, Massachusetts, site, November 1989.

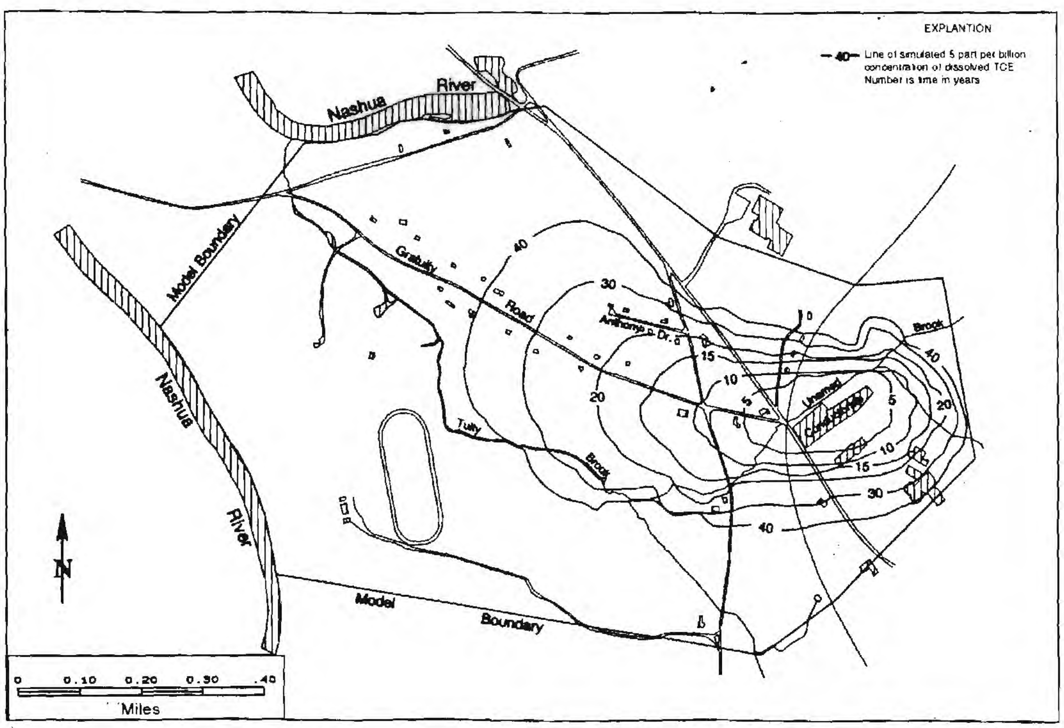


Application of Environmental Transport Models to Study Area

The environmental transport models described previously were used to evaluate transport of the contaminant TCE at the Gratuity Road site. The site is underlain by a stratified glacial-drift, water-table aquifer that varies in thickness from a few feet to more than 50 feet. Historical data indicate that TCE contamination of groundwater from the Conductorlab area (Figure 1) began during the mid-1960s (HMM Associates, Inc. 1988, 1990). A 1985 environmental investigation revealed significant TCE contamination of groundwater. By the summer of 1987, all Gratuity Road residences were connected to the Groton municipal water supply system. Thus, ongoing contamination of groundwater with TCE and exposure of the population to the contaminated groundwater occurred for approximately 20 years.

Our analysis began with a steady-state groundwater flow calibration using November 1989 water levels to determine flow field characteristics. The SLAM (Steady Layered Aquifer Model) code (Aral 1990a) was used to simulate the groundwater flow field. The finite element idealization (or mesh) using three-nodal triangular elements is shown in Figure 2. For this study, the mesh consisted of 3,828 elements and 2,010 nodes. The selected model boundary and calibrated water levels, based on November 1989 field data, are shown in Figure 3. The boundary adjacent to the Nashua River was simulated as a Dirichlet boundary and assigned a value of 200 ft (referenced to sea level datum), the stage of the river. The eastern boundary was simulated as a Neuman boundary and assigned a value of 0.002 feet per day (ft/d). The top and bottom boundaries were also simulated as Neuman boundaries and assigned a value

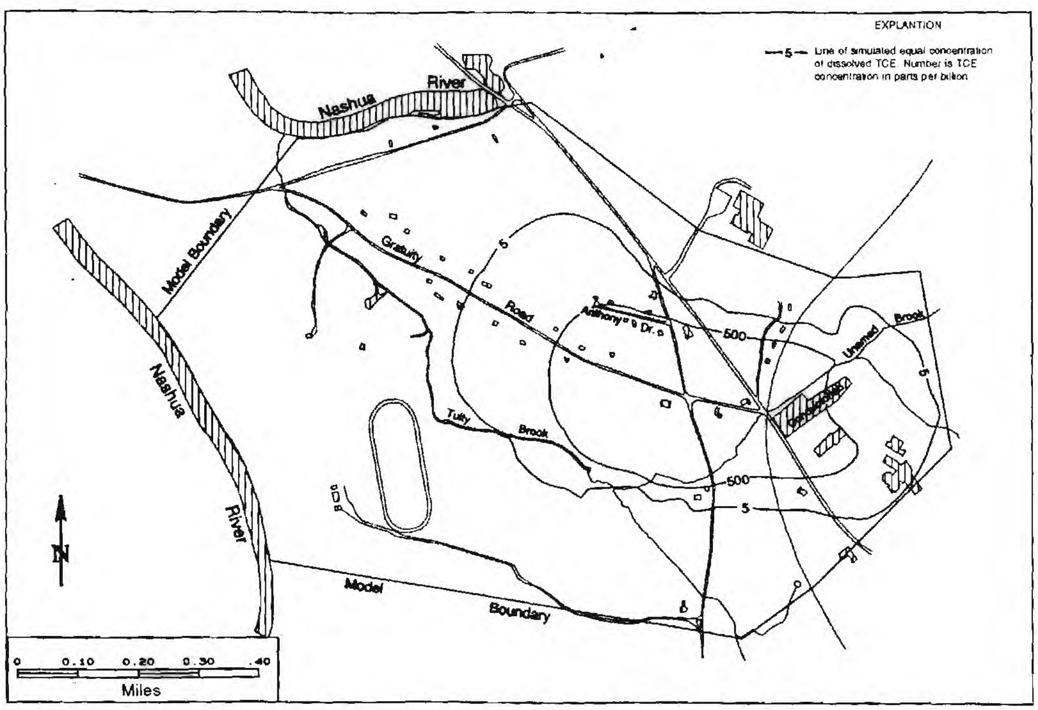
Figure 4. Movement of the 5 ppb trichloroethylene concentration contour at the Groton, Massachusetts, site.



of zero (no-flow). The calibrated infiltration rate due to precipitation was assumed to be constant over the model area and was assigned a value of 8.5 inches per year. Calibrated hydraulic conductivity values ranged from 0.5 to 22 ft/d, which were consistent with and within the range of field- and laboratory- derived values (HMM Associates, Inc. 1988, 1990). As shown in Figure 3, the flow field is characterized by groundwater and surface-water interaction as indicated by the curvature of water-level contours near Tuity and Unamed Brooks. Graphical display of the calibrated velocity field and simulation of alternative flow-field scenarios are not presented here because of space limitations.

Aquifer contamination and proposed remediation were simulated by investigating two contaminant transport scenarios using the CLAM (Contaminant transport in Layered Aquifer Media) code (Tang and Aral 1992). In all simulations, we assumed a constant porosity of 0.35, a retardation factor of 3 for the dissolved TCE (HMM Associates 1990) with no volatilization or biodegradation, and longitudinal and transverse dispersivities (α_L, α_T) of 64 and 8 ft, respectively. In the first scenario, we conducted a 40-year simulation with a maximum source concentration of 50,000 parts per billion (ppb) located at the assumed point of contamination in the Conductorlab area. Results of this simulation are shown in Figure 4 as temporal distributions of TCE. The contour lines represent the U.S. Environmental Protection Agency's (EPA) maximum contaminant level (MCL) for TCE of 5 ppb for times of 5, 10, 15, 20, 30, and 40 years. Model results indicate that, after 20 years, groundwater contaminated with TCE has migrated into the Gratuity Road and Anthony Drive areas and has encroached into nearby surface-water streams (Tuity Brook and Unamed Brook).

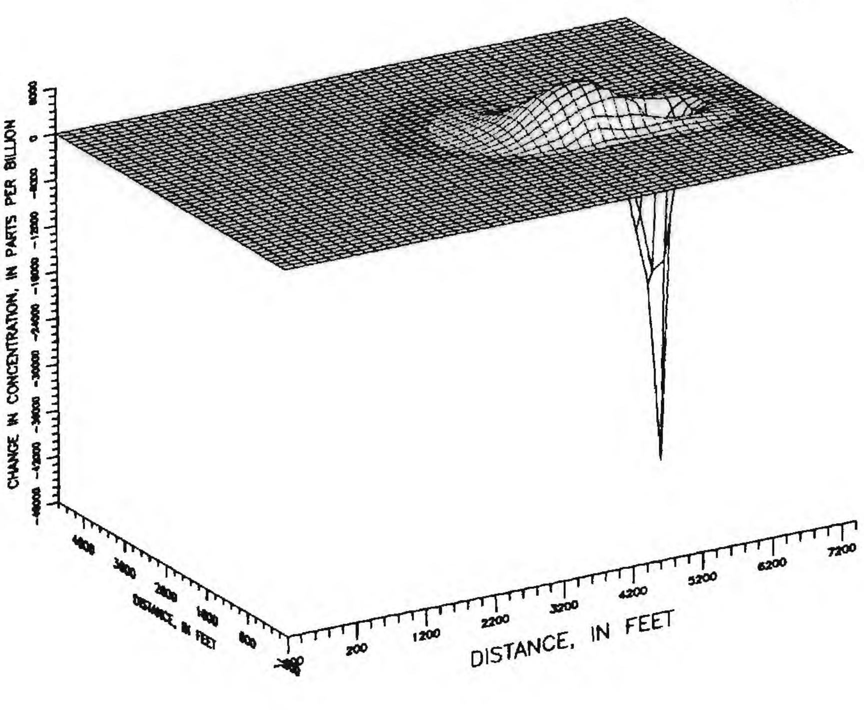
Figure 5. Location of the 5 and 500 ppb trichloroethylene concentration contours after 20 years of contamination and 20 years of remediation at the Groton, Massachusetts, site.



In the second scenario, we simulated a proposed pump-and-treat remediation plan by conducting a 20-year simulation with a maximum source concentration of 50,000 ppb and then removing the source from the site and pumping and injecting 20 gallons per minute (gpm) of water for another 20 years. Figure 5 shows the location of the 500 ppb and 5 ppb TCE contours after 40 years (20 years of contamination and 20 years of pump-and-treat technology). Results indicate that, after 40 years, TCE concentrations in part of the source area have been reduced to less than 50 ppb. Downgradient of the site near Gratuity Road and Anthony Drive, however, an area of TCE contamination of more than 500 ppb now exists, which represents the historical TCE contamination that has escaped the pump-and-treat remediation process (Aral et al. 1993). Figure 6, a three-dimensional surface plot of the change in TCE concentration in the aquifer after 20 years of remediation, clearly illustrates the effect of remediation at the site (depression) and the downgradient migration of the noncaptured historical contamination (mound). The darker area surrounding the mound represents an increase in TCE concentration of 5-50 ppb after 20 years of remediation in areas of the aquifer previously uncontaminated.

Results of contaminant transport simulations indicate that, after 20 years of contamination, some people living in the Gratuity Road area and using groundwater were probably exposed to TCE that exceeded the MCL (5 ppb). Additionally, the simulations suggest that although pump-and-treat technology may clean up the site and source area (Figure 6, depression area), populations downgradient from the site may still be at risk of exposure

Figure 6. Change in trichloroethylene concentration after 20 years of remediation, showing effect of site remediation (depression area) and downgradient migration of non-captured historical contamination (mound area) at the Groton, Massachusetts, site.



from TCE that exceeds the MCL (Figure 6, mound area).

Variation of Hydraulic and Transport Parameters

Because measured values of hydraulic and transport parameters are unknown at every location within the modeling domain (Figure 2), understanding and recognizing the effect of possible variation in the parameter values on modeling results is important. For example, use of November 1989 water levels was justified by comparing long-term (1951-1980) monthly mean precipitation (3.99 inches) from the Ashburn, Massachusetts, weather station with monthly precipitation for November 1989 (4.1 inches). Because no large-scale regional pumping occurs near Groton, groundwater levels are influenced by increases and decreases in precipitation that result in increased or decreased infiltration to the aquifer. Thus, to simulate a period of higher groundwater levels (for example, May 1989), infiltration input to the model would have to be increased.

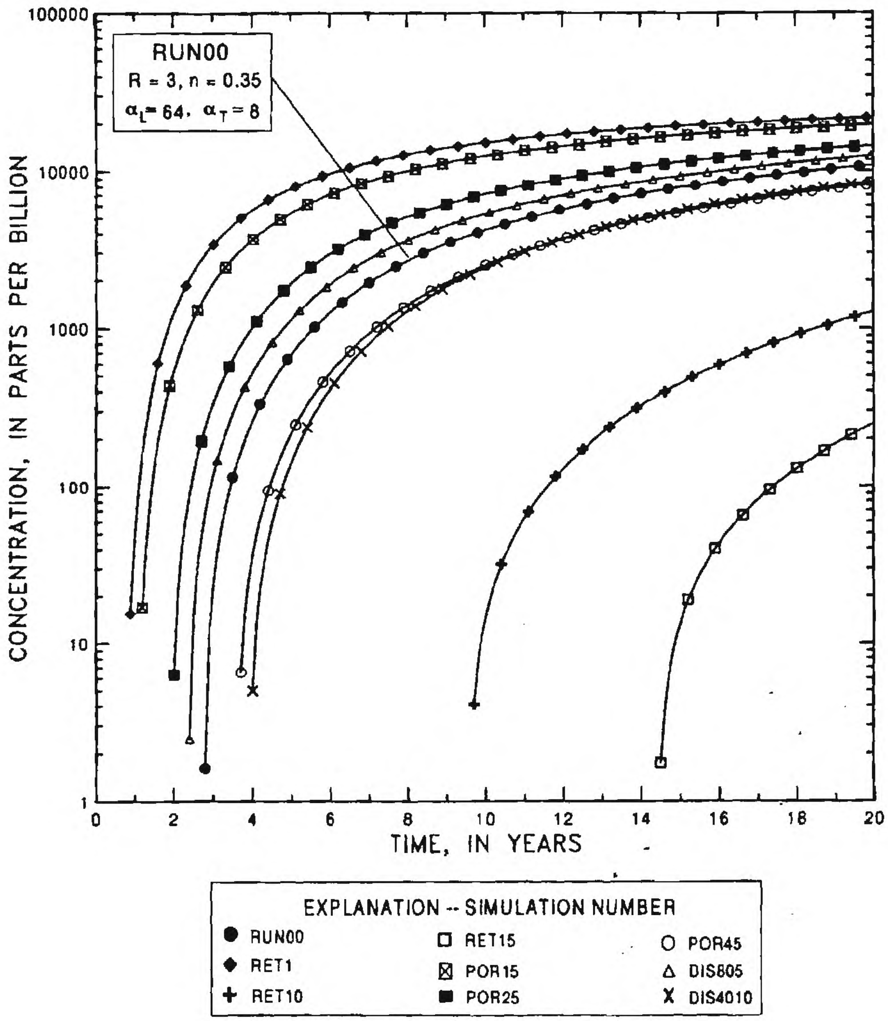
Although variation of any parameter value may cause some change in simulation results, by far the most significant changes occur (with respect to movement of TCE) when transport parameters such as retardation (R), porosity (n), and dispersivity (a_L, a_T) are changed in value. A sensitivity analysis was conducted by varying the values of retardation, porosity, and longitudinal and transverse dispersivity from the values previously described. A series of simulations was conducted and values of the parameters are listed in Table 1 for each simulation. Results of the simulations are displayed as a series of line graphs of time (in years) on the abscissa and TCE concentration on the ordinate (Figure 7). With simulation number "RUN00" being the original parameter values previously described, the most sensitive parameter to variation is retardation. A change in this parameter value has the effect of reducing or increasing movement of the contaminant with respect to the mean velocity of groundwater. The value of the porosity of the aquifer is also sensitive to change because it results in an increase or decrease of the fluid (pore) velocity, thereby advecting more or less contaminant. Thus, to improve the simulation, more refined estimates (based on field observations and measurements) of retardation and porosity would be necessary.

Table 1. Variation of trichloroethylene transport parameter values at the Groton, Massachusetts, site.

Run Number	Retardation	Porosity	Dispersivity (feet)	
			Longitudinal	Transverse
RUN00*	3	0.35	64	8
RET1	1	0.35	64	8
RET10	10	0.35	64	8
RET15	15	0.35	64	8
POR15	3	0.15	64	8
POR25	3	0.25	64	8
POR45	3	0.45	64	8
DIS805	3	0.35	80	5
DIS4010	3	0.35	40	10

* Simulation using aquifer and transport parameters described above in section on "Application of Environmental Transport Models to Study Area"

Figure 7. Response of trichloroethylene concentration to variation in transport parameters at the Groton, Massachusetts, site (See Table 1 for explanation of simulation number.)



Exposure Model

Exposure models attempt to quantify a person's contact with a contaminant at a specific concentration for a specified duration of time. Total human exposure is composed of contributions from all environmental media (water, soil, air, and plants) that contain the contaminant, and all routes of entry to the human body (dermal contact, ingestion, and inhalation). From a mathematical perspective, total human exposure may be defined by the equation

$$E = \int_{t_1}^{t_2} C(t)\, dt \qquad (14)$$

where *E* is the exposure, *C(t)* is the time-varying concentration of a contaminant, and *dt* is the time increment from t_1 to t_2.

Although total human exposure is described by Equation (14), data are usually insufficient to account for exposure from all environmental media and by every route of entry. Consequently, researchers and regulators have, in the past, focused their attention on exposure to hazardous substances from potable water supplies by the ingestion route. However, when contaminants (such as TCE) belonging to the class of compounds known as volatile organic compounds (VOCs) are considered, evidence is mounting that entry by the route of inhalation may be as important as ingestion. For example, laboratory experiments using standard shower conditions have indicated that an average of 80% to 85% of TCE contained in the water supply for the shower volatilized into air (Wilder 1986). Therefore, exposure by the inhalation route should be accounted for in exposure assessment studies involving VOCs.

For the present study, we will be using empirical equations that were derived from results of laboratory shower experiments in which TCE was added to the shower water supply to determine volatilization and inhalation characteristics. Because of space limitations, details of the laboratory experiments will not be provided here, but can be found in Andelman (1990) and Wilder (1986). The maximum contaminant concentration in air during a shower can be described by the equation

$$Ca_{max} = k\, t\, C_w / V_a \quad (15)$$

where Ca_{max} is the maximum contaminant concentration in the shower air in milligrams per liter (mg/L), k is the volatilization mass transfer coefficient in liters per minute (L/min), t is time in the shower in hours (h), C_w is the contaminant concentration in the shower water supply (mg/L), and V_a is the volume in liters of the shower room. Assumptions for laboratory shower experiments are in Table 2.

Using these standard assumptions, Equation (15) reduces to the equation

$$Ca_{max} = 4.5 \times 10^{-3}\, C_w \quad (16)$$

It can also be shown that for the given shower assumptions used in the laboratory experiments, after the shower period of time t, the average TCE concentration in the air C_a that an individual is exposed to is equal to Ca_{max} at time t (at the end of the shower) (Andelman 1990). Inhalation exposures in the shower can be defined as the product of concentration of the contaminant in air, breath-

Table 2. Assumptions about trichloroethylene (TCE) exposure used for laboratory shower experiments (Wilder 1986).

Shower	Contaminant	Human
Flow rate in the shower: 8 L/min.	Fraction volatilization rate of TCE from shower water: 0.90.	Adult body weight: 70 kg.
Air exchange rate in the shower room: 0.53/hr.	Rate of volatilization during the shower is constant.	Ingestion: 1.3 L of domestic water per day.
Volume of shower and shower room: 10,000 L.	Rate of decay of TCE in the shower room after shower is constant.	Inhalation rate at rest: 1,000 L of air per hour.
	Shower and shower room treated as a one-compartment model.	Takes one 6-minute shower per day, 365 days per year.
		Remains in shower room for 15 minutes after showering.

ing rate (for an adult), and exposure time, such that

$$E_i = C_a B t \tag{17}$$

where E_i is exposure (mg), B is breathing rate (L/h), and C_a and t are as previously defined. Assuming a human adult takes one shower per day (Table 2), using results of the laboratory experiments, inhalation exposure to TCE during showering can be defined by the equation

$$E_i = 1.35\ C_w \tag{18}$$

where E_i is now defined as exposure from inhalation of TCE in mg/d.

Application of Exposure Model to Study Area

As a result of environmental transport simulations, the temporal and spatial distribution of TCE contamination for the study area was known. Thus, if the domestic water supply was obtained from groundwater, the concentration of TCE in the water supply, C_w, for a specific point in time at a specific location would be known. Equation (14) can be solved using concentration data derived from the environmental transport model to compute exposure to TCE. However, for illustrative purposes, we will compute exposure for only one point in time. After 20 years of remediation, the concentration of TCE in groundwater at a certain location in the study area is 250 ppb or 0.25 mg/L. Letting C_w = 0.25 mg/L, and inserting this value into Equation (15), the exposure an adult receives by the route of inhalation during and after a shower is computed as

$$1.35\ \text{L/d} \times 0.25\ \text{mg/L} = 0.34\ \text{mg/d}$$

Alternatively, if an adult ingests 1.3 liters of water per day, then exposure by the ingestion route can be computed as

$$0.25\ \text{mg/L} \times 1.3\ \text{L/d} = 0.33\ \text{mg/d}$$

Therefore, using concentration data from the study area in conjunction with laboratory-determined inhalation parameters indicate that an adult would receive nearly the same exposure by the inhalation route during and after showering as from ingestion of groundwater contaminated with TCE.

Summary and Conclusions

In this study, a type frequently encountered by ATSDR, groundwater and surface-water contamination have occurred near the Gratuity Road site in the town of Groton, Massachusetts. A petitioned public health assessment for the Gratuity Road site identified the primary contaminants as trichloroethylene (TCE), 1,1,1-trichloroethane (TCA), hexavalent chromium (Cr^{+6}), chromium (Cr), and lead (Pb) (ATSDR 1992). The health assessment also indicated that off-site residential groundwater wells had been contaminated with TCE and TCA. Because direct measures of historical exposure to TCE are unavailable for the Gratuity Road site, computational models were used to reconstruct and predict exposure to TCE. These computational models included environmental transport and exposure models. For the environmental transport models, numerical methods were used to approximate the equations of groundwater flow and contaminant transport.

Results of using environmental transport models provided us with the spatial and temporal database necessary to conduct an exposure analysis. This database indicated that groundwater concentrations of TCE typically exceeded EPA's MCL of 5 ppb for TCE. The study demonstrated that although a hazardous waste site can be remediated, nearby populations may experience significant exposure because of historical contamination, which will not be captured by remediation activities.

The exposure analysis used simulated concentrations of TCE predicted by environmental transport models. These concentrations were used to compare exposure to TCE from inhalation in a one-compartment model shower with exposure from ingestion of domestic water contaminated by TCE. The exposure model indicated that exposure to TCE by the inhalation route during showering is nearly identical to exposure by ingestion of domestic water supplies contaminated with TCE. As a result, entry by inhalation route is as important as entry by ingestion route when conducting exposure analyses of contamination from volatile organic compounds such as TCE.

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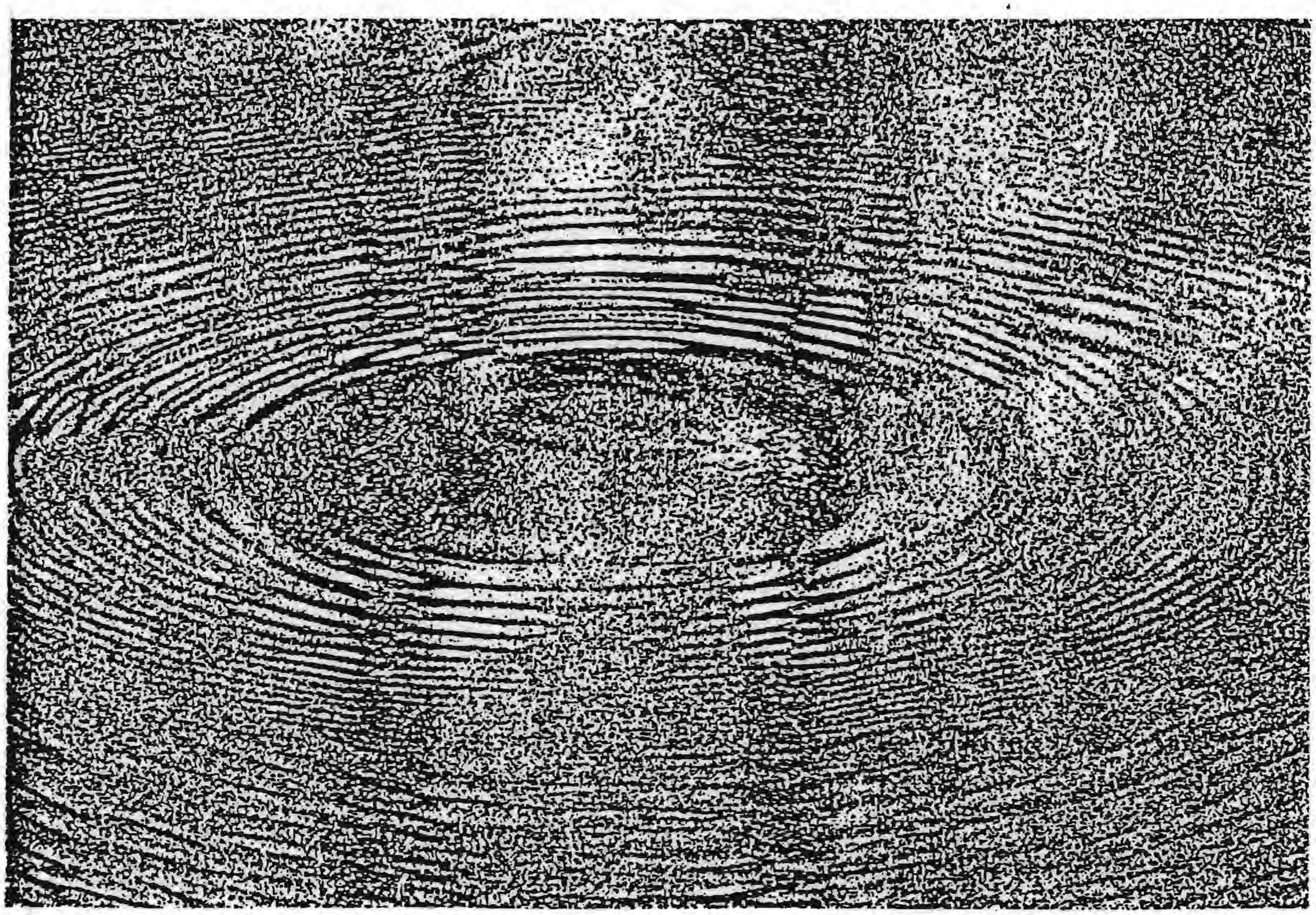

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EXPOSURE ASSESSMENT OF POPULATIONS USING ENVIRONMENTAL MODELING, DEMOGRAPHIC ANALYSIS, AND GIS[1]

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STRACT: Simulation of ground-water flow and fate of contami- nts in the subsurface environment constitutes a major phase of st environmental assessment and site remediation studies. ese simulation studies yield information on spatial and temporal tributions of contaminants in the subsurface media. An impor- t use of this information is to conduct exposure assessment dies. Spatial and temporal distributions of both chemical con- trations and exposed populations render this integrated expo- e analysis task rather difficult. Geographic Information Systems S), on the other hand, provide a platform in which layered, spa- ly distributed databases can be manipulated with ease, thereby plifying exposure analysis tasks significantly. In this paper, we cribe procedures that combine the simulation models and demo- phic databases under a GIS platform to automate the exposure essment phase of a typical health assessment study. Procedures eloped herein significantly simplify the post-processing phase of analysis, and render the overall task more "user friendly." A -specific application is included as a demonstration of the pro- ed process.
Y TERMS: ground-water flow; contaminant transport; environ- ital modeling; hazardous waste; geographic information sys- s; demographic analysis; exposure assessment.)

INTRODUCTION

n the past, environmental modeling analyses ducted in concert with remedial investigation/ sibility studies have concentrated primarily on nstructing historical contaminant levels in the surface and on predicting future contaminant lev- as a result of planned or ongoing remediation vities. These studies rarely have addressed the e of human exposure to historical and ongoing off- environmental contamination. On the other hand, health and epidemiologic studies have concentrated their efforts on biologic measurements and monitoring of populations by direct methods in order to estimate the effect or impact that exposure to environmental factors (such as subsurface contamination) may have had on the population. In recent years, however, there have been efforts to link contamination from environmental sources with increased health risk to humans. These exposure assessment studies require the interpretation and integration of spatial and temporal environmental data with demographic and epidemiologic data.

Geographic Information Systems (GIS) provide the platform in which layered, spatially distributed databases can be manipulated easily and whereby certain topological attributes, which are not known *a priori*, may be queried to obtain the spatial relationship between environmental parameters and demographic distributions. Thus, the purpose of this paper is to present procedures for automating the process of conducting exposure assessment of populations and to provide a site-specific case history that demonstrates the use and application of these automated procedures.

In this paper, we present a case study of the type frequently encountered by the Agency for Toxic Substances and Disease Registry (ATSDR), a Public Health Service agency, U.S. Department of Health and Human Services. ATSDR is mandated by Congress to evaluate the threat to public health of hazardous waste sites by using environmental and health outcome data (information on community-wide rates of illness, disease, and death compared with

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national and state rates) and community concerns (reports from the public about how a site affects their health or quality of life). Results of this public health assessment process are published and disseminated to interested parties. For this study, we used the Gratuity Road site, located in the town of Groton, Massachusetts (Figure 1). Ground-water and surface-water contamination have occurred near Gratuity Road in the town of Groton. A petitioned public health assessment (a health assessment conducted for a site that is not listed on the National Priorities or Superfund List) for the Gratuity Road site (ATSDR, 1992) identified the primary contaminants as trichloroethylene (TCE), 1,1,1-trichloroethane (TCA), hexavalent chromium (Cr^{+6}), chromium (Cr), and lead (Pb). The study also indicated that off-site residential ground-water wells had been contaminated with TCE and TCA. For the present study, we analyzed exposure through one environmental medium, ground water, for a single contaminant, TCE (dissolved in ground water).

GIS AND CONTAMINANT TRANSPORT MODELING ENVIRONMENT

The Federal Interagency Coordinating Committee on Digital Cartography (FICCDC, 1988) defines a GIS as follows: *A system of computer hardware, software, and procedures designed to support the capture, management, manipulation, analysis, modullary and display of spatially referenced data for solving complex planning and management problems.* Thus for exposure assessment studies, a GIS should be designed to store, retrieve, manage, display, and analyze geographic and spatial data – such as spatial and temporal distributions of environmental data (measured and/or computer simulated) and selected census areas containing demographic, hydrologic, and environmental attributes. To construct the GIS interface, we chose the GisPlus software package (Caliper Corporation, 1992) that runs on a personal computer (DOS machine) platform. Some of the features of GisPlus include the following:

- a menu-driven interface,
- a spreadsheet view of databases,
- graphic display of databases,
- geographic editing and querying,
- statistical analysis and cross tabulations,
- integration of user customized analysis routines, and
- automatic TIGER/Line file translation.

Throughout this paper, we will be providing illustrations that are images (screen images or dumps) of procedures used by the GIS to produce results discussed herein. A useful feature of the software is a menu-driven program that automates the building of point, line, and area databases (coverages) required by a GIS to conduct a spatial analysis. This program allows the user to specify the type of database, the number of layers, and the number and type of fields (attributes) that will be associated with the database. For example, if a database using data from the TIGER/Line files (TIGER/Line Census files, 1991) is to be built, then once the database specifications have been entered, the user selects the TIGER/Line Create command from the pull-down menu, and the program translates the TIGER/Line files and creates all necessary files required by the area database. Then the user can link the newly created database with census data on population. GisPlus also has the ability to create area databases for address matching and geocoding analyses.

The ground-water flow and contaminant transport modeling environment usually consists of a source code or a sequence of source codes that contain instructions to solve a particular problem expressed in terms of a set of mathematical models. The approximate solution of the problem is obtained by using numerical procedures if mathematical models describing the problem are too complex. For simpler mathematical models, closed-form solutions are utilized to obtain exact solutions to less complex problems. In either case, to implement the model, the computer code will require an input data file prepared in a proper format following the instructions of the input statements of the source code. As an output, the computer code will generate information on the spatial and temporal distribution of contaminant concentrations at a particular geographic location.

In most numerical simulations, the input and output database management requirements are complex if the simulation is to be accurate and reliable. For example, if the finite element method is used as the numerical procedure to solve governing mathematical models, the first task is the idealization of the solution domain into a computational mesh using spatially and most often non-uniformly distributed sub-regions called elements. To automate this process, the user can apply rather sophisticated mesh generation routines that can be found in the finite element literature. These routines simplify the generation of the coordinates of the nodes of the finite element idealization and also the development of the connectivity matrix for these elements. These are essential elements of the overall numerical procedure. The mesh generation programs, however, are not particularly useful when either (1) element values of the field data

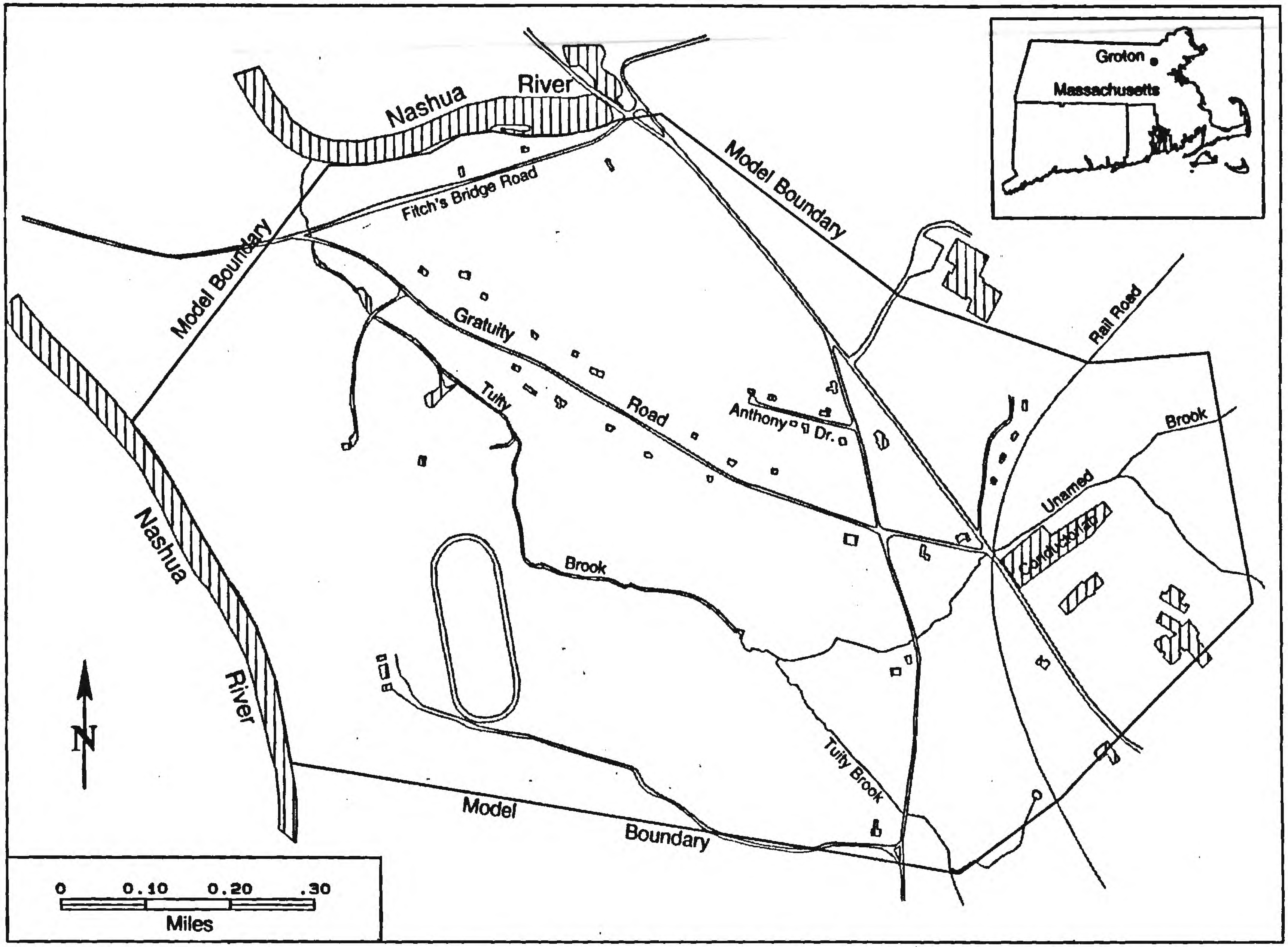

Figure 1. Location of Study Area, Groton, Massachusetts.

need to be prepared following a particular input format required by the source code; or (2) the nodal coordinates need to be referenced to a specific geographic location instead of an arbitrary Cartesian coordinate system.

A practical solution to this complex data preparation problem is interfacing finite element mesh generation algorithms and coordinate system transformation programs with GIS databases and developing algorithms to spatially interpret the GIS databases based on the mesh generated in the finite element idealization of the solution domain. In this overlay, through the use of appropriate algorithms and codes, every element of the idealization could be geographically associated with an attribute of a spatially distributed field variable. Because field variables can be stored in different layers of the GIS database, algorithms associated with different layers of the database could be used to extract various nodal or elemental data structures. These data structures could then be invoked by a source code to properly execute the code. Although such algorithms and codes are utilized in this study, the automated pre-processing phase of environmental databases used for the numerical solutions will not be described in this paper due to space limitations.

Numerical results obtained after executing the source code might also be stored in other layers of the GIS as additional databases or coverages. These output database files could be interpreted by using the GIS interface. For example, associating contaminant distribution database output obtained from a contaminant transport model with population distribution databases would yield very important information for an exposure analysis. This type of information is essential for evaluating increased health risk and health outcome data of environmental pollution. The two stages of pre- and post-processing of environmental data are of significant importance in a typical exposure assessment study. In this paper, we concentrate on the post-processing phase of the numerical modeling output by using a GIS interface.

APPLICATION OF ENVIRONMENTAL TRANSPORT MODELS

In the mathematical model used for this study, the flow and contaminant transport equations are solved by using a finite element Galerkin procedure with three nodal triangular elements. Because this method is well established in the ground-water literature, only a brief review of the development of the governing equations is provided below. A more detailed description of the methodology can be found in a number of texts, including Pinder and Gray (1977).

The governing equation for two dimensional, vertically averaged, steady-state flow in an unconfined aquifer is:

$$\frac{\partial}{\partial x_i}\left(K_{ij} h \frac{\partial h}{\partial x_j}\right) - \sum_{m=1}^{w} Q_m \delta(x_m, y_m) - I = 0 \tag{1}$$

where convention for tensor notation applies to indices i and j (i,j = 1,2 designate x, y respectively), K_{ij} represents the hydraulic conductivity tensor of the unconfined aquifer, h is the piezometric head in the aquifer, w is the number of wells, Q_m is the pumping rate for well m, $\delta(x_m,y_m)$ is the Dirac delta function evaluated at (x_m,y_m), and I is the infiltration or leakage flux in or out of the aquifer, which is a function of piezometric head distribution in adjacent aquifers. The governing equation for an unconfined aquifer is nonlinear due to the unknown location of the position of the water table, which must be determined as a part of the solution through an iterative process. The associated boundary conditions for the ground-water flow problem can be given in terms of Dirichlet, Neuman, and Cauchy conditions, which are shown below for an unconfined aquifer:

$$h = h_c \quad (x,y) \in \Gamma_1^{\,h}$$

$$n_i\left(hK_{ij}\frac{\partial h}{\partial x_j}\right) = f_h \quad (x,y) \in \Gamma_2^{\,h}$$

$$n_i\left(hK_{ij}\frac{\partial h}{\partial x_j}\right) = F_1 + F_2 h \quad (x,y) \in \Gamma_3^{\,h} \tag{2}$$

where n_i is the component of the outward normal to the boundary of the solution domain, and f_h, F_1, F_2, and h_c are functions defined on the boundary, Γ.

The governing equation for the two dimensional, vertically averaged, convective-dispersive transport of a miscible contaminant can be given as:

$$R\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - V_i\frac{\partial C}{\partial x_i}$$

$$+\sum_{m=1}^{w}\frac{Q_m\left(C - C_p\right)}{Bn}\delta(x_m, y_m) - \lambda C \tag{3}$$

where C is the contaminant concentration, R is the retardation factor, D_{ij} is the hydrodynamic dispersion tensor, V_i are the pore velocities in x and y directions, C_p is the concentration of the pumped water, B is the aquifer thickness, n is the aquifer porosity, λ is the first order decay constant, and Q_m, w, and $\delta(x_m,y_m)$ are as defined in Equation (1). Boundary and initial conditions for a contaminant transport problem can be defined as:

$$C = C_o \quad (x,y) \in \Omega \ ; \ t = t_o$$

$$C = C_c \quad (x,y) \in \Gamma_1 \ ; \ t \geq t_o$$

$$n_i\left[nB\left(V_i - D_{ij}\frac{\partial C}{\partial x_j}\right)\right] = f_c \quad (x,y) \in \Gamma_2 \quad ; \quad t \geq t_o \qquad (4)$$

where Ω represents the solution domain and Γ the boundary of the solution domain.

The retardation factor, R, is equal to $(1 + K_s)$, where K_s is the adsorption solubility rate constant defined in terms of the bulk density and porosity of the soil and the partition coefficient, which is a function of organic carbon content of soil and octanol water partition coefficient of the chemical constituent. The pore velocities are defined using Darcy's Law:

$$V_x = -\frac{K_{xx}}{n}\frac{\partial h}{\partial x}$$

$$V_Y = -\frac{K_{yy}}{n}\frac{\partial h}{\partial y} \qquad (5)$$

where K_{xx} and K_{yy} are the hydraulic conductivities in the x and y directions as defined in Equation (1).

The diffusion tensor terms may be defined using the identities of Schiedegger (1961):

$$D_{xx} = \frac{\alpha_L V_x^2 + \alpha_T V_y^2}{|V|}$$

$$D_{yy} = \frac{\alpha_L V_y^2 + \alpha_T V_x^2}{|V|}$$

$$D_{xy} = D_{yx} = \frac{(\alpha_L - \alpha_T)V_x V_y}{|V|} \qquad (6)$$

where α_L and α_T are the longitudinal and transverse dispersivities of the porous media, and $|V|$ is the magnitude of the velocity vector.

In finite element analysis the solution domain is idealized by a network of elements. It is then assumed that the differential equation can be approximated by a series of independent basis functions defined in terms of the nodal values of the unknown function in each element. For example, when solving Equation (1), the piezometric head can be approximated as follows:

$$h = \sum_{i=1}^{n} N_i h_i \qquad (7)$$

where N_i is the basis function at node i, n is the total number of nodes for an element, and h_i is the approximate value of the piezometric head at node i.

When Equation (7) is substituted in Equation (1) a residual will be generated. The best approximation is then achieved when the residuals are minimized by using the method of weighted residuals process. The Galerkin method, a typical weighted residual method, minimizes residuals using the basis functions as the weighting functions. This residual or orthogonality condition can be defined as:

$$\sum_{e}^{N} \int_{A^e} N_k L(h) dA^e = 0 \qquad (8)$$

where L is the differential operator defined as Equations (1) or (3), and N_k is the weighting functions. The integration is performed over an element, and the summation indicates the assembly of all elemental integral evaluations.

Utilizing this process, Equation (1) can be written as follows for a typical element:

$$\iint_{A^e} N_l\left[\frac{\partial}{\partial x}\left(K_{xx}h\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial y}\left(K_{yy}h\frac{\partial h}{\partial y}\right) - \sum_{m=1}^{w} Q_m \delta(x_m, y_m) - I\right]dA = 0; \quad l = i,j,k \qquad (9)$$

where i, j, and k refer to the nodal numbers of the element. The minimization of the residual over each element, the assembly of all elemental matrices, and the introduction of boundary conditions yield the global matrix system given below.

$$[S]\{h\} = \{F\} \ . \qquad (10)$$

Equation (10) may now be solved for the piezometric head at each node after the introduction of boundary conditions.

The contaminant transport equation may also be analyzed using a similar process. In this case the contaminant transport solution is tied to the ground-water flow solution through Darcy velocity terms. Thus, in this sequential solution process Equation (1) needs to be solved first. The weighted integral residual of the convective transport equation can be given as:

$$\iint_{A^e} N_l \left[R\frac{\partial C}{\partial t} - \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial C}{\partial x} + D_{xy}\frac{\partial C}{\partial y}\right) - \frac{\partial}{\partial y}\left(D_{yy}\frac{\partial C}{\partial y} + D_{xy}\frac{\partial C}{\partial x}\right) + V_x\frac{\partial C}{\partial x} + V_y\frac{\partial C}{\partial y} + \sum_{i=1}^{w}\frac{Q_m(C-C_p)}{Bn}\delta(x_m, y_m) + \lambda C \right] dA = 0 ;$$

$$l = i, j, k . \tag{11}$$

Minimization of the residual over each element and the assembly of all elemental matrices yield the resultant matrix equations given below:

$$[M]\left[\frac{\partial C}{\partial t}\right] + [S][C] = [F] . \tag{12}$$

After the introduction of boundary conditions, finite difference techniques are used in the solution of the above equation to determine the concentration at each node at each time step. This sequential solution process yields spatial and temporal distribution of contaminants at each node over the solution domain. This equation may be given as:

$$([M] + (1-\alpha)\Delta t[S])[C]^{t+\Delta t} = ([M] - \alpha\Delta t[S])[C]^t + \left(F^t\right) + \left(F^{t+\Delta t}\right) \tag{13}$$

where Δt is the time step, α is a weighting factor, which may vary from zero to one, and the superscripts identify the time at which matrices or vectors in Equation (13) are defined. Selecting $\alpha = 1$ corresponds to forward differencing, selecting $\alpha = 0.5$ corresponds to central differencing, and selecting $\alpha = 0$ corresponds to backward differencing (Aral, 1990a; b).

APPLICATION OF METHODOLOGY TO STUDY AREA

The ground-water flow and contaminant transport equations and the numerical method described above were used to evaluate the transport of the contaminant TCE at the Gratuity Road site. The site is underlain by a stratified glacial drift water-table aquifer that varies in thickness from a few feet to more than 50 feet. Historical data indicate that TCE contamination of ground water from the Conductorlab area (Figure 1) began during the mid-1960s (HMM Associates, Inc., 1988; 1990), at which time all residences were using ground water for their domestic water supplies. A 1985 environmental investigation revealed TCE contamination of ground water in excess of 50 parts per billion (ppb) extending west of the Conductor Lab area into the Gratuity Road area. By the summer of 1987 all Gratuity Road residences, originally using ground water for domestic supplies, were connected to the Groton municipal water supply system. Thus, ongoing contamination of ground water with TCE and exposure of the population to the contaminated ground water occurred for approximately 20 years.

Our analysis began with a steady-state ground-water flow calibration using November 1989 water levels to determine flow field characteristics. The SLAM (Steady Layered Aquifer Model) code (Aral, 1990a) was used to simulate the ground-water flow field. The selected model boundary and calibrated water levels are shown in Figure 2. The boundary adjacent to the Nashua River was simulated as a Dirichlet boundary and assigned a value of 200 feet (referenced to sea level datum), the stage of the river. The eastern boundary was simulated as a Neuman boundary and assigned a value of 0.002 ft/d (feet per day). The top and bottom boundaries also were simulated as Neuman boundaries and assigned a value of zero (no-flow). The calibrated infiltration rate due to precipitation was assumed to be constant over the model area and was assigned a value of 8.5 inches per year. Calibrated hydraulic conductivity values ranged from 0.5 to 22 ft/d, which were consistent with and within the range of field and laboratory derived values (HMM Associates, Inc., 1988; 1990). As shown in Figure 2, this flow field is characterized by ground-water and surface-water interaction as indicated by the curvature of water-level contours near Tuity and Unamed Brooks. Graphical display of the calibrated velocity field and simulation of alternative flow-field scenarios are not presented here owing to brevity, but can be found in Maslia *et al.* (1993).

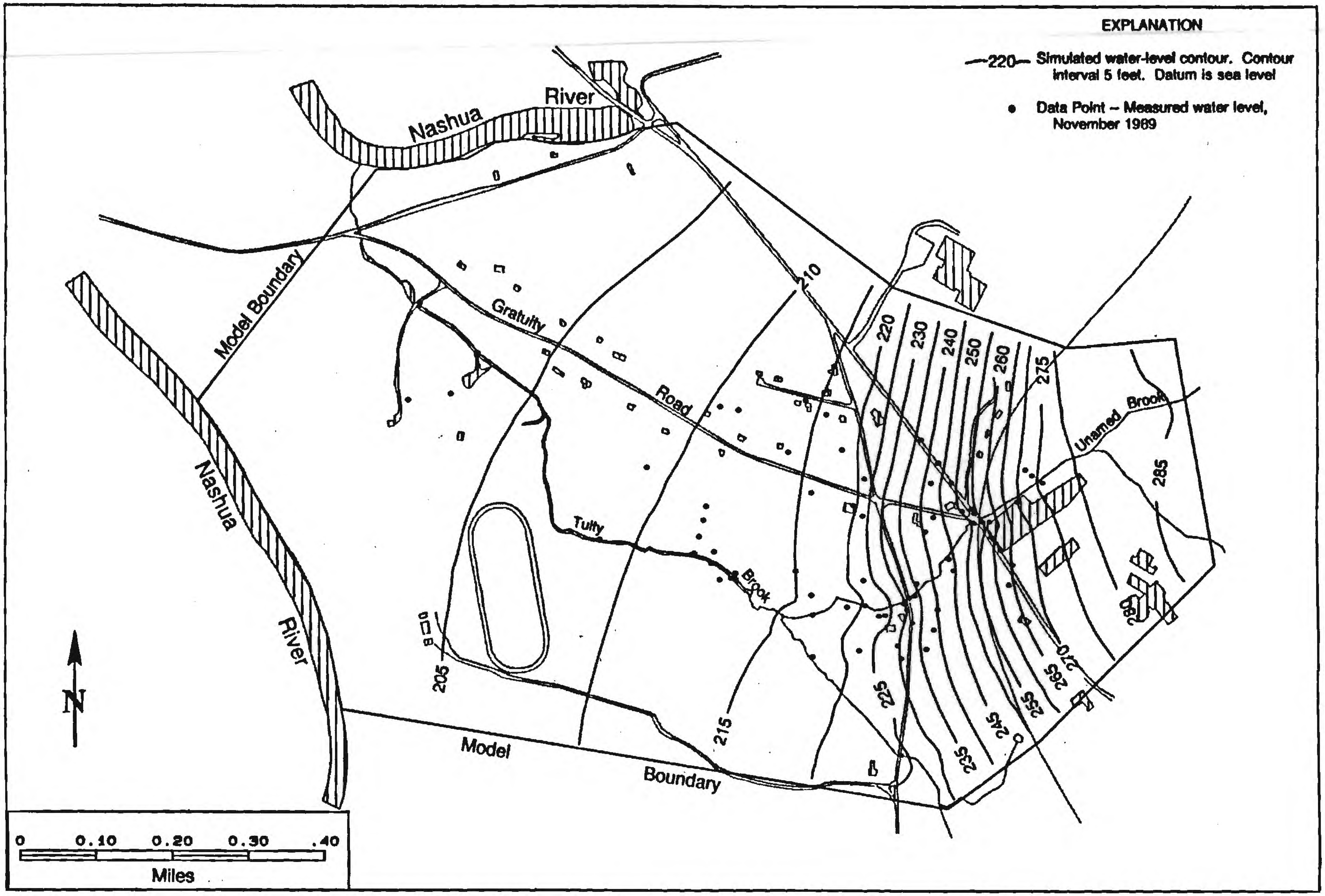

Figure 2. Calibrated Ground-Water Levels for the Groton Area Based on November 1989 Data.

Aquifer contamination and proposed remediation were simulated by investigating two contaminant transport scenarios using the CLAM (Contaminant transport in Layered Aquifer Media) code (Tang and Aral, 1992). In all simulations, we assumed a constant porosity of 0.35, a retardation factor of 3 for the dissolved TCE (HMM Associates, 1990), no volatilization or biodegradation, and longitudinal and transverse dispersivities (α_L, α_T) of 64 and 8 feet, respectively. In the first scenario, we conducted a 40-year simulation with a maximum source concentration of 50,000 parts per billion (ppb) located at the assumed point of contamination in the Conductorlab area. Results of this simulation are shown in Figure 3 as temporal distributions of TCE. The contour lines represent the U.S. Environmental Protection Agency's (USEPA) maximum contaminant level (MCL) for TCE of 5 ppb for times of 5, 10, 15, 20, 30, and 40 years. Model results indicate that after 20 years ground water contaminated with TCE has migrated into the Gratuity Road and Anthony Drive areas and has encroached into nearby surface-water streams (Tuity Brook and Unamed Brook).

In the second scenario, we simulated a proposed pump-and-treat remediation plan by conducting a 20-year simulation with a maximum source concentration of 50,000 ppb and then removing the source from the site and pumping and injecting 20 gallons per minute (gpm) of water for another 20 years. Figure 4 shows the location of the 500 and 5 ppb TCE contours after 40 years (20 years of contamination and 20 years of pump-and-treat technology). Results indicate that, after 40 years, in part of the source area, TCE concentrations have been reduced to less than 50 ppb. Downgradient of the site near Gratuity Road and Anthony Drive, however, an area of TCE contamination of more than 500 ppb which represents the historical TCE contamination that has escaped the pump-and-treat remediation process, now exists (Aral *et al.*, 1993].

Results of the contaminant transport simulations indicate that, after 20 years of contamination, some people living in the Gratuity Road area and using ground water were exposed to TCE that exceeds the MCL (5 ppb). Additionally, the simulations suggest that although the pump-and-treat technology may clean up the site and source area, populations downgradient from the site may still be at risk of exposure from TCE that exceeds the MCL (Figure 4). Numerical results obtained from the ground-water flow and contaminant transport model generated the databases that were used to compose several of the GIS layers.

The next step in an exposure assessment study is to determine the spatial distribution of the population for Groton, Massachusetts, by using digital census data and the GIS. Clearly, in this analysis we have assessed potential exposure solely for one environmental medium, ground water. The downgradient population may come into contact with TCE contamination through other environmental media and pathways such as surface water, soil, and plant uptake. Thus, a more refined analysis would be needed to identify multimedia exposure trends. A research program that concentrates on developing multimedia exposure assessment capability and applying it to hazardous waste sites is currently underway at ATSDR.

DEMOGRAPHIC ANALYSIS

The smallest subdivision of reportable census data occurs at the block level. The 1990 census data at the block level are available for the Groton area. Therefore, these data were used to determine the demographics of the study area. Census data were obtained by using the Summary Tape File 1B Extract (STF1BX) for the Groton area (Census of Population and Housing, 1991). Visualizing the distribution of the census blocks and data required a method of graphically displaying the location of the census blocks relative to the Gratuity Road site. This was accomplished in a two-step process by using the GisPlus software package (Caliper Corporation, 1992).

The first step in the process was to determine the location of the census block level areas and boundaries for the Groton area. This was accomplished by using the GisPlus internal translator for the TIGER/Line census files to translate the 1990 TIGER/Line census files for Middlesex County, Massachusetts (TIGER/Line Census Files, 1991). Once the block level areas and boundaries were translated, they were graphically displayed. Figure 5 is a screen image showing the block level areas and boundaries for the Groton area (for state, county, and tract code 250173261). The 3-digit number within each block (for example, 602) is the block number. Note, Gratuity Road is classified as a block boundary that divides blocks 602 and 603.

The second step in the process was to relate the STF1BX data to the appropriate census block. Again, this was accomplished through the use of the GIS software. Once the STF1BX data were related to the census blocks, the spatial query capabilities of GisPlus were used to query each census block. Figure 6 is a screen image showing the spatial querying of census block 121. This query was executed by first selecting the Query option from the main menu of the GisPlus program. The GIS then outlines the selected block area and displays the information shown on the left

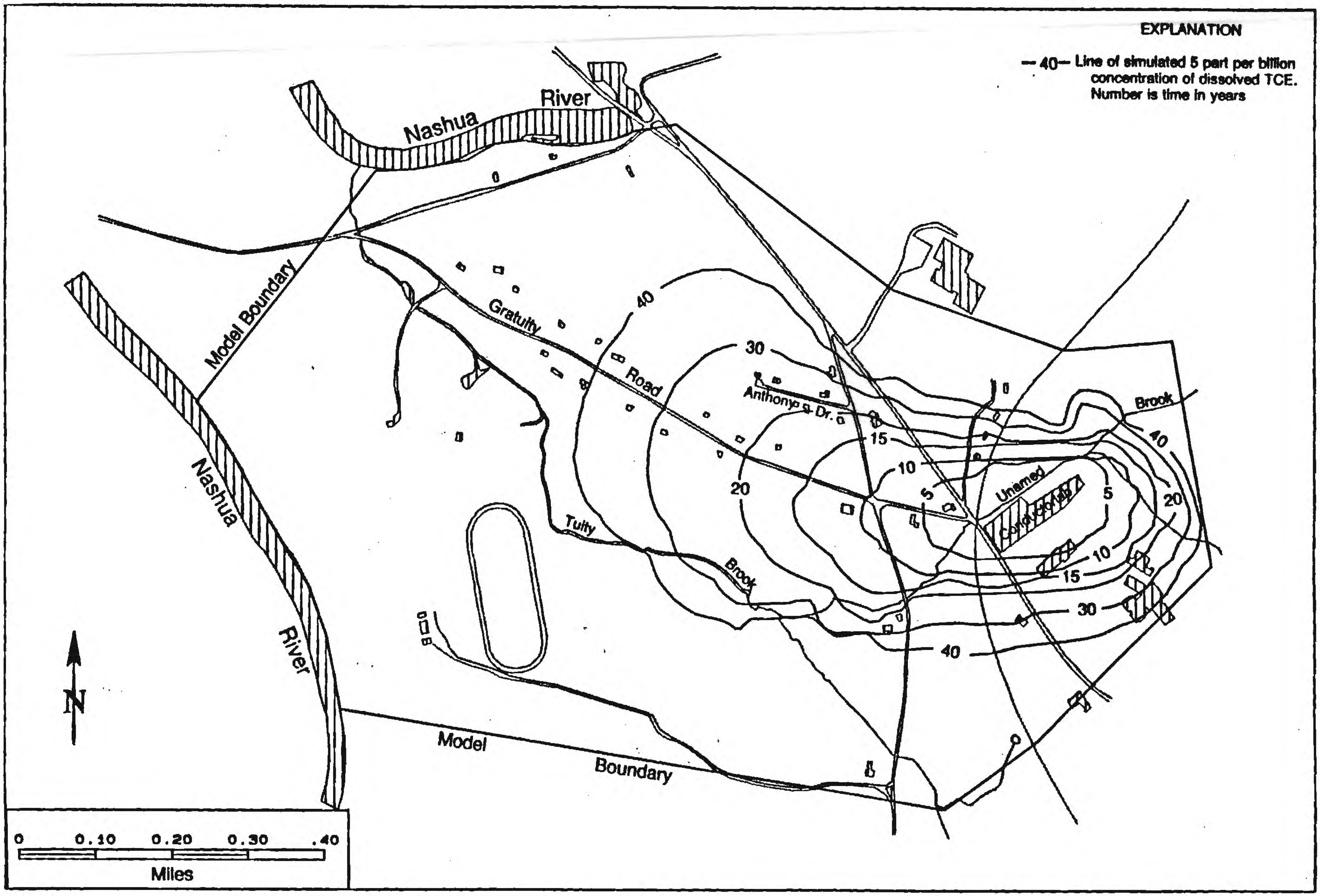

Figure 3. Simulated Temporal Distribution of the 5 Part-Per Billion Contour for Dissolved TCE (40 years of simulation time).

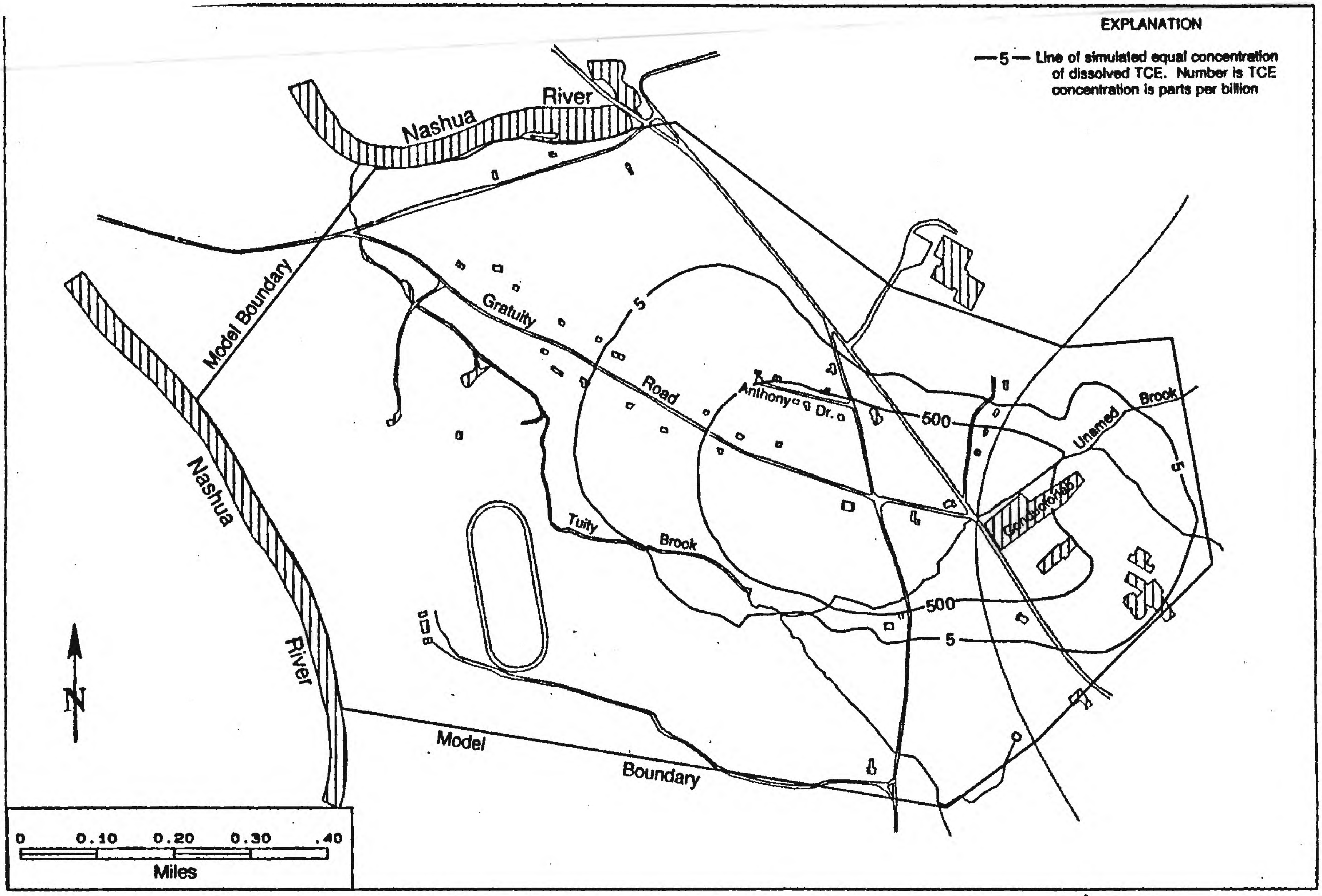

Figure 4. Simulated Distribution of Dissolved TCE After 40 Years (20 years of contamination and 20 years of remediation).

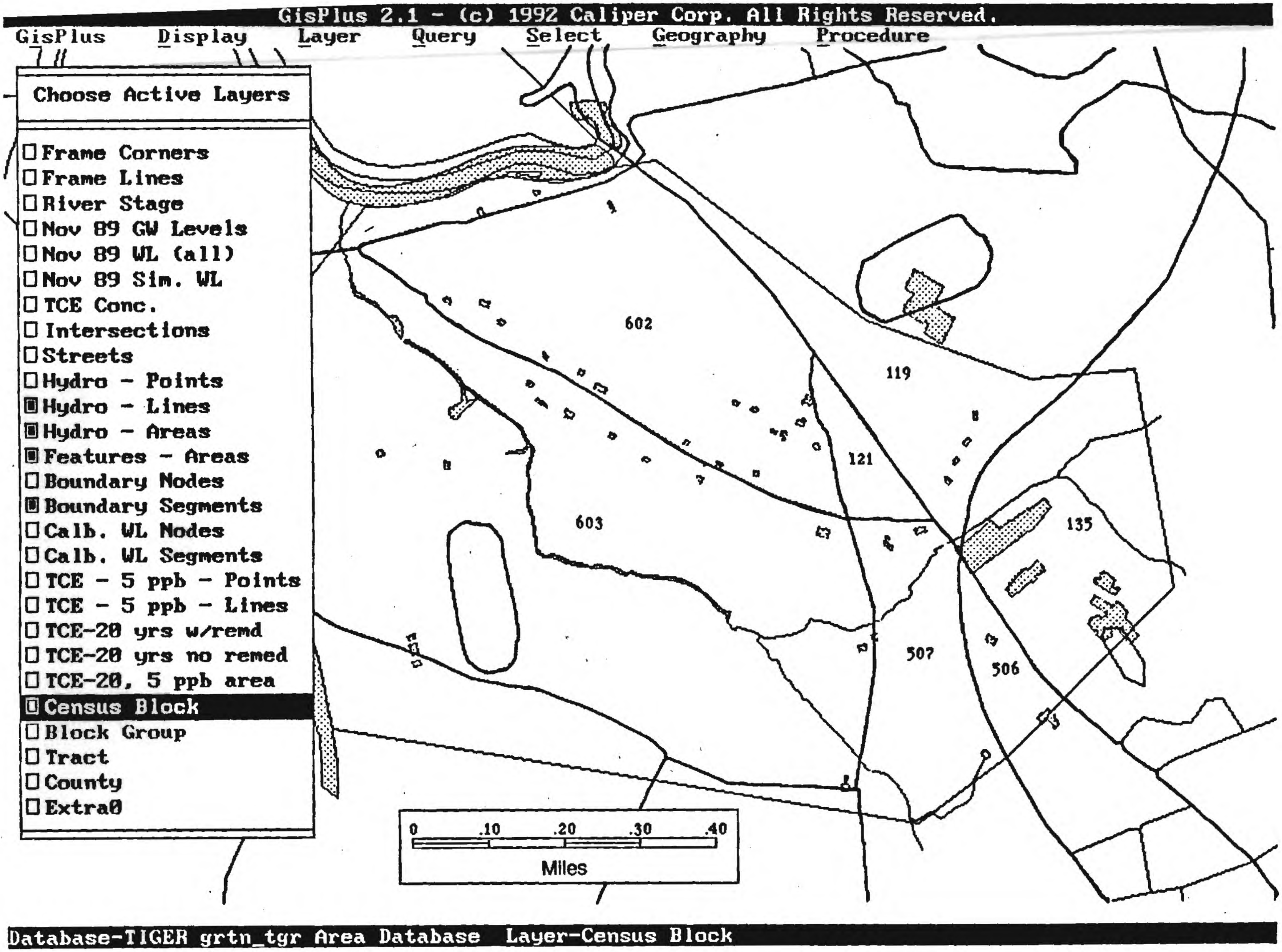

Figure 5. Screen Image of the TIGER/Line Census Block Area Database for Groton, Massachusetts, Area (state, county, and tract code 250173261).

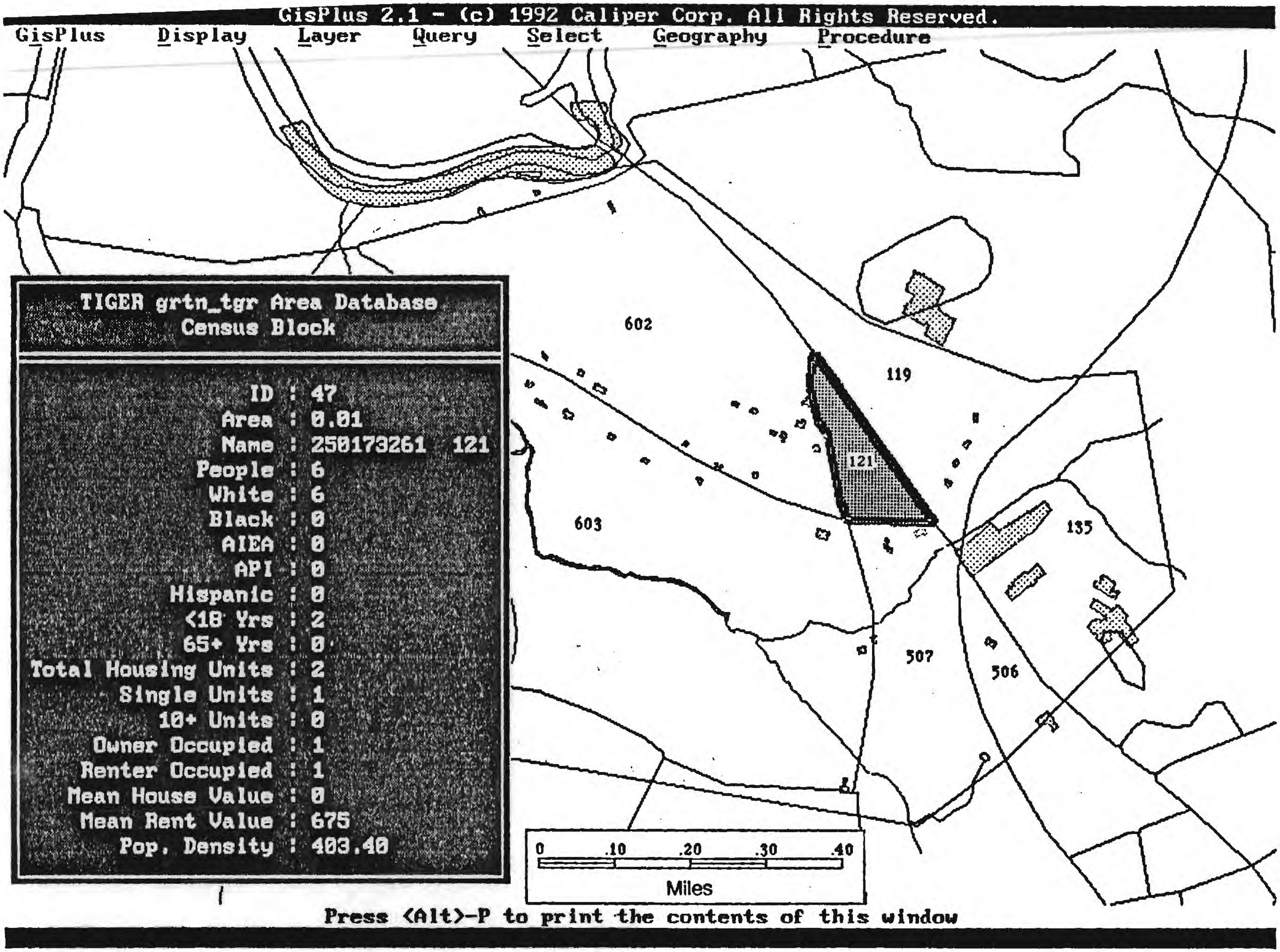

Figure 6. Screen Image of Census Block Areas and Demographic Data Query.

ide of Figure 6. Additionally, several census block reas can be selected and the census data from the elected blocks can be stored in a table or a file for ater use. Population and area statistics for each of he Groton census blocks are listed in Table 1.

As part of the process described above, the area of ach census block (in square miles) was also obtained. 'hus, the values for population density were comput-d using the equation entry capability of GisPlus and omputing population density according to the formu-a:

$$Population\ Density = People\ /\ Area \qquad (14)$$

'here population density is defined as the number of eople per square mile of census block area (column 4, 'able 1).

INTEGRATED SYSTEM

The last step in the exposure assessment process 'as to spatially integrate results of the contaminant 'ansport analysis databases (location of the 5 ppb or reater area of TCE contamination, Figure 3) with ie demographic analysis for the Groton area. If done ianually, this is a complex and time consuming ffort. However, when accomplished by using the spa-ial query capabilities of a GIS, this task becomes a mple operation. Figure 7 shows the relation between CE contamination after 20 years (environmental 'ansport, first scenario) with the 1990 census block vel areas (demographic analysis) derived by con-ıcting a spatial analysis using the GIS. The result-ıg parameter is the area of the census blocks that ıs TCE contamination that equals or exceeds the MCL (5 ppb). Conducting a spatial query on the hatchured areas within each census block (Figure 7) yielded the area of a particular census block that had been contaminated. Results of this spatial query are listed in Table 1 (column 5) for each census block.

The population that may been exposed to the contaminated ground water for each census block was obtained by multiplying the population density for each block (column 4, Table 1) by the area of contamination within each block (column 5, Table 1). Based on this approach, we estimated that nearly 36 people (the sum of all entries for column 6 of Table 1) may have been exposed to ground water contaminated with TCE that exceeds the MCL (5 ppb) after 20 years of contamination. This method enumerates only the population living in the area of concern as of the 1990 census while assuming those persons are uniformly distributed throughout the census block areas. To assess potential population exposure over time requires linking past census data with current area boundaries and estimating area migration (White, 1984). Census tracts are most suitable for this type of small area longitudinal analysis because tracts are relatively stable statistical area boundaries (Shryock and Siegel, 1976). We are currently evaluating different approaches to utilizing historical demographic information in conjunction with historical contaminant exposure. Nevertheless, comparison of historical and 1990 census data for the Groton area have indicated a rather stable population. Therefore, we believe that the procedures outlined above provide an acceptable estimate of population exposure for this case study and will serve as the basis for future studies when more rigorous analysis techniques are developed.

TABLE 1. 1990 Census Data, Area Statistics, and Population Exposed to TCE Contaminated Ground Water, Groton, Massachusetts.

Census Block Number*	Total People	Block Area (square miles)	Population Density	Census Block Area Contaminated With TCE (square miles)	Estimated Exposed Population
119	62	0.22985	269.74	0.00761	2.1
121	6	0.01487	403.40	0.00914	3.7
135	66	0.29954	254.29	0.03859	9.8
506	33	0.04261	774.47	0.00232	1.8
507	39	0.10842	359.71	0.01688	6.0
602	106	0.14087	752.45	0.01035	7.8
603	62	0.39453	157.15	0.02826	4.4
				Total Exposed Population	35.6

ıte, county, and track code 250173261.

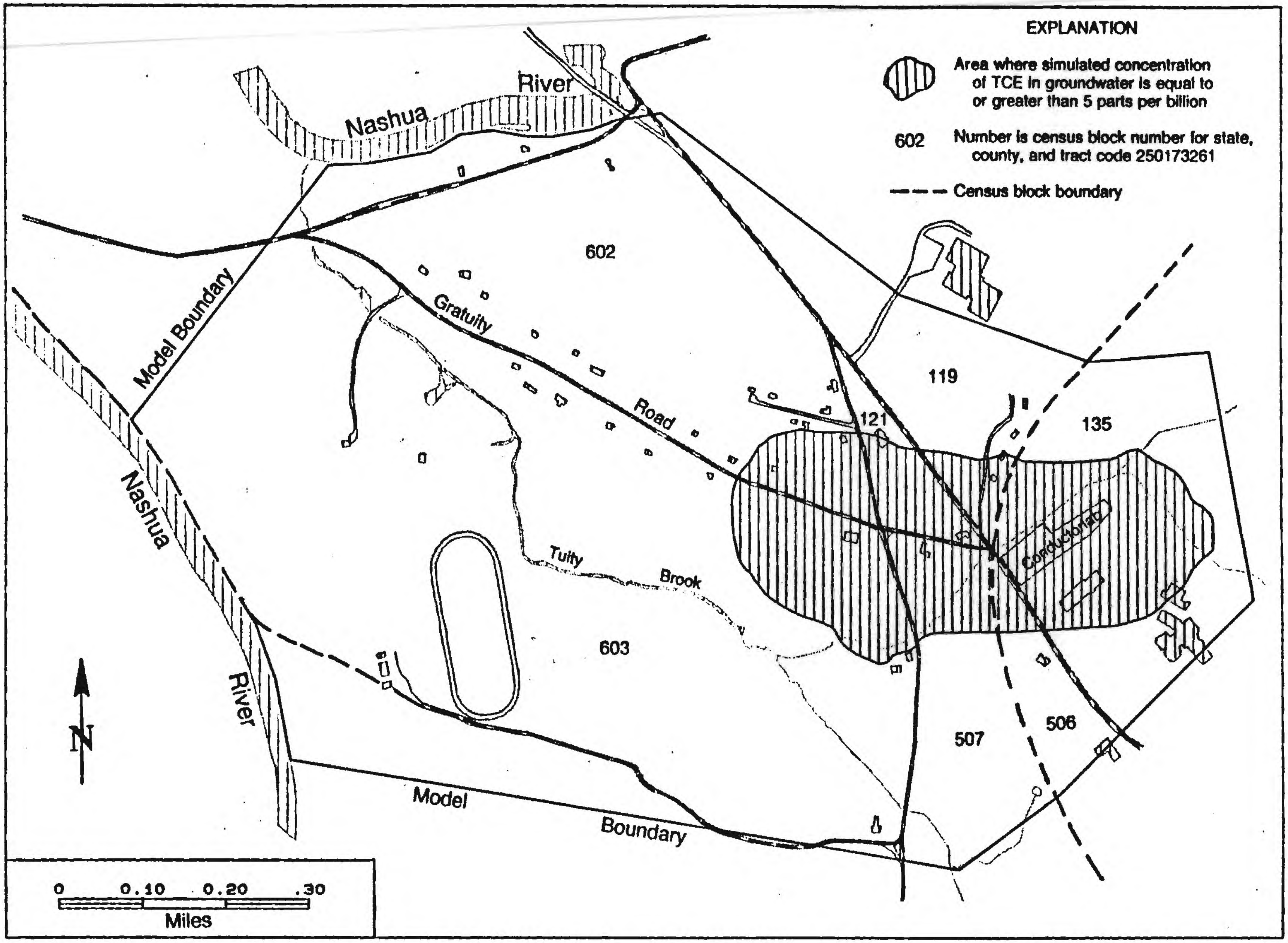

Figure 7. Relation of TCE Dissolved in Ground Water with Census Block Areas After 20 Years of Contamination.

Exposure Model

Exposure models attempt to quantify a person's contact with a contaminant at a specific concentration for a specified duration of time. Total human exposure is composed of contributions from all environmental media (water, soil, air, and plants) that contain the contaminant, and all routes of entry to the human body (dermal contact, ingestion, and inhalation). From a mathematical perspective, total human exposure may be defined by the following equation:

$$E = \int_{t_1}^{t_2} C(t)dt \tag{15}$$

where E is the exposure, $C(t)$ is the time-varying concentration of a contaminant, and dt is the time increment from t_1 to t_2.

Although total human exposure is described by Equation (15), data are usually insufficient to account for exposure from all environmental media and by every route of entry. Consequently, researchers and regulators have, in the past, focused their attention on exposure to hazardous substances from potable water supplies by the ingestion route. However, when contaminants (such as TCE) belonging to the class of compounds known as volatile organic chemicals (VOCs) are considered, evidence is mounting that entry by the route of inhalation may be as important as ingestion. For example, laboratory experiments using standard shower conditions have indicated that an average of 80 percent to 85 percent of TCE contained in the water supply for the shower volatilized into air (Wilder, 1986). Therefore, exposure by the route of inhalation should be accounted for in exposure assessment studies involving VOCs.

For the present study, we will be using empirical equations that were derived from results of laboratory shower experiments in which TCE was added to the shower water supply to determine volatilization and inhalation characteristics. Because of space limitations, details of the laboratory experiments will not be provided herein but can be found in Andelman (1975) and Wilder (1986). The maximum contaminant concentration in the air during the shower can be described by the following equation:

$$C_{a_{max}} = ktC_w / V_a$$

where $C_{a_{max}}$ is the maximum contaminant concentration in the shower air in milligrams per liter (mg/L), k is the volatilization mass transfer coefficient in liters per minute (L/min), t is time in the shower in hours (h), C_w is the contaminant concentration in the shower water supply (mg/L), and V_a is the volume of the shower room (L). Assumptions used for the laboratory shower experiments are listed below in Table 2. Using these standard assumptions, Equation (16) reduces to the following equation:

$$C_{a_{max}} = 4.5\text{x}10^{-3}\, C_w\,.$$

It can also be shown that for the given shower assumptions used in the laboratory experiments, after the shower period of time t, the average TCE concentration in the air C_a that an individual is exposed to is equal to $C_{a_{max}}$ at time t (at the end of the shower) (Andelman, 1975).

Inhalation exposures in the shower can be defined as the product of the concentration of the contaminant in the air, the breathing rate (for an adult), and the exposure time, such that:

TABLE 2. Assumptions Used for Laboratory Shower Experiments (Wilder, 1986).

Shower	Contaminant	Human
'low rate in the shower: 8 L/min.	Fraction volatilization rate of TCE from shower water: 0.90.	Adult body weight: 70 kg.
ir exchange rate in the shower and hower room: 0.53/hr.	Rate of volatilization during the shower is constant.	Ingestion: 1.3 L of domestic water per day.
olume of shower and shower room: 0,000 L.	Rate of decay of TCE in the shower room after shower is constant.	Inhalation rate at rest: 1,000 L of air per hour.
	Shower and shower room treated as a one-compartment model.	Takes one 6-minute shower per day, 365 days per year.
		Remains in shower room for 15 minutes after showering.

$$E_i = C_a B t \tag{18}$$

where E_i is the exposure (mg), B is the breathing rate (L/h), and C_a and t are as previously defined. Assuming a human adult takes one shower per day (Table 2), using results of the laboratory experiments, inhalation exposure to TCE during showering can be defined by the following equation:

$$E_i = 1.35 C_w \tag{19}$$

where E_i is now defined as the exposure from inhalation of TCE in mg/d.

Application of Exposure Model to Study Area

As a result of the environmental transport simulations, the temporal and spatial distribution of TCE contamination for the study area was known. Thus, if the domestic water supply was obtained from ground water, the concentration of TCE in the water supply, C_w, for a specific point in time at a specific location would be known. Equation (15) can be solved using the concentration data derived from the environmental transport model to compute exposure to TCE. For illustrative purposes, however, we will compute exposure for only one point in time. After 20 years of simulated remediation, the concentration of TCE in ground water at a certain locations along Gratuity Road in the study area is 250 ppb or 0.25 mg/L. Letting C_w = 0.25 mg/L, and inserting this value into Equation (19), the exposure an adult receives by the route of inhalation during and after a shower is computed as follows:

$$1.35 \text{ L/d} \times 0.25 \text{ mg/L} = 0.34 \text{ mg/d} .$$

Alternatively, if an adult ingests 1.3 liters of water per day, then the exposure by the route of ingestion can be computed as follows:

$$0.25 \text{ mg/L} \times 1.3 \text{ L/d} = 0.33 \text{ mg/d} .$$

Therefore, using concentration data from the study area in conjunction with laboratory determined inhalation parameters indicates that an adult would receive nearly the same exposure by the route of inhalation during and after showering as from ingestion of ground water contaminated with TCE. This analysis, in conjunction with the demographic and spatial analysis techniques previously described, may allow one to identify sub-populations that could be further studied for potential exposures and adverse health effects resulting from contact with environmental contaminants.

CONCLUSIONS

The impact of environmental pollution on populations and the accurate assessment of this impact is an important part of determining the potential for increased health risk to humans. In the study summarized in this paper, adverse environmental impacts on populations were evaluated by conducting an exposure assessment using the ground-water medium as the primary pathway of exposure. In this assessment, ground-water flow and contaminant transport models were integrated with spatial demographic analysis tools through the use of a GIS interface. Procedures used to develop this integrated approach are innovative and quite promising for use in more detailed and elaborate analyses. Results of this study demonstrate the novel and very useful information that can be obtained from accurate evaluation of exposure patterns derived from spatially distributed databases. For the present analysis, spatial and temporal distributions of TCE dissolved in ground water were integrated with 1990 census data derived from the Summary Tape File 1B Extract for the Groton, Massachusetts, area. Availability of additional demographic information on the distribution and mobility of households would facilitate the generation of more precise spatial and temporal exposure patterns that could easily be accommodated by methodology described herein.

The exposure analysis used the simulated concentrations of TCE predicted by the environmental transport models. These concentrations were used to compare exposure to TCE from inhalation in a one-compartment model shower with exposure from ingestion of domestic water contaminated by TCE. The exposure model indicated that exposure to TCE by the inhalation route during showering is nearly identical to exposure by ingestion of domestic water supplies contaminated with TCE. As a result, entry by route of inhalation is as important as entry by route of ingestion when conducting exposure analyses due to contamination from volatile organic chemicals such as TCE.

ACKNOWLEDGMENTS

The research described in this paper was supported by Cooperative Agreement award number U50/ATU499828-01 for the Research Program for Exposure-Dose Reconstruction between the Agency for Toxic Substances and Disease Registry (ATSDR) and the Georgia Institute of Technology. The authors would like to express their appreciation to Dr. Barry L. Johnson, Assistant Administrator, ATSDR, for his continued support of the project.

TRADEMARKS

The use of brand or trade names in this paper is for identification purposes only and does not constitute endorsement by the Agency for Toxic Substances and Disease Registry (ATSDR).

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GEORGIA TECH RESEARCH CORPORATION
GEORGIA INSTITUTE OF TECHNOLOGY
OFFICE OF CONTRACT ADMINISTRATION
PROGRAM INITIATION DIVISION
ATLANTA, GEORGIA 30332-0420
USA

Telex: 542507 GTRC OCA ATL
Fax: (404) 894-6956

Phone: (404) 894-4817

Refer to: JLG/02.108.002.95.004
E-20-X79
2

19 May 1995

Mr. Henry S. Cassell, III
Centers for Disease Control & Prevention
Grants Management Office
255 E. Paces Ferry Road, NE
Room 300, MS E-13
Atlanta, Georgia 30305

Attention: Ms. Maggie Slay

Subject: Research Proposal Entitled, "Research Program on Exposure-Dose Reconstruction"

Reference: U61/ATU499828-03

Dear Mr. Cassell:

The GEORGIA TECH RESEARCH CORPORATION desires to submit for your consideration the subject proposal prepared by Dr. Mustafa M. Aral,School of Civil and Environmental Engineering, Georgia Institute of Technology.

A description of the research program, the time required and program cost are included in the proposal. Should additional information be desired, please do not hesitate to contact Dr. Aral at 404/894- 2243 regarding technical matters or the undersigned at 404/894-4817 for administrative concerns.

We appreciate the opportunity of submitting this continuation application and look forward to hearing from you.

Sincerely,

Jarlis L. Goddard
Contracting Officer

JLG/bb
Addressee: Three copies
Enclosure: Proposal - Three copies

Georgia Tech

School of Civil and Environmental Engineering

Georgia Institute of Technology
Atlanta, Georgia 30332-0355
USA
404•894•2201
404•894•2278 FAX

404•894•2243 (Direct)
maral@ce.gatech.edu (e-mail)

MEMORANDUM

To : **Mr. Henry S. Cassell, III**
Grants Management Officer, Grants Management Branch
Centers for Disease Control and Prevention
Ms. Maggie Slay
Project Specialist, Grants Management Branch
Centers for Disease Control and Prevention

From : **Dr. M. M. Aral**
Project Director, School of Civil Engineering, Georgia Tech

Date : **May 8, 1995**

Subject : Your reference: Award No. U61/ATU499828-02
Progress Report and Application for Extension

Per your letter dated 29 March, 1995, enclosed please find an original and two copies of the continuation application I am submitting for the Fiscal Year 1995. The application package titled "Progress Report and Application for Extension - RESEARCH PROGRAM FOR EXPOSURE-DOSE RECONSTRUCTION" include the following information:

- A summary of progress made during the second project year;
- Scheduled activities of the third project year;
- A list of technical publications which are the outcome of the research effort; and,
- Proposed budget and justification.

I am looking forward to hearing from you regarding this application. If you have any questions please do not hesitate to contact me at the above address and telephone numbers.

Annual Progress Report for Project Period 2
and
Application for Extension for Project Year: 3

RESEARCH PROGRAM FOR EXPOSURE-DOSE RECONSTRUCTION

Submitted to:

Agency for Toxic Substances and Disease Registry (ATSDR)

Project Officer: Allan S. Susten, Ph.D. (DHAC, MS E-32)
Technical Project Officer: Morris L. Maslia, P.E. (DHAC, MS E-32)

Centers for Disease Control and Prevention and ATSDR
Award Reference No. U61/ATU499828-02

Submitted by:

Mustafa M. Aral, Ph.D.

Principal Investigator
School of Civil and Environmental Engineering
Georgia Institute of Technology
Atlanta, Georgia 30332

June 27, 1995

TABLE OF CONTENTS

OMB Approval No. 0348-0043

APPLICATION FOR FEDERAL ASSISTANCE

2. DATE SUBMITTED May 12, 1995

Applicant Identifier

3. DATE RECEIVED BY STATE

State Application Identifier

4. DATE RECEIVED BY FEDERAL AGENCY

Federal Identifier

1. TYPE OF SUBMISSION:

Application
☐ Construction
XX Non-Construction

Preapplication
☐ Construction
☐ Non-Construction

5. APPLICANT INFORMATION

Legal Name: GEORGIA TECH RESEARCH CORP

Organizational Unit: School of Civil and Env. Eng.

Address (*give city, county, state, and zip code*):
Office of Contract Adm.
Georgia Institute of Tech.
Atlanta, Fulton Georgia 30332-0420

Name and telephone number of the person to be contacted on matters involving this application (*give area code*):
Dr. Mustafa M. Aral
(404) 894 2243

6. EMPLOYER IDENTIFICATION NUMBER (EIN): 58 – 0603146

7. TYPE OF APPLICANT: (*enter appropriate letter in box*) I

A. State
B. County
C. Municipal
D. Township
E. Interstate
F. Intermunicipal
G. Special District
H. Independent School Dist.
I. State Controlled Institution of Higher Learning
J. Private University
K. Indian Tribe
L. Individual
M. Profit Organization
N. Other (Specify) ______

8. TYPE OF APPLICATION:

☐ New XXX Continuation ☐ Revision

If Revision, enter appropriate letter(s) in box(es): ☐ ☐

A. Increase Award B. Decrease Award C. Increase Duration
D. Decrease Duration Other (*specify*):

9. NAME OF FEDERAL AGENCY:
ATSDR-US Department of Health and Human Serv.

10. CATALOG OF FEDERAL DOMESTIC ASSISTANCE NUMBER: 93-161

TITLE: Program announcement no 326

11. DESCRIPTIVE TITLE OF APPLICANT'S PROJECT:
Research Program on Exposure-Dose econstruction

12. AREAS AFFECTED BY PROJECT (*cities, counties, states, etc.*):
NONE - General Method Development

13. PROPOSED PROJECT:

Start Date	Ending Date
Sept, 1993	Sept, 1997

14. CONGRESSIONAL DISTRICTS OF:

a. Applicant: V
b. Project: General

15. ESTIMATED FUNDING:

a. Federal	$ 295,272.00	.00
b. Applicant	$ ----	.00
c. State	$ 15,425.00	.00
d. Local	$ ----	.00
e. Other	$ ----	.00
f. Program Income	$ ----	.00
g. TOTAL	$ 310,697.00	.00

16. IS APPLICATION SUBJECT TO REVIEW BY STATE EXECUTIVE ORDER 12372 PROCESS?

a. YES THIS PREAPPLICATION/APPLICATION WAS MADE AVAILABLE TO THE STATE EXECUTIVE ORDER 12372 PROCESS FOR REVIEW ON

DATE ______

b. NO XXX PROGRAM IS NOT COVERED BY E.O. 12372

☐ OR PROGRAM HAS NOT BEEN SELECTED BY STATE FOR REVIEW

17. IS THE APPLICANT DELINQUENT ON ANY FEDERAL DEBT?

☐ Yes If "Yes," attach an explanation. XXXX No

18. TO THE BEST OF MY KNOWLEDGE AND BELIEF, ALL DATA IN THIS APPLICATION/PREAPPLICATION ARE TRUE AND CORRECT, THE DOCUMENT HAS BEEN DULY AUTHORIZED BY THE GOVERNING BODY OF THE APPLICANT AND THE APPLICANT WILL COMPLY WITH THE ATTACHED ASSURANCES IF THE ASSISTANCE IS AWARDED

a. Typed Name of Authorized Representative: Janis Goddard

b. Title: Contracting Off.

c. Telephone number: 404-894-4817

d. Signature of Authorized Representative:

e. Date Signed: 5/19/95

Previous Editions Not Usable

Standard Form 424 (REV 4-88)
Prescribed by OMB Circular A-102

INSTRUCTIONS FOR THE SF 424

This is a standard form used by applicants as a required facesheet for preapplications and applications submitted for Federal assistance. It will be used by Federal agencies to obtain applicant certification that States which have established a review and comment procedure in response to Executive Order 12372 and have selected the program to be included in their process, have been given an opportunity to review the applicant's submission.

Item:	Entry:
1.	Self-explanatory.
2.	Date application submitted to Federal agency (or State if applicable) & applicant's control number (if applicable).
3.	State use only (if applicable).
4.	If this application is to continue or revise an existing award, enter present Federal identifier number. If for a new project, leave blank.
5.	Legal name of applicant, name of primary organizational unit which will undertake the assistance activity, complete address of the applicant, and name and telephone number of the person to contact on matters related to this application.
6.	Enter Employer Identification Number (EIN) as assigned by the Internal Revenue Service.
7.	Enter the appropriate letter in the space provided.
8.	Check appropriate box and enter appropriate letter(s) in the space(s) provided: — "New" means a new assistance award. — "Continuation" means an extension for an additional funding/budget period for a project with a projected completion date. — "Revision" means any change in the Federal Government's financial obligation or contingent liability from an existing obligation.
9.	Name of Federal agency from which assistance is being requested with this application.
10.	Use the Catalog of Federal Domestic Assistance number and title of the program under which assistance is requested.
11.	Enter a brief descriptive title of the project. if more than one program is involved, you should append an explanation on a separate sheet. If appropriate (e.g., construction or real property projects), attach a map showing project location. For preapplications, use a separate sheet to provide a summary description of this project.

Item:	Entry:
12.	List only the largest political entities affected (e.g., State, counties, cities).
13.	Self-explanatory.
14.	List the applicant's Congressional District and any District(s) affected by the program or project.
15.	Amount requested or to be contributed during the first funding/budget period by each contributor. Value of in-kind contributions should be included on appropriate lines as applicable. If the action will result in a dollar change to an existing award, indicate *only* the amount of the change. For decreases, enclose the amounts in parentheses. If both basic and supplemental amounts are included, show breakdown on an attached sheet. For multiple program funding, use totals and show breakdown using same categories as item 15.
16.	Applicants should contact the State Single Point of Contact (SPOC) for Federal Executive Order 12372 to determine whether the application is subject to the State intergovernmental review process.
17.	This question applies to the applicant organization, not the person who signs as the authorized representative. Categories of debt include delinquent audit disallowances, loans and taxes.
18.	To be signed by the authorized representative of the applicant. A copy of the governing body's authorization for you to sign this application as official representative must be on file in the applicant's office. (Certain Federal agencies may require that this authorization be submitted as part of the application.)

OMB Approval No. 0348-0044

BUDGET INFORMATION — Non-Construction Programs

SECTION A - BUDGET SUMMARY

Grant Program Function or Activity (a)	Catalog of Federal Domestic Assistance Number (b)	Estimated Unobligated Funds: Federal (c)	Estimated Unobligated Funds: Non-Federal (d)	New or Revised Budget: Federal (e)	New or Revised Budget: Non-Federal (f)	New or Revised Budget: Total (g)
1. ATSDR-U61/ATU4	99828-02	$ 0.0	$ 0.0	$ 295,272.00	$ 15,425.00	$310,697.00
2. Researh Prog.93	.161					
3. Continuation pr	oject					
4.						
5. TOTALS		$ 0.0	$ 0.0	$ 295,272.00	$ 15,425.00	$310,697.00

SECTION B - BUDGET CATEGORIES

6. Object Class Categories	Grant Program, Function or Activity (1)	(2)	(3)	(4)	Total (5)
a. Personnel	$ 167,500.00	$	$	$	$ 167,500.00
b. Fringe Benefits 24.7 %	11,980.00				11,980.00
c. Travel	4,000.00				4,000.00
d. Equipment	30,000.00				30,000.00
e. Supplies	6,000.00				6,000.00
f. Contractual	0.00				0.00
g. Construction	0.00				0.00
h. Other	0.00				0.00
i. Total Direct Charges (sum of 6a - 6h)	219,480.00				219,480.00
j. Indirect Charges	75,792.00				75,792.00
k. TOTALS (sum of 6i and 6j)	$ 295,272.00	$	$	$	$ 295,272.00
7. Program Income	$ 0.00	$	$	$	$ 0.00

Standard Form 424A (4-88)
Prescribed by OMB Circular A-102

SECTION C - NON-FEDERAL RESOURCES

(a) Grant Program	(b) Applicant	(c) State	(d) Other Sources	(e) TOTALS
8. ATSDR-U61/ATU499828-02 Continuation project	$ 0.00	$ 15,425.00	$ 0.00	$ 15,425.00
9.				
10.				
11.				
12. TOTALS (sum of lines 8 and 11)	$ 0.00	$ 15,425.00	$ 0.00	$ 15,425.00

SECTION D - FORECASTED CASH NEEDS

	Total for 1st Year	1st Quarter	2nd Quarter	3rd Quarter	4th Quarter
13. Federal	$ 295,272.00	$ 73,818.00	$ 73,818.00	$ 73,818.00	$ 73,818.00
14. NonFederal	15,425.00	5,142.00	5,142.00	5,141.00	----
15. TOTAL (sum of lines 13 and 14)	$310,697.00	$ 78,960.00	$ 78,959.00	$ 78,959.00	$ 73,818.00

SECTION E - BUDGET ESTIMATES OF FEDERAL FUNDS NEEDED FOR BALANCE OF THE PROJECT

(a) Grant Program	FUTURE FUNDING PERIODS (Years)			
	(b) First	(c) Second	(d) Third	(e) Fourth
16.	$ 300,000.00	$	$	$
17.				
18.				
19.				
20. TOTALS (sum of lines 16-19)	$ 300,000.00	$	$	$

SECTION F - OTHER BUDGET INFORMATION

(Attach additional Sheets if Necessary)

21. Direct Charges:

22. Indirect Charges: 40%

23. Remarks

OMB Approval No. 0937-0189
Expiration Date: March 31, 1995

CERTIFICATIONS

1. CERTIFICATION REGARDING DEBARMENT AND SUSPENSION

The undersigned (authorized official signing for the applicant organization) certifies to the best of his or her knowledge and belief, that the applicant, defined as the primary participant in accordance with 45 CFR Part 76, and its principals:

(a) are not presently debarred, suspended, proposed for debarment, declared ineligible, or voluntarily excluded from covered transactions by any Federal Department or agency;

(b) have not within a 3-year period preceding this proposal been convicted of or had a civil judgment rendered against them for commission of fraud or a criminal offense in connection with obtaining, attempting to obtain, or performing a public (Federal, State, or local) transaction or contract under a public transaction; violation of Federal or State antitrust statutes or commission of embezzlement, theft, forgery, bribery, falsification or destruction of records, making false statements, or receiving stolen property;

(c) are not presently indicted or otherwise criminally or civilly charged by a governmental entity (Federal, State, or local) with commission of any of the offenses enumerated in paragraph (b) of this certification; and

(d) have not within a 3-year period preceding this application/proposal had one or more public transactions (Federal, State, or local) terminated for cause or default.

Should the applicant not be able to provide this certification, an explanation as to why should be placed after the assurances page in the application package.

The applicant agrees by submitting this proposal that it will include, without modification, the clause titled "Certification Regarding Debarment, Suspension, Ineligibility, and Voluntary Exclusion—Lower Tier Covered Transaction" (Appendix B to 45 CFR Part 76) in all lower tier covered transactions (i.e., transactions with subgrantees and/or contractors) and in all solicitations for lower tier covered transactions.

2. CERTIFICATION REGARDING DRUG-FREE WORKPLACE REQUIREMENTS

The undersigned (authorized official signing for the applicant organization) certifies that it will provide a drug-free workplace in accordance with 45 CFR Part 76 by:

(a) Publishing a statement notifying employees that the unlawful manufacture, distribution, dispensing, possession or use of a controlled substance is prohibited in the grantee's workplace and specifying the actions that will be taken against employees for violation of such prohibition;

(b) Establishing a drug-free awareness program to inform employees about—
  (1) The dangers of drug abuse in the workplace;
  (2) The grantee's policy of maintaining a drug-free workplace;
  (3) Any available drug counseling, rehabilitation, and employee assistance programs; and
  (4) The penalties that may be imposed upon employees for drug abuse violations occurring in the workplace;

(c) Making it a requirement that each employee to be engaged in the performance of the grant be given a copy of the statement required by paragraph (a) above;

(d) Notifying the employee in the statement required by paragraph (a), above, that, as a condition of employment under the grant, the employee will—
  (1) Abide by the terms of the statement; and
  (2) Notify the employer of any criminal drug statute conviction for a violation occurring in the workplace no later than five days after such conviction;

(e) Notifying the agency within ten days after receiving notice under subparagraph (d)(2), above, from an employee or otherwise receiving actual notice of such conviction;

(f) Taking one of the following actions, within 30 days of receiving notice under subparagraph (d)(2), above, with respect to any employee who is so convicted—

(1) Taking appropriate personnel action against such an employee, up to and including termination; or
(2) Requiring such employee to participate satisfactorily in a drug abuse assistance or rehabilitation program approved for such purposes by a Federal, State, or local health, law enforcement, or other appropriate agency;

(g) Making a good faith effort to continue to maintain a drug free workplace through implementation of paragraphs (a), (b), (c), (d), (e), and (f), above.

3. CERTIFICATION REGARDING LOBBYING

Title 31, United States Code, Section 1352, entitled "Limitation on use of appropriated funds to influence certain Federal contracting and financial transactions," generally prohibits recipients of Federal grants and cooperative agreements from using Federal (appropriated) funds for lobbying the Executive or Legislative Branches of the Federal Government in connection with a SPECIFIC grant or cooperative agreement. Section 1352 also requires that each person who requests or receives a Federal grant or cooperative agreement must disclose lobbying undertaken with non-Federal (non-appropriated) funds. These requirements apply to grants and cooperative agreements EXCEEDING $100,000 in total costs (45 CFR Part 93).

The undersigned (authorized official signing for the applicant organization) certifies, to the best of his or her knowledge and belief, that:

(1) No Federal appropriated funds have been paid or will be paid, by or on behalf of the undersigned, to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the awarding of any Federal contract, the making of any Federal grant, the making of any Federal loan, the entering into of any cooperative agreement, and the extension, continuation, renewal, amendment, or modification of any Federal contract, grant, loan, or cooperative agreement.

(2) If any funds other than Federally appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with this Federal contract, grant, loan, or cooperative agreement, the undersigned shall complete and submit Standard Form-LLL, "Disclosure of Lobbying Activities," in accordance with its instructions. (If needed, Standard Form-LLL, "Disclosure of Lobbying Activities," its instructions, and continuation sheet are included at the end of this application form.)

(3) The undersigned shall require that the language of this certification be included in the award documents for all subawards at all tiers (including subcontracts, subgrants, and contracts under grants, loans and cooperative agreements) and that all subrecipients shall certify and disclose accordingly.

This certification is a material representation of fact upon which reliance was placed when this transaction was made or entered into. Submission of this certification is a prerequisite for making or entering into this transaction imposed by Section 1352, U.S. Code. Any person who fails to file the required certification shall be subject to a civil penalty of not less than $10,000 and not more than $100,000 for each such failure."

4. CERTIFICATION REGARDING PROGRAM FRAUD CIVIL REMEDIES ACT (PFCRA)

The undersigned (authorized official signing for the applicant organization) certifies, to the best of his or her knowledge and belief, that the statements herein are true, accurate, and complete, and agrees to comply with the Public Health Service terms and conditions if an award is issued as a result of this application. Willful provision of false information is a criminal offense (Title 18, U.S. Code, Section 1001). Any person making any false, fictitious, or fraudulent statement may, in addition to other remedies available to the Government, be subject to civil penalties under the Program Fraud Civil Remedies Act of 1986 (45 CFR Part 79).

SIGNATURE OF AUTHORIZED CERTIFYING OFFICIAL	TITLE
Janis L. Goddard	Contracting Officer
APPLICANT ORGANIZATION	DATE SUBMITTED
Georgia Tech Research Corporation	5/19/95

ASSURANCES — NON-CONSTRUCTION PROGRAMS

Note: Certain of these assurances may not be applicable to your project or program. If you have questions, please contact the awarding agency. Further, certain Federal awarding agencies may require applicants to certify to additional assurances. If such is the case, you will be notified.

As the duly authorized representative of the applicant I certify that the applicant:

1. Has the legal authority to apply for Federal assistance, and the institutional, managerial and financial capability (including funds sufficient to pay the non-Federal share of project costs) to ensure proper planning, management and completion of the project described in this application.

2. Will give the awarding agency, the Comptroller General of the United States, and if appropriate, the State, through any authorized representative, access to and the right to examine all records, books, papers, or documents related to the award; and will establish a proper accounting system in accordance with generally accepted accounting standards or agency directives.

3. Will establish safeguards to prohibit employees from using their positions for a purpose that constitutes or presents the appearance of personal or organizational conflict of interest, or personal gain.

4. Will initiate and complete the work within the applicable time frame after receipt of approval of the awarding agency.

5. Will comply with the Intergovernmental Personnel Act of 1970 (42 U.S.C. §§ 4728-4763) relating to prescribed standards for merit systems for programs funded under one of the nineteen statutes or regulations specified in Appendix A of OPM's Standards for a Merit System of Personnel Administration (5 C.F.R. 900, Subpart F).

6. Will comply with all Federal statutes relating to nondiscrimination. These include but are not limited to: (a) Title VI of the Civil Rights Act of 1964 (P.L. 88-352) which prohibits discrimination on the basis of race, color or national origin; (b) Title IX of the Education Amendments of 1972, as amended (20 U.S.C. §§ 1681-1683, and 1685-1686), which prohibits discrimination on the basis of sex; (c) Section 504 of the Rehabilitation Act of 1973, as amended (29 U.S.C. § 794), which prohibits discrimination on the basis of handicaps; (d) the Age Discrimination Act of 1975, as amended (42 U.S.C. §§ 6101-6107), which prohibits discrimination on the basis of age; (e) the Drug Abuse Office and Treatment Act of 1972 (P.L. 92-255), as amended, relating to nondiscrimination on the basis of drug abuse; (f) the Comprehensive Alcohol Abuse and Alcoholism Prevention, Treatment and Rehabilitation Act of 1970 (P.L. 91-616), as amended, relating to nondiscrimination on the basis of alcohol abuse or alcoholism; (g) §§ 523 and 527 of the Public Health Service Act of 1912 (42 U.S.C. 290 dd-3 and 290 ee-3), as amended, relating to confidentiality of alcohol and drug abuse patient records; (h) Title VIII of the Civil Rights Act of 1968 (42 U.S.C. § 3601 et seq.), as amended, relating to nondiscrimination in the sale, rental or financing of housing; (i) any other nondiscrimination provisions in the specific statute(s) under which application for Federal assistance is being made; and (j) the requirements of any other nondiscrimination statute(s) which may apply to the application.

7. Will comply, or has already complied, with the requirements of Titles II and III of the Uniform Relocation Assistance and Real Property Acquisition Policies Act of 1970 (P.L. 91-646) which provide for fair and equitable treatment of persons displaced or whose property is acquired as a result of Federal or federally assisted programs. These requirements apply to all interests in real property acquired for project purposes regardless of Federal participation in purchases.

8. Will comply with the provisions of the Hatch Act (5 U.S.C. §§ 1501-1508 and 7324-7328) which limit the political activities of employees whose principal employment activities are funded in whole or in part with Federal funds.

9. Will comply, as applicable, with the provisions of the Davis-Bacon Act (40 U.S.C. §§ 276a to 276a-7), the Copeland Act (40 U.S.C. § 276c and 18 U.S.C. §§ 874), and the Contract Work Hours and Safety Standards Act (40 U.S.C. §§ 327-333), regarding labor standards for federally assisted construction subagreements.

10. Will comply, if applicable, with flood insurance purchase requirements of Section 102(a) of the Flood Disaster Protection Act of 1973 (P.L. 93-234) which requires recipients in a special flood hazard area to participate in the program andto purchase flood insurance if the total cost of insurable construction and acquisition is $10,000 or more.

11. Will comply with environmental standards which may be prescribed pursuant to the following: (a) institution of environmental quality control measures under the National Environmental Policy Act of 1969 (P.L. 91-190) and Executive Order (EO) 11514; (b) notification of violating facilities pursuant to EO 11738; (c) protection of wetlands pursuant to EO 11990; (d) evaluation of flood hazards in floodplains in accordance with EO 11988; (e) assurance of project consistency with the approved State management program developed under the Coastal Zone Management Act of 1972 (16 U.S.C. §§ 1451 et seq.); (f) conformity of Federal actions to State (Clear Air) Implementation Plans under Section 176(c) of the Clear Air Act of 1955, as amended (42 U.S.C. § 7401 et seq.); (g) protection of underground sources of drinking water under the Safe Drinking Water Act of 1974, as amended, (P.L. 93-523); and (h) protection of endangered species under the Endangered Species Act of 1973, as amended, (P.L. 93-205).

12. Will comply with the Wild and Scenic Rivers Act of 1968 (16 U.S.C. §§ 1271 et seq.) related to protecting components or potential components of the national wild and scenic rivers system.

13. Will assist the awarding agency in assuring compliance with Section 106 of the National Historic Preservation Act of 1966, as amended (16 U.S.C. 470), EO 11593 (identification and protection of historic properties), and the Archaeological and Historic Preservation Act of 1974 (16 U.S.C. 469a-1 et seq.).

14. Will comply with P.L. 93-348 regarding the protection of human subjects involved in research, development, and related activities supported by this award of assistance.

15. Will comply with the Laboratory Animal Welfare Act of 1966 (P.L. 89-544, as amended, 7 U.S.C. 2131 et seq.) pertaining to the care, handling, and treatment of warm blooded animals held for research, teaching, or other activities supported by this award of assistance.

16. Will comply with the Lead-Based Paint Poisoning Prevention Act (42 U.S.C. §§ 4801 et seq.) which prohibits the use of lead based paint in construction or rehabilitation of residence structures.

17. Will cause to be performed the required financial and compliance audits in accordance with the Single Audit Act of 1984.

18. Will comply with all applicable requirements of all other Federal laws, executive orders, regulations and policies governing this program.

SIGNATURE OF AUTHORIZED CERTIFYING OFFICIAL	TITLE
Janis L. Goddard Janis L. Goddard	Contracting Officer

APPLICANT ORGANIZATION	DATE SUBMITTED
Georgia Tech Research Corporation	5/19/95

1. REVIEW OF RESEARCH ACTIVITIES FOR PROJECT YEAR 2

The cooperative agreement on Exposure-Dose Reconstruction Project (EDRP) was awarded to Dr. M. M. Aral, School of Civil and Environmental Engineering, Georgia Institute of Technology, towards the end of September 1993. Since then our efforts focused on several tasks of the research program in order to start the project in a most efficient and cost effective manner. We have successfully completed the first project period during the 1993-1994 academic year. The progress made during the first year of the research program was submitted to ATSDR, USDHHS, in an Annual Progress Report on June 27, 1994. We are now in the second project period (1994-1995) of the research program. A description of administrative efforts, research activities and the progress made in each activity during the second year of the research program are described in this Annual Progress Report. This report also includes the budget and non competitive Application for Extension of the Project to the Third Project Period.

- **Purchase of the computational equipment**:

  The second phase of the purchase of the computer equipment necessary for the project has been completed. We anticipate that we will be adding to this equipment throughout the duration of the project as future needs arise. The equipment purchased for the Exposure Dose Reconstruction Research program is compatible with the present standards and other computational equipment used by ATSDR. With this equipment, direct communication between ATSDR and Ga. Tech has been established through ethernet communication platform. It is also anticipated that the compatibility established between the equipment at both sites will enhance the technology transfer phase of the research program which is anticipated to occur during later stages of the research program.

- **Development of the analytical framework for the prediction of contaminant migration scenarios in multiple exposure pathways**:

  It is anticipated that the contaminant migration analysis (the forward pathway calculation environment) will include several analytical tools to evaluate the contaminant concentration levels in multiple and interactive pathways. These pathways, at a minimum, will include the following:

  (i) air pathway;
  (ii) ground-water pathway;
  (iii) surface water pathway; and,
  (iv) soil pathway.

  According to the proposed schedule of the research program, the analytic tools for these pathways will be developed throughout the duration of the project. During the first project year, it was extremely important to conceptualize the overall system and develop a unified analytical structure and a user friendly framework for this computational environment. As parts of the overall system are developed, and several analytical tools are put together, this unified structure will provide the framework necessary for a user friendly computational environment. This approach will also minimize the revisions that will be necessary during the later stages of the research program. Major portion of this task was completed during the first project year. Although this software development effort may not be in its final form, the initial computational tool developed for the ground-water pathway and submitted to ATSDR during the first project period, indicate our line of taught for the general computational environment we are developing in this effort. During the second project period, the first years initial effort was modified significantly resulting in a major upgrade of the overall product. The new version of the software was submitted to ATSDR for beta testing during April 1995 (ACTS version 1.2). This version of the software is now more user friendly and more computationally efficient. In this tool several analytic solutions for the ground-water pathway and also the air pathway was developed along with a graphical and text output format interphase which may be used to interpret the results. This version now also includes the Monte Carlo simulations for the air pathway analysis as described in more detail below. This is an essential component of for this pathway since the inherent uncertainties of the computations in the air pathway is much more pronounced. This software will be updated throughout the project period to include analytical tools for other pathways mentioned above as well as other revisions that may be recommended by ATSDR. In it's present form the computational tool submitted to ATSDR can be used to evaluate concentration distributions in site specific cases for the ground-water pathway and air pathway. This software can be installed in ATSDR's network system for immediate access by all health professionals. At the present this computational tool is tested and used successfully in several site specific applications by ATSDR professionals.

- **Monte Carlo simulations in analytic contaminant migration analysis**

As was proposed in our first year progress report, an important component of the second project period effort was the incorporation of evaluation of the uncertainties involved in analytic contaminant migration simulations. Evaluation of the effect of these uncertainties on the numerical results generated can be accomplished using Monte Carlo methods.

Implementation of analytical tools in all pathways requires a number of input parameters including source-specific, media-specific, and chemical-specific variables. Typically, the values of these parameters are not known exactly due to measurement errors and/or inherent spatial and temporal variability. Therefore, it is often more appropriate to express these parameter values in terms of a probability distribution rather than a single deterministic value and use an uncertainty propagation model to assess the effect of the variability on the output of the models. Most suitable method that can be employed for this purpose is the Monte Carlo method. Based on the principles of this approach, the following procedure is incorporated to the software developed for ATSDR.

Whatever the source of the parameter uncertainty, the uncertainty can be quantified using a cumulative probability distribution. Thus, for each parameter to be analyzed as an uncertain variable, the user may select and assign a probability distribution (normal, log normal, uniform, exponential, triangular) for the variable and specify the parameters that describe the distribution. In Monte Carlo simulations, data sets randomly generated from these distributions form the basis of the data sets that will be used in deterministic models which in turn will generate a population of model outputs. This series of outputs can than be analyzed to yield a cumulative probability distribution of expected model results. This distribution quantitatively describes the uncertainty in the model output and can be used in decision making.

During the second project year, considerable effort was devoted to introduce Monte Carlo simulation tools into the overall computational framework developed in the first project year. With this component added to the system, users will have the choice to select between direct calculations (deterministic mode computations) and Monte Carlo simulations in pathway analysis exercises based on the confidence they have on the parameters they are using in their applications. With the addition of Monte Carlo methods, the flexibility and reliability of the computational system is improved and the applicability of the overall system is enhanced. At the present this computational system is included into the air pathway calculations.

- **An application study for contaminant transport analysis in pipe network systems and GIS based evaluation of exposure assessment for a site specific case**

ATSDR and the Connecticut Department of Health Services (CDHS) are collaborating in a study of cancer incidence in the Town of Southington, Hartford County, Connecticut. As part of the study, ATSDR is determining population exposure to contaminated groundwater that was distributed in the town's water distribution system. To address the complex engineering issues associated with exposure assessment, ATSDR relied on the resources of the Exposure-Dose Reconstruction Cooperative Agreement Project. The main problem in addressing this issue was the time limitations imposed on ATSDR to find a solution to the problem. A solution to the problem was requested by CDHS within a period of 4 to 6 months. Based on this request ATSDR Exposure-Dose Reconstruction project officer contacted Ga Tech research program during September 1994 an requested us to devote our efforts to solve the problem and provide them with the analysis results within a period of 4 to 6 months. In order to address this urgent problem Ga Tech principal investigator decided to allocate all resources of the project to finding a solution to this problem and providing ATSDR with reliable estimates of exposure using GIS integrated pipe network analysis. The project was completed in time and the results were submitted to ATSDR in a final report titled "A Public Health Analysis of Exposure to Contaminated Municipal Water Supplies at Southington, Hartford County, Connecticut."

This research effort, was not included to the initial research program proposed by the principal investigator, and was undertaken as an additional effort at the request of ATSDR project officers. Since the problem posed to ATSDR by the CDHS is an extremely important health assessment problem with nationwide applications and the engineering analysis provided by Ga. Tech is an extremely useful and practical but preliminary solution to the problem at hand, the Ga Tech principal investigator recommends that ATSDR may like to pursue this research in the future. This unplanned research effort requested by ATSDR delayed the ongoing efforts at Ga Tech by two quarters during the second year of the research program.

- **Development of user friendly GIS interface programs:**

It is our understanding that ATSDR's needs for computational tools in the area of health assessment is multilevel. The range of complexity of these tools may vary between screening tools, similar to the analytical computational environment described above, to the sophisticated GIS integrated multimedia modeling tools which may be used to analyze more complex cases. Given the number of sites that needs to be analyzed by ATSDR periodically and given the variability in complexity of the contaminant migration pathways in these sites, there would be a need for sophisticated approaches as well as the screening tools. Thus, in addition to the analytical tool development phase of the project, we are also in the process of developing user friendly GIS interface programs to simplify the analysis steps necessary in these complex cases. Our initial efforts in category was concentrated towards the development of a shell structure for the GISPlus software which is presently used by ATSDR. This shell program will simplify the manipulation of data structures within a GIS integrated computation and the interaction of the complex simulation tools with the GIS system. The preliminary shell structure submitted to ATSDR during the first period of the project may describe our line of thought in this effort. Although this shell program will be updated throughout the project period, in its present form it is being tested and used to evaluate site specific conditions for the ground-water pathway at ATSDR and Ga. Tech. In this effort, in addition to the general shell structure submitted to ATSDR, certain coordinate transformation routines and data base generation routines, compatible with the existing ground-water flow and contaminant transport models, has been developed and submitted to ATSDR for beta testing. These codes were tested and used successfully in site specific applications by ATSDR professionals. This aspect of the research program is still under development and revisions to the code will be supplied to ATSDR for their beta testing.

- **Adaptation of existing ground-water flow models to GISPlus software:**

The PC-based GIS system in use at ATSDR is the GISPlus system. The implementation of existing ground-water pathway analysis tools required substantial revision of these codes to make them compatible with the GISPlus system. Although this is an ongoing task, our initial efforts provided ATSDR with these tools which are now in use in predicting ground-water flow patterns in several sites of interest to ATSDR. We are in the process of adding contaminant transport models to this system in the area of subsurface analysis. These codes were tested and used in site specific applications by ATSDR professionals during the second period of the research program and the results are shared with several federal and state agencies involved in the program.

2. PRODUCTS SUBMITTED TO ATSDR, USDHHS

During the second year of the cooperative agreement the following computational software were submitted to ATSDR for their evaluation and beta testing. Some of this software are still in the development stage and should not be considered to be a final product. All of these products are presently used by ATSDR health assessors in evaluating health consequences of contaminants released to subsurface pathways.

(i) Analytical Contaminant Transport analysis System (ACTS Version 1.20)
(ii) GIS Interphase SYStem (GIS-SYS Version 1.20)

3. RESEARCH ACTIVITIES FOR PROJECT YEAR 3

As the second year effort, the progress made in all of the activities summarized above are substantial. This progress was in addition to an unplanned GIS based Pipe Network Analysis research activity requested by ATSDR. Ga Tech project director welcomes such requests since in our cooperative agreement the basic goal is to satisfy the technical needs of ATSDR as they arise and provide ATSDR with expertise utilizing resources of Ga. Tech. This effort was an excellent example of this cooperation.

Our ongoing efforts will be directed towards the completion of the tasks and improving the tools we are developing for ATSDR during the next two years of the project period. In this effort, additional pathways described above will be incorporated into the computational environment. These tools will be periodically submitted to ATSDR for their evaluation and beta testing.

The primary pathway that will be analyzed during the third project period is selected to be the surface water pathway. Analytical tools that will be developed to evaluate exposure in this pathway will include, near field far field surface water diffusion dispersion models. Monte Carlo simulations will also be incorporated into this analysis. Details of this computational processes were described in the original proposal submitted to ATSDR which will not be repeated here.

4. TECHNICAL PUBLICATIONS

Based on the progress made during the second year of the research program, several technical publications and reports were published or submitted for publication. These research reports or technical papers are the outcome of the research effort of the second project year. The following technical publications were accepted for publication in refereed journals or were accepted for inclusion in the proceedings of the conferences listed below.

1. M. L. Maslia, M. M. Aral, R. C. Williams, R., A. Susten and J. L. Heitgerd, "Exposure Assessment of Populations Using Environmental Modeling, Demographic Analysis, and GIS," *Water Resources Bulletin*, Vol. 30, No. 6, pp. 1025-1041, 1994.

2. Maslia, M. L. and Aral, M. M., "Application of Geographic Information Systems and Numerical Models to Exposure Assessment", Sixth Joint Conference of the International Society for Environmental Epidemiology and International Society for Exposure Analysis, The University of North Carolina at Chapel Hill, September 18-21, 1994.

3. Aral, M. M. and M. L. Maslia, "A Public Health Analysis of Exposure to Contaminated Municipal Water Supplies at Southington, Hartford County, Connecticut," School of Civil Engineering, Georgia Institute of Technology Final Report submitted to ATSDR as a part of Exposure-Dose Reconstruction Research Program, p 42, December 20, 1994.

4. Aral, M. M. and M. L. Maslia, "A Public Health Analysis of Exposure to Contaminated Municipal Water Supplies at Southington, Hartford County, Connecticut," *Archives of Environmental Health*, (submitted for publication)1994.

5. PROPOSED BUDGET AND JUSTIFICATION

With this proposal continuation of the cooperative agreement between ATSDR USDHHS and Georgia Institute of Technology is proposed. The third year budget for the services of the personnel and other resources are itemized below. The budget proposed for the third project year is not significantly different than the one proposed for the second year. Main differences reflect the changes in faculty salaries as anticipated.

Budget summary for third year :

	ATSDR Funds Allocated to the Project	Matching Funds Source GA.TECH
a. Salaries and Wages :		
Principal Investigator	$ 33,000.00	$ 9,000.00
Research Faculty	$ 13,000.00	--
7 full time Ph.D. students	$ 105,000.00	--
Two full time M.S. students	$ 14,000.00	--
Secretarial Support	$ 2,500.00	--
Total (excluding students)	$ 48,500.00	$ 9,000.00
Total (including students)	$167,500.00	
b. Fringe Benefits :		
24.7 % of salaries (excluding students)	$ 11,980.00	$ 2,259.00
c. Supplies :	$ 6,000.00	--
d. Publication costs :	$ 0.00	--
e. Travel :	$ 4,000.00	--
f. Equipment (computer/hardware):	$ 30,000.00	--
g. Total direct costs :	$219,480.00	$ 11,259.00
h. Indirect costs :		
40 % of Direct Costs (excluding equipment)	$ 75,792.00	$ 4,166.00
i. Total amount proposed :	$295,272.00	$ 15,425.00

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j. GA.TECH share for the third year :	--	$ 15,425.00
k. ATSDR share for the third year:	$ 295,272.00	--

Justification of Budget :

The proposed budged will be primarily used to underwrite graduate and post-graduate student research funds, and secondarily to support release time for the research faculty. This approach will foster the training of professionals specialized in this much needed area of research and increase the awareness of engineering and science students on health related issues. This trained resource pool will be of vital importance to ATSDR's and also to other federal and state health organization's needs in the future. Part of the research funds requested will be used to purchase certain computer equipment and software. The main purpose of this purchase is to develop the proposed simulation tools on computational platforms which are similar to the computational and data processing environment available at ATSDR and utilize the most recent and advanced software available in the literature. The compatibility between the computational systems at ATSDR and Ga. Tech is essential and will definitely simplify the technology transfer phase of the proposed study. These dedicated computational equipment will only be used by the graduate students and research scientists for the exclusive purposes of the proposed study.

Budget Breakdown:

Personnel	Annual Salary	Percentage of effort	No. of Months	Amount Requested(Federal Funds)
Principal Inv.	$ 72,000	46 %	5	$ 33,000.00
Research Fac.	$ 70,000	19 %	2	$ 13,000.00
1 PhD Student	$ 15,000	33 %	12	
Total PhD Students (7)				$ 105,000.00
1 MS Student	$ 7,000	33 %	9	
Total MS Students (2)				$ 14,000.00
Secretary	$ 25,000	10 %	1.5	$ 2,500.00

Principal Investigator : Dr. M. M. Aral is the principal investigator of the Exposure Dose Reconstruction Research program. He is the main contributor and the coordinator for all research activities in the proposed program. His contribution and time will form the nucleus of all research activities proposed in this program.

Research Faculty: On an as needed basis services of several other faculty members will be requested under this category.

PhD Students (7 students) Contribution of several PhD students are an essential element of this research program. At the present there are five PhD students working in the program. It is anticipated that this number will increase to seven during the third project year.

MS Students (2 students) — Contribution of several MS students are an essential element of this research program. At the present there are two MS students working in the program. We do not anticipate an increase in this number.

Fringe Benefits:

Fringe benefits are applicable to direct salaries and wages of all personnel excluding students. The present fringe benefit rate is 24.7 %. This rate may change during the academic year 1994-95. However, this change will not effect the total amount requested from federal funds for the third year of the cooperative agreement.

Travel:

	Travel	Lodging and Meals	Registration
Conference 1 (Europe)	$ 1,500.00	$ 450.00	$ 200.00
Conference 2 (USA)	$ 400.00	$ 250.00	$ 200.00
Conference 3 (USA)	$ 550.00	$ 250.00	$ 200.00

Total Travel Budget : $ 4,000.00

It is expected that the principal investigator will participate in at least three conferences during the academic year 1995-96 related to the research program topic. The funds in this category will be only used by the principal investigator for this purpose. The total cost of this category will be within the range allocated for the program.

Equipment:

Unit #	Quantity	Unit Cost	Total Cost
Dell Pentium PC.	2	8,333.00	16,666.00
MacIntosh Comp	1	8,333.00	8,334.00
Slide Dev.	1	5,000.00	5,000.00

Total Equipment Budget : $ 30,000.00

We anticipate that we will be adding to the initial equipment purchased throughout the duration of the project as future needs arise. The equipment purchased for the Exposure Dose Reconstruction Research program is compatible with the present standards and other computational equipment which is used by ATSDR and will remain the property of ATSDR. We anticipate to purchase three computers, and a slide developer for the research program. The total cost of this equipment will be within the range allocated for the program.

Supplies:

The computational tools developed for the program requires special software as utility tools. We anticipate to purchase these tools and use them in or research efforts. The total cost of this supplies purchase will be within the limits allocated for the program ($ 6,000.00).

Contractual: None

Consultant: None

Other: None

Indirect Costs:

Overhead rates are applicable to direct salaries and wages of all personnel and other expenses excluding equipment purchases. The present overhead rate is 40 %. This rate may change during the academic year 1994-95. However, this change will not effect the total amount requested from federal funds for the third year of the cooperative agreement.

Unobligated Funds:

We anticipate that there will not be any unobligated funds remaining from the second project year.

BIOGRAPHICAL SKETCH

Dr. Mustafa M. Aral

Personal Data Summary

Born	: February 26, 1945, Ankara, Turkey
Citizenship	: U.S.A.
Home Address	: 2974 Cravey Dr. NE., Atlanta, GA. 30345

Business Address

School of Civil Engineering
Georgia Institute of Technology
Atlanta, Georgia 30332
Buss. Phone : (404) 894-2243 / (404) 894-5111

Professional Registration

Professional Engineer : GA : 15254
Professional Ground Water Hydrologist, National Registration : No.: 649

Educational Background

School of Civil Engineering, Georgia Institute of Technology, Ph.D. in Water Resources Engineering with minor in Numerical Analysis and Applied Mathematics, September 1971.

School of Civil Engineering, Georgia Institute of Technology, M.S. in Civil Engineering with major in Environmental and Water Resources Engineering, June 1969.

Department of Civil Engineering, Middle East Technical University (Ankara, Turkey), B.S. in Civil Engineering, June 1967.

Professional Experience

1983-Present	Associate Professor	School of Civil Engineering, Georgia Institute of Technology.
1978-1983	Visiting Professor	School of Civil Engineering, Georgia Institute of Technology.
1974-1983	Adjunct Professor	At Marine Sciences Department, Civil Engineering Department, Engineering Science Department, Middle East Technical University.
1977-1983	Associate Professor	Mathematics Department, Middle East Technical University.

Professional Experience (cont.)

1975-1978	Assistant Chairman	Mathematics Department, Middle East Technical University.
1971-1977	Assistant Professor	Mathematics Department, Middle East Technical University.

Publications

42. **Aral, M. M.**, Ground Water Modeling in Multilayer Aquifers - Steady Flow, *Lewis Publishers Inc.*, February, 1990 (Book).

43. **Aral, M. M.**, Ground Water Modeling in Multilayer Aquifers - Unsteady Flow, *Lewis Publishers Inc.*, March, 1990 (Book).

44. Tang, Y., and **Aral, M. M.**, Contaminant Transport in Layered Porous Media: A. General Solution, *Water Resources Research*, Vol. 28, No. 5, pp. 1389-1397, 1992.

45. Tang, Y., and **Aral, M. M.**, Contaminant Transport in Layered Porous Media: B. Applications, *Water Resources Research*, Vol. 28, No. 5, pp. 1399-1406, 1992.

46. Ratzlaff, S., **Aral, M. M.**, and Alkhayyal, F., Optimal Capture Zone Design Using Segmental Velocity Direction Constraints, *Groundwater Journal*, Vol. 30, No. 4, pp. 607-612, 1992.

47. **Aral, M. M.**, and Tang, Y. Flow Against Dispersion in Two Dimensional Aquifers, *Journal of Hydrology*, Vol. 140, pp. 261-277, 1992.

48. Maslia, M., **Aral, M. M.**, and Houlihan, M., "Evaluation of Ground-Water Flow Regime at a Landfill with Liner System," *Journal of Environmental Science and Health*, Vol. A27, No. 7, pp. 1793-1816, 1992.

49. Maslia, M., **Aral, M. M.**, and Gill, H. E., "The Importance of Hydrogeologic Controls on Remedial Action Alternatives," *Geophysical Society of America*, Southeastern Section Meeting, Contaminant Hydrogeology Session, Vol. 24, No. 2, pp. 53, 1992.

50. Maslia, M., **Aral, M. M.**, Williams, R., Williams, S., Hayes, L. and Wilder, L., "Use of Computational Models to Determine Health Implications of Human Exposure Resulting from Remediation Activities at Hazardous Waste Sites," Report for: *Division of Health Assessment and Consultation, DHHS-ATSDR*, 20p, November 5, 1992.

51. **Aral, M. M.**, Maslia, M. and Williams, R., "Integration of GIS and Environmental Transport Models for Exposure Assessment of Populations," *Water Resources Bulletin*, (submitted for publication), 1993.

52. Maslia, M., **Aral, M. M.**, Williams, R., Williams, S., Hayes, L. and Wilder, L., "Use of

Computational Models to Determine Human Exposure Resulting from Remediation Activities at Hazardous Waste Sites," Proceedings of the Water Environment Federation Specialty Conference *How Clean is Clean*, 85p, January 10-13, 1993.

53. Maslia, M., **Aral, M. M.**, Williams, R., Williams, S., Hayes, L. and Wilder, L., "Use of Computational Models to Reconstruct and Predict Trichloroethylene Exposure," Proceedings of the International Congress on the Health Effects of Hazardous Waste, 22p, 1993.

54. **Aral, M. M.**, Maslia, M., and Williams, R., "Ground-Water Remediation Using Smart Pump-and Treat," *Ground Water Journal*, Discussion, Vol. 31, No. 4, pp. 680-681, 1993.

55. **Aral, M. M.**, C. Shea and Al-Khayyal, F., "Optimization Methods in Ground Water Management," Review Chapter in Volume 9, "Applications of Management Science: Network Optimization Applications," JAI Press Inc., 1993 (in publication).

56. Maslia, M. L. and **Aral, M. M.**, "Health Implications Associated with Hazardous Waste Site Clean-Up Goals: A Case Study of Trichloroethylene (TCE) Contamination", Proceedings of the Annual Meeting of the Geological Society of America, Boston, 1993.

57. Maslia, M. L. and **Aral, M. M.**, "Conducting Exposure Assessment of Populations by Integrating Environmental Transport Models, Demographic Analysis, and Geographic Information Systems", Proceedings of the International Symposium on Assessing and Managing Health Risks from Drinking Water Contamination: Approaches and Applications, Rome, Italy, September 1994.

Expertise Areas

Research, teaching and engineering experience in the following specific areas :

- Fluid mechanics, Hydraulics Engineering
- Environmental simulations and fate
- Analytical and numerical studies in surface water, ground-water and air pollution
- Evaluation of ground water and surface water monitoring data
- Ground water flow and contaminant transport modeling in aquifers
- Ground water resources evaluation and management
- Disposal and ground water quality effects of hazardous substances, aquifer remediation
- Saturated and unsaturated ground water flow analysis
- Miscible and immiscible ground water flow analysis
- GIS applications in environmental systems

Goddard

DEPARTMENT OF THE NAVY
OFFICE OF NAVAL RESEARCH
800 NORTH QUINCY STREET
ARLINGTON. VA 22217-5660

IN REPLY REFER TO

NEGOTIATION AGREEMENT

Institution: Georgia Institute of Technology
Georgia Tech Research Corporation
Atlanta, GA 30332

The Indirect Cost Rates and Fringe Benefit rates contained herein are for use on grants and contracts with all Federal Agencies in accordance with the cost principles mandated by Office of Management and Budget (OMB) Circular A-21, and in accordance with OMB Circular A-88. These rates shall be used for forward pricing and billing purposes for Georgia Institute of Technology's/Georgia Tech Research Corporation's Fiscal Year 1995. This rate agreement supersedes all previous rate agreements/determinations for Fiscal Year 1995.

SECTION I: Rate-Type: Provisional, Predetermined (Pred.), Fixed with Carryforward (Fixed)

INDIRECT RATES

Type	From	To	Rate	Base	Applicable to	Location
Provisional	07/01/94	Until Amended	47.0%	(a)	Organized Research (1)	GTRI
Provisional	07/01/94	Until Amended	44.0%	(a)	Organized Research (2)	GTRI
Provisional	07/01/94	Until Amended	46.0%	(a)	Organized Research (1)	Resident Instruction
Provisional	07/01/94	Until Amended	40.0%	(a)	Organized Research (2)	Resident Instruction
Pred.	07/01/94	06/30/95	33.0%	(a)	All Programs	Public Service

FRINGE BENEFIT RATES

Type	From	To	Rate	Base	Applicable to	Location
Fixed	07/01/94	06/30/95	24.7%	(b)	All Programs	All units
Fixed	07/01/94	06/30/95	1.5%	(c)	All Programs	All units

DISTRIBUTION BASE

(a) Modified Total Direct Cost Base consisting of salaries and wages, fringe benefits,Program Management Cost (PMC), Allocated Project Level Cost (APLC), materials and supplies, services, travel and subcontracts and subgrants up to $25,000 each.

(b) Salaries and wages of (i) regular full-time faculty, (ii) principal investigators, (iii) professional and administrative staff, (iv) joint staff, (v) temporary academic or research professionals covered by the Teachers Retirement System (TRS) and group health and life insurance, (vi) bi-weekly permanent employees and (vii) part-time employees who work 50 percent but less than 100 percent of a full-time work schedule.

(c) Salaries and wages of employees who participate in the social security program but do not participate in the TRS or group health and life insurance plans. This rate covers (i) temporary classified persons, (ii) temporary academic or research professionals not eligible for TRS or group health or life insurance coverage and (iii) part-time employees employed for less than 50% of a full work schedule.

NOTE: Fringe benefits are not applicable to student employees.

APPLICABLE TO

(1) Applies to all DoD contracts awarded on or after November 30, 1993 in accordance with and under the authority of DFARS 231.303(1). See Section II, part F hereof.

(2) Applies to DoD contracts awarded or issued before November 30, 1993, all Non-DoD Instruments and all DoD Grants. See Section II, part F hereof.

SECTION II - GENERAL

A. **LIMITATIONS:** Use of the rates contained in this agreement is subject to any statutory or administrative limitations and is applicable to a given grant or contract only to the extent that funds are available. Acceptance of the rates agreed herein is predicated upon all of the following conditions: (1) that no costs other than those incurred by the grantee/contractor were included in this indirect cost pool as finally accepted and that such costs are legal obligations of the grantee/contractor and allowable under governing cost principles, (2) that the same costs that have been treated as indirect costs are not claimed as direct costs, (3) that similar types of costs have been accorded consistent accounting treatment, and (4) that the information provided by the grantee/contractor which was used as a basis for acceptance of the rates agreed to herein is not subsequently found to be materially incomplete or inaccurate.

B. **ACCOUNTING CHANGES:** The rates contained in this agreement are based on the accounting system in effect at the time the agreement was negotiated. Changes to the method of accounting for costs which affect the amount of reimbursement resulting from the use of these rates require the prior approval of the authorized representative of the cognizant negotiation agency. Such changes include but are not limited to changes in the charging of a particular type of costs from indirect to direct. Failure to obtain such approval may result in subsequent cost disallowances.

C. **USE BY OTHER FEDERAL AGENCIES:** The rates contained herein were negotiated in accordance with the authority set forth in OMB Circular A-88 and should be applied to the extent provided in such Circular, to grants and contracts to which OMB Circular A-21 applies, subject to any limitations in paragraph A, above. Copies of this document may be provided by the Institution to other Federal Agencies having grants and contracts using this rate as a means of providing them with early notification of the agreement contained herein.

D. FIXED RATES AND CARRY-FORWARD PROVISIONS: The fixed fringe benefits rates contained in this agreement are based on estimates of the costs for FY 1995. When the actual costs for this period have been determined, adjustments shall be made to the fringe benefits rates of the next subsequent rate negotiation to compensate for the difference between the FY 1995 costs used to establish the fixed rates and the negotiated actual FY 1995 costs.

E. PREDETERMINED RATE: The predetermined rate in this agreement is not subject to adjustment in accordance with the provisions of OMB Circular A-21, subject to the limitations contained in Part A of this section.

F. APPLICATION OF INDIRECT COST RATES TO DOD CONTRACTS/SUBCONTRACTS: In accordance with DFARS 231.303, no limitation (unless waived by the institution) may be placed on the reimbursement of otherwise allowable indirect costs incurred by an institution of higher education under a DoD contract awarded on or after November 30, 1993, unless the same limitation is applied uniformly to all other organizations performing similar work. It has been determined by the Department of Defense that such limitation is not being uniformly applied. Accordingly, the rates cited (1) of Section I, as explained under the title "APPLICABLE TO" (1), do not reflect the application of the 26% limitation on administrative indirect cost imposed by OMB A-21 where (2) does so.

G. SPECIAL REMARKS:

1. The Government's agreement with these rates is not an acceptance of the Institution's accounting systems, cost classifications, allocation methodologies, cost analysis and special studies, and the reasonableness of any specific proposed cost.

2. Signature of this agreement does not constitute Government acceptance of the proposed repayment plan for the actual over recoveries from FYs 1987 through 1991 as set forth in the Institution's letter of 17 June 1994.

For the Institution:	For the Government:
Signature	Signature
J.W. Dees Associate Vice President for Research & Director, Office of Contract Administration, Assistant Secretary	Andrew D. Holland Contracting Officer
Date July 1, 1994	Date July 1, 1994

OMB Approval No. 0937-0189
Expiration Date: March 31, 1995

CHECKLIST

Public Burden Statement: Public reporting burden for this collection of information is estimated to average 10 minutes per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate, or any other aspect of this collection of information, including suggestions for reducing this burden, to PHS Reports Clearance Officer, ATTN: PRA, Hubert H. Humphrey Bldg., Room 721-B, 200 Independence Ave., S.W., Washington, D.C. 20201, and to the Office of Management and Budget, Paperwork Reduction Project (0937-0189), Washington, D.C. 20503.

NOTE TO APPLICANT: This form must be completed and submitted with the original of your application. Be sure to complete both sides of this form. Check the appropriate boxes and provide the information requested. This form should be attached as the last page of the signed original of the application. This page is reserved for PHS staff use only.

Type of Application: ☐ NEW ☒ Noncompeting Continuation ☐ Competing Continuation ☐ Supplemental

PART A: The following checklist is provided to assure that proper signatures, assurances, and certifications have been submitted.

	Included	NOT Applicable
1. Proper Signature and Date for Item 18 on SF 424 (FACE PAGE)	☒	
2. Proper Signature and Date on PHS-5161-1 "Certifications" page	☒	
3. Proper Signature and Date on appropriate "Assurances" page, i.e., SF-424B (Non-Construction Programs) or SF-424D (Construction Programs)	☒	

4. If your organization currently has on file with DHHS the following individual assurances, please identify which have been filed by indicating the date of such filing on the line provided. Georgia Tech is audited annually by the Office of Federal Compliance Programs.
   - ☐ Civil Rights Assurance (45 CFR 80) ____
   - ☐ Assurance Concerning the Handicapped (45 CFR 84) ____
   - ☐ Assurance Concerning Sex Discrimination (45 CFR 86) ____
   - ☐ Assurance Concerning Age Discrimination (45 CFR 90 & 45 CFR 91) ____

	Included	NOT Applicable
5. Human Subjects Certification, when applicable (45 CFR 46)	☐	☒

PART B: This part is provided to assure that pertinent information has been addressed and included in the application.

	YES	NOT Applicable
1. Has a Public Health System Impact Statement for the proposed program/project been completed and distributed as required?	☐	☒
2. Has the appropriate box been checked for Item #16 on the SF-424 (FACE PAGE) regarding intergovernmental review under E.O. 12372 ? (45 CFR Part 100)	☒	
3. Has the entire proposed project period been identified in Item #13 of the FACE PAGE ?	☒	
4. Have biographical sketch(es) with job description(s) been attached, when required ?	☒	☐
5. Has the "Budget Information" page, SF-424A (Non-Construction Programs) or SF-424C (Construction Programs), been completed and included ?	☒	
6. Has the 12 month detailed budget been provided ?	☒	☐
7. Has the budget for the entire proposed project period with sufficient detail been provided ?	☐	☒
8. For a Supplemental application, does the detailed budget only address the additional funds requested ?	☐	☒
9. For Competing Continuation and Supplemental applications, has a progress report been included ?	☒	☐

PART C: In the spaces provided below, identify the applicant organization's administrative official to be notified if an award is made and the individual responsible for directing the proposed program/project.

Name, title, organization, address and telephone number of the administrative official to be notified if an award is to be made.	Name, title, organization, address and telephone number of the program director/project director/principal investigator designated to direct the proposed project or program.
Janis L. Goddard, Contracting Officer Georgia Tech Research Corporation Georgia Institute of Technology Atlanta, Georgia 30332-0420 (404) 894-4817	Dr. M. M. Aral, Associate Professor School of Civil & Environmental Engineering Georgia Institute of Technology Atlanta, GA 30332 (404) 894-2243

DHHS 12 DIGIT EIN FOR APPLICANT ORGANIZATION (If already assigned)	SOCIAL SECURITY NUMBER	HIGHEST DEGREE EARNED
1 5 8 0 6 0 3 1 4 6 A 1	252-88-3587	Ph.D.

(OVER)

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PART D: A private, nonprofit organization must include evidence of its nonprofit status with the application. Any of the following is acceptable evidence. Check the appropriate box or complete the "Previously Filed" section, whichever is applicable.

☐ (a) A reference to the organization's listing in the Internal Revenue Service's (IRS) most recent list of tax-exempt organizations described in section 501(c)(3) of the IRS Code.

☐ (b) A copy of a currently valid Internal Revenue Service Tax exemption certificate.

☐ (c) A statement from a State taxing body, State Attorney General, or other appropriate State official certifying that the applicant organization has a nonprofit status and that none of the net earnings accrue to any private shareholders or individuals.

☐ (d) A certified copy of the organization's certificate of incorporation or similar document if it clearly establishes the nonprofit status of the organization.

☐ (e) Any of the above proof for a State or national parent organization, and a statement signed by the parent organization that the applicant organization is a local nonprofit affiliate.

If an applicant has evidence of current nonprofit status on file with an agency of PHS, it will not be necessary to file similar papers again, but the place and date of filing must be indicated.

Previously Filed with: *(Agency)*	on *(Date)*

INVENTIONS

If this is an application for continued support, include: (1) the report of inventions conceived or reduced to practice required by the terms and conditions of the grant; or (2) a list of inventions already reported, or (3) a negative certification.

EXECUTIVE ORDER 12372

Effective September 30, 1983, Executive Order 12372 (Intergovernmental Review of Federal Programs) directed OMB to abolish OMB Circular A-95 and establish a new process for consulting with State and local elected officials on proposed Federal financial assistance. The Department of Health and Human Services has implemented the Executive Order through regulations at 45 CFR Part 100 (Intergovernmental Review of Department of Health and Human Services Programs and Activities). The objectives of the Executive Order are to (1) increase State flexibility to design a consultation process and select the programs it wishes to review, (2) increase the ability of State and local elected officials to influence Federal decisions and (3) compel Federal officials to be more responsive to State concerns, or explain the reasons.

The regulations at 45 CFR Part 100 were published in the Federal Register on June 24, 1983, along with a notice identifying the Department's programs that are subject to the provisions of Executive Order 12372. Information regarding PHS programs subject to Executive Order 12372 is also available from the appropriate awarding office.

States participating in this program establish State Single Points of Contact (SPOCs) to coordinate and manage the review and comment on proposed Federal financial assistance. Applicants should contact the Governor's office for information regarding the SPOC, programs selected for review, and the consultation (review) process designed by their State.

Applicants are to certify on the face page of the SF-424 (attached) whether the request is for a program covered under Executive Order 12372 and, where appropriate, whether the State has been given an opportunity to comment.