United States
Environmental Protection
Agency

Office of Solid Waste
and Emergency Response
(OS-110)

EPA-500-B-92-006
October 1992

EPA

Ground-Water Modeling Compendium

Model Fact Sheets, Descriptions, Applications and Assessment Framework

OSWER Information Management

Purpose of This Compendium

The Ground-Water Modeling Compendium increases the reader's awareness of ground-water models and modeling in general. The Compendium also provides a convenient source of information on overseeing modeling projects.

The Compendium provides an Assessment Framework for planning and assessing modeling applications, summary descriptions of model applications that were used to test the Assessment Framework and summary and detailed descriptions of four ground-water models.

The use of this Compendium by technical support staff and remedial project managers will help to promote the appropriate use of models and therefore sound and defensible modeling within the hazardous waste/Superfund programs.

Who May Benefit From This Compendium

This Compendium is intended for use by:

- Technical Support Staff
- Remedial Project Managers

This Compendium may also help:

- OSWER and Regional Management
- EPA Contractors
- Other Consultants

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Section 1.0 - Introduction

1.0

Introduction

Background

This *Ground-Water Modeling Compendium* has been prepared as part of the Models Management Initiative being conducted by EPA's Office of Solid Waste and Emergency Response (OSWER). OSWER's Resource Management and Information Staff (RMIS) is directing this effort in order to promote improved usage of environmental models -- initially focusing on hazardous waste/Superfund programs, and in the future, supporting Agency-wide efforts.

Objective and Intended Use

During FY 1991-92, OSWER has been conducting a pilot project on ground-water modeling with the primary objective of providing useful information on existing modeling practices and models to EPA staff, contractors, and the regulated community. OSWER recognizes that ground-water models are being used in a variety of ways and under different circumstances and constraints. Models can be used to guide and complement field investigations, thereby improving the understanding of the consequences of site-specific hydrogeologic conditions. However, models should not be used in lieu of field investigations and care must be taken to ensure that models are not misused. The intention of this Compendium is to:

- promote the appropriate use of models by increasing users' awareness about the strengths, weaknesses and inherent uncertainties associated with ground-water models and modeling in general; and

- support model users and decision-makers by providing a convenient source of information on how to oversee modeling projects, how certain models have been applied in the context of hazardous waste/Superfund programs, and the characteristics of four specific ground-water models.

The contents of the *Compendium* have been reviewed extensively by ground-water modeling experts both within and external to EPA. OSWER recommends this document as a reference source for promoting sound and defensible modeling methods and approaches. This document does not, however, constitute official EPA guidance, nor should it be construed as an endorsement of specific models.

Organization and Structure

The *Compendium* is organized into four distinct sections designed to meet the needs of various audiences, including project/site managers, technical reviewers, and model users. The four sections of the Compendium are:

- 1.0, this section, is the **Introduction** describing the Compendium's purpose and organization.

- 2.0, **Assessment Framework for Ground-Water Model Applications,** provides a framework for planning and assessing model applications. The framework is organized into eight categories (e.g., Project Management, Model Setup and Input Estimation). Each category contains a series of criteria that can be used to assess a model application after the fact (i.e., by using existing documentation and the knowledge of the participants to determine how actual modeling practices compare to the criteria), or to guide a team in an ongoing or future application (i.e., by conducting the project in the manner indicated by the criteria). This framework has been developed by the pilot project team in conjunction with recognized modeling experts. Also included in Section 2.0 are footnotes for some of the criteria, a glossary of technical terms, and a list of potential sources of information on EPA modeling guidance.

- 3.0, **Model Applications,** provides summary descriptions of the model applications used to test the assessment framework. These tests were performed to gain insight into the effectiveness of the assessment framework in different modeling situations. Each description discusses the decision objective, regulatory context, site characteristics (e.g., geology, ground-water contamination), modeling activities and results, interesting features of the application, and the names of EPA staff to contact for more details. This section is intended to help readers understand the variety of modeling applications used to test the assessment framework.

- 4.0, **Model Descriptions,** provides summary and detailed descriptions for the four selected models. The summary descriptions are contained on a series of Fact Sheets, each of which is a double-sided encapsulation of the important characteristics of the model and sources of additional information. The detailed model information contained in the latter part of the section includes names of the developers, names and addresses of the custodian, technical features, and solution methods. This information has been extracted from a database of ground-water models developed and maintained by the International Ground Water Modeling Center (IGWMC).

Future Plans

This *Compendium* may be expanded as additional information is collected, analyzed, and organized. This edition focuses on ground-water modeling, reflecting the scope of the OSWER pilot project. Later editions could be expanded or modified in order to:

- enhance the assessment framework;

- include case studies of model applications that illustrate both appropriate and less appropriate modeling methodologies;

- include summary and detailed descriptions for additional models;
- address other modeling domains; and
- modify the format or contents to meet specific requests for information.

If you have any comments about this edition or would like to identify sources of additional information, please contact Mary Lou Melley at OSWER/RMIS (202-260-6860).

Acknowledgements

The OSWER Pilot Project has benefitted since its inception from input by a team of ground-water modeling experts that includes Dr. Mary Anderson, University of Wisconsin, Dr. Paul van der Heijde, International Ground Water Modeling Center, and Dr. Luanne Vanderpool, EPA Region V. These individuals were instrumental in developing the assessment framework provided in Section 2 of the *Compendium*, and their insights led to many improvements in the other sections.

Darcy Campbell and Jon Lutz, of Region VIII, contributed to the contents of the "EPA Publications Related to Ground-Water Modeling" in Section 2.0.

A committee, representing model users in the EPA Regional offices, in OSWER, and other program offices, has been serving as a review group and providing suggestions for the *Compendium*. Its members include:

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Section 2.0 - Assessment Framework for Ground-Water Model Applications

2.0

Assessment Framework for Ground-Water Model Applications

Introduction

This section provides a framework for assessing ground-water model applications. The framework contains a series of assessment criteria, grouped into eight categories:

- Modeling Application Objectives
- Project Management
- Conceptual Model Development
- Model (code) Selection
- Model Setup and Input Estimation
- Simulation of Scenarios
- Post Simulation Analysis
- Overall Effectiveness.

The objective of the assessment framework is to support the use of models as tools for aiding decision-making under conditions of uncertainty. A manager, reviewer, or modeler can use these criteria to assess modeling work that has already been performed, or they can use the criteria to guide a current or future effort. These criteria cover a wide range of conceivable technical and management issues that might be encountered in a variety of modeling applications. For certain types of problems, some of the criteria may not be applicable. For the more complex modeling applications, some criteria may have to be modified or expanded.

The criteria address the activities and thought processes that should be part of a modeling application and the subsequent documentation of that activity or process. Consequently, some of the following criteria are preceded with an asterisk "*" indicating that the analysis, the process, or the data referred to in the question should be documented to assure the defensibility of the modeling application.

Some of the criteria are followed by footnotes referencing other sources of information. The criteria also contain numerous technical terms that may require additional explanation. These terms are italicized the first time they appear. A glossary that follows the criteria contains the definitions for these terms in the context in which they are used in the criteria. In other contexts, alternative definitions of these terms may be more appropriate.

Assessment Criteria

Modeling Application Objectives

1 ☐ *Management's decision objectives and the *modeling objectives* should be clearly specified up-front.

2 ☐ *Management's decision objectives should be based upon existing information about the physical characteristics of the site (e.g., hydrogeologic system) and the source and location of the contamination.

3 ☐ *The function of the model (e.g., data organization, understanding the system, planning additional *field characterization* or evaluation of remediation alternatives) should be defined during the development of the modeling objectives.

4 ☐ *The potential solutions to be evaluated (e.g., *containment* and *remediation* solutions) should be identified prior to the initiation of the modeling.

5 ☐ The level of analysis required (e.g., *numerical model, analytical model* or graphical techniques) should be determined during the definition of the modeling objectives.

6 ☐ *Management, in consultation with a professional ground-water scientist, should specify the time period (e.g., one year, ten years or hundreds of years) for which model predictions are required.

7 ☐ The level of confidence (quantitative or qualitative) required of the modeling results should be specified.

8 ☐ *Performance targets* (e.g., allowable head error) for the model application should be specified up-front.

9 ☐ *An analysis should be performed of the incremental costs associated with expanding these study objectives (e.g., expanding the size of the study area, the number of remedial technologies modeled or the performance targets of the model) and the consequent incremental improvement in supporting management's decision objectives.

10 ☐ Management's decision objectives should be reaffirmed throughout the modeling process.

11 ☐ *The modeling objectives should be reviewed, after the development of the conceptual model and prior to the initiation of the modeling, to ensure that they support management's decision objectives.

12 ☐ The level of analysis required should be reviewed during the course of the project and if necessary modified.

13 ☐ The function of the model should be reviewed during the course of the project and if necessary modified.

Project Management

14 ☐ The individuals who are actually performing the modeling, managing the modeling effort and performing the *peer review* should have the ground-water modeling experience required for the project. Specifically, for their role on the project, each should have the appropriate level of:

- Formal training in modeling and hydrogeology
- Work experience modeling *physical systems*
- Field experience characterizing site hydrogeology
- Modeling project management experience.

15 ☐ These individuals should be organized as a cohesive modeling team with well defined roles, responsibilities and level of participation.

16 ☐ The organization of the team should be appropriate for the application.

17 ☐ *An independent quality assurance (QA) process should be established at the beginning of the project.

18 ☐ *This QA process should include ongoing peer review of the:

- Modeling objectives development
- Conceptual model development
- Model code selection
- Model setup and calibration
- Simulation of scenarios
- Post simulation analysis.

19 ☐ This QA process should be implemented.

20 ☐ A procedure should be established up front for documenting the model application.

21 ☐ *The documentation should include a discussion of the:

- General setting of the site
- Physical systems of interest
- Potential solutions to be evaluated
- Modeling objectives and time frame for model predictions
- Quality assurance and peer review process
- Composition of the modeling team
- Data sources and data quality
- *Conceptual model*
  - *Hydrostratigraphy*
  - *Ground-water flow system*
  - *Hydrologic boundaries*
  - *Hydraulic properties*
  - *Sources and sinks*

  - *Contaminant source, loading and areal extent*
  - *Contaminant transport* and transformation processes
- Selection of the computer code
  - Description of the code
  - *Reliability*
  - Usability
  - Transportability
  - Performance
  - Public Domain vs. Proprietary Models
  - Limitations
  - Related Applications
- Ground-water model construction
  - Code modifications
  - *Model grid*
  - Hydraulic parameters
  - *Boundary conditions*
  - Simplifying Assumptions
- *Calibration, sensitivity analysis, and verification*
- Predictive simulations
  - Scenarios
  - Implementation of the scenarios
  - Discussion of the results of each run
- *Uncertainty analysis*
- Discussion of results related to management's information needs as formulated in the decision objectives
- Executive summary (in terms of the decision objectives)
- References
- Input and output files.

See Footnote 1.

22 ☐ The documentation should provide the information required for an independent reviewer to complete a post application assessment.

Conceptual Model Development

23 ☐ An initial *conceptual model* of both the local and regional hydrogeological system should be developed prior to any computer modeling.

24 ☐ *The conceptual model should be based upon a quantification of field data as well as other qualitative data that includes information on the:

- Aquifer system (Distribution and configuration of aquifer and *aquitard* units)
  - Thickness and continuity of relevant units
  - Areal extent
  - Interconnections between units
- Hydrologic boundaries
  - Physical extent of the aquifer system
  - Hydrologic features that impact or control the ground-water system
    - *Ground-water divides*
    - *Surface water bodies*
- Hydraulic properties (Including, where relevant, homogeneous and isotropic characteristics)
  - *Transmissivity*
  - *Porosity*
  - *Hydraulic conductivity*
  - *Storativity*
  - *Specific yield*
- Sources and Sinks
  - Recharge to the aquifer (e.g., *Infiltration*)
  - *Evapotranspiration*
  - Drains
  - Ground-water discharges (e.g., flow to surface water bodies)
  - Wells (e.g., water supply, injection or irrigation wells)
- *Fluid Potential* (i.e., the potentiometric surface, the magnitude and direction of the hydraulic gradient within each model layer)
- Contaminant
  - Source
  - Loading
  - Areal extent
  - Physical properties
  - Chemical interactions
  - Biotransformations
- Soils.

See Footnote 2.

25 ☐ *The quantity, quality and completeness of the field data should be analyzed as part of the development of the conceptual model.

26 ☐ If there are data gaps (e.g., missing water level or hydraulic conductivity information), additional field work and other attempts to fill in these gaps should be documented.

27 ☐ *If there are data gaps, the tradeoff should be analyzed between the cost of acquiring additional data and the consequent improvement in meeting management's decision objectives.

28 ☐ *The data sources should be documented.

29 ☐ *The quality of the data should be examined and documented and the influence of their quality on the project's results should be assessed.

30 ☐ *Any and all potential interactions with other physical systems (e.g., surface water systems or agricultural systems) should be evaluated, prior to the beginning of the modeling, by means of a water budget, a chemical mass balance or other analytical techniques.

31 ☐ The manner in which existing and future engineering (e.g., wells or slurry walls) must be represented in the numeric or analytic model should be explicitly incorporated into the conceptual model.

32 ☐ Sufficient contaminant sources should be identified to account for the contaminant mass in the plume.

33 ☐ *A clear statement of the location, type and state of the boundary conditions; justification of their formulation; and the source(s) of information on the boundary conditions should be included as part of the conceptual model.

34 ☐ *All conceptual model parameters and reasonable parameter ranges should be specified prior to beginning the calibration of the numerical model.

Model (code) Selection

35 ☐ *The selected model (code) should be described with regard to its flow and transport processes, mathematics, hydrogeologic system representation, boundary conditions and input parameters.

36 ☐ *The *reliability* of the model (code) should be assessed including a review of:

- Peer reviews of the model's theory (e.g., a formal review process by an individual or organization acknowledged for their expertise in ground-water modeling or the publication of the theory in a peer-reviewed journal)
- Peer reviews of the model's code (e.g., a formal review process by an individual or organization acknowledged for their expertise in assessing ground-water computer models)
- *Verification studies* (e.g., evaluation of the model results against laboratory tests, analytical solutions or other well accepted models)
- Relevant field tests (i.e., the application and evaluation of the model to site specific conditions for which extensive data sets are available)
- The model's (code) acceptability in the user community as evidenced by the quantity and type of use.

37 ☐ *The usability of the model (code) should be assessed including the availability of:

- The model binary code
- The model source code
- Pre and post processors
- Existing data resources
- Standardized data formats
- Complete user instruction manuals
- Sample problems
- Necessary hardware
- Transportability across platforms
- User support.

38 ☐ *The tradeoff should be analyzed between model (code) performance (e.g., accuracy and processing speed) and the human and computer resources required to perform the modeling.

39 ☐ *The model (code) should be in the public domain or at least readily accessible to all interested parties. If not, the modelers should explain how the inaccessibility would not detract from the study objectives and the regulatory process.

40 ☐ *The assumptions in the model (code) should be analyzed with regard to their impact upon the modeling objectives.

41 ☐ *Any and all discrepancies between the modeling requirements (i.e., as indicated by the decision objectives, conceptual model and available data) and the capabilities of the selected model should be identified and justified. The modelers should explain why the modeling objectives and/or the conceptual model did or did not need to be modified. For example, the implications of the selected code supporting one, two or three dimensional modeling; providing steady versus unsteady state modeling; or requiring simplifications of the conceptual model should be discussed.

42 ☐ *If the modeling objectives are modified due to such discrepancies, those modifications should be documented.

43 ☐ *If the model source code is modified, the following tests should be performed and the testing methodology and results should be justified:

- Reliability testing (See criteria #36)
- Usability evaluation (See criteria #37)
- *Performance testing.*

See Footnote 3.

Model Setup And Input Estimation

44 ☐ *The overall grid resolution (e.g., average spacing of 100 feet versus 1000 feet) should be analyzed with respect to the dependent variable accuracy required to meet management's objectives. For example, the grid should be fine enough to allow the hydraulic gradient to be accurately represented.

See Footnote 7.

45 ☐ *The *finite element* or *finite difference* grid design should be analyzed with respect to the modeling objectives such as the need to locate or model wells, existing and future engineering or contaminant sources and plumes.

See Footnote 7.

46 ☐ *The grid should be designed with respect to the physical system. For example:

- The main grid orientation should be aligned with the principal directions of hydraulic conductivity and/or transmissivity.
- A finer grid should be used in areas where results are needed (e.g., in the area of highest pollution or drawdown) or areas having large:
  - Changes in transmissivity
  - Changes in hydraulic head
  - Concentration gradients
- A coarser grid should be used where data are scarce and for those parts of the study area that are not of particular interest.

See Footnotes 4 and 7.

47 ☐ *The grid spacing and time step size should be analyzed with respect to numerical accuracy. For example:

- If a finite difference model with variable grid spacing was used the grid should be expanded towards distant boundaries by less than a factor of 2.
- If a finite element model was used the following should be analyzed with regard to their impact on the numerical accuracy of the model application:
  - Length to width ratio of each element
  - Size difference between neighboring elements
  - The Peclet number ($P_e = v \bullet \Delta X/D$).
- The Courant number ($C_r = v \bullet \Delta t/\Delta X$) should be ≤ 1

  Where:

  D = Dispersion Coefficient (l^2/t)

  Δt=Time Step

  V = Velocity (l/t)

  ΔX = Grid spacing (l).

- If Random Walk particle tracking was used the grid spacing and particle mass should be analyzed with respect to the contaminant resolution required.

See Footnotes 5 and 7.

48 ☐ *The mapping of the location of the boundary conditions on the grid should be evaluated. For example:
- The boundaries should be located far enough away from the areas of interest to dampen any instability in the model.
- The manner in which the boundaries are represented in the grid should ensure the fineness of the grid, the accuracy of the geometry and the accuracy of the boundary conditions.
- For finite element grids, internal and external boundaries should coincide with element boundaries.

See Footnotes 6 and 7.

49 ☐ Well nodes should be located near the physical location of the wells.

50 ☐ *The data sources, the data collection procedures and the data uncertainty for the model input data should be evaluated and documented in the project report or file.

51 ☐ *All model inputs should be defined as to whether they are measurements, estimates or assumptions including:
- The *constitutive coefficients and parameters* (i.e., parameters that are not generally observable but must be inferred from observations of other variables, for example the distribution of transmissivity and specific storage)
- The *forcing terms* (e.g., sources and sinks of water and dissolved contaminants)
- The boundary conditions
- The initial conditions.

52 ☐ The input estimation process whereby data are converted into model inputs (e.g., spatial and temporal interpolation and extrapolation or *Kriging*) should be described and the spatial location and the associated values of the data used to perform the interpolation should be shown on a map or provided in a table.

See Footnote 7.

53 ☐ The uncertainty associated with the input estimation process should be specified, explained and documented.

54 ☐ The model should be *calibrated*.

55 ☐ *If the model is not calibrated, the reasoning for not calibrating the model should be explained.

56 ☐ *The criteria being used to terminate the calibration process (i.e., the definition of an adequate match between observed and modeled values) should be justified with regard to the modeling objectives.

See Footnote 7.

57 ☐ *The calibration should be performed in a generally acceptable manner. Specifically:

- A *sensitivity analysis* should be performed to determine the key parameters and boundary conditions to be investigated during calibration.
- The calibration should include a calculation of *residuals* between simulated and measured values.
- The calibration should include an evaluation of both spatial and temporal residuals.
- The calibration should be performed in the context of the physical features (e.g., were residuals analyzed with respect to the pattern of ground-water contours including mounds or depressions or indications of surface water discharge or recharge).

See Footnote 8.

58 ☐ If a water budget is developed, the results and their use in calibrating the model should be explained.

59 ☐ *All changes in initial model parameter values due to calibration should be justified as to their reasonableness.

60 ☐ *Any discrepancies between the calibrated model parameters and the parameter ranges estimated in the conceptual model should be justified.

61 ☐ *If the conceptual model is modified as a result of the model calibration, all changes in the conceptual model should be justified. Whenever feasible, the calibrated model should be verified with an independent set of field observations.

Simulation Of Scenarios

62 ☐ *For each modeling scenario, the model inputs and the location of features in the model grid should be justified. For example:

- If a pumping well was not located at a node, the allocation of well discharges among neighboring nodes should be justified.
- If a slurry wall is a remedial alternative, the representation in the model of the wall's geometric and hydraulic properties should be justified.
- If cleanup times are calculated, all assumptions about the location, quantity and state of the contaminants should be justified.
- When a remedial action, such as extraction wells, affects the flow, such effects should be determined, including the downgradient distance to the stagnation point and the lateral reach of each modeled extraction well.

Post Simulation Analysis

63 ☐ *The success of the model application in simulating the site scenarios should be assessed.

64 ☐ This assessment should include an analysis of:

- Whether the modeling simulations were realistic
- Whether the simulations accurately reflected the scenarios
- Whether the hydrogeologic system was accurately simulated
- Which aspects of the conceptual model were successfully modeled.

65 ☐ *The sensitivity of the model results to uncertainties in site specific parameters and the level of error in the model calibration should be examined and quantified. For example the modeling scenarios should be simulated for the range of possible values of the more sensitive hydrogeologic parameters. Moreover, the range of error in the model calibration should be considered when drawing conclusions about the model results.

66 ☐ The post-processing should be analyzed to ensure that it accurately represents the modeling results and interpolation and smoothing methods should be documented where appropriate.

67 ☐ The post-processing results should be analyzed to ensure that they support the modeling objectives.

68 ☐ The final presentation should effectively and accurately communicate the modeling results.

69 ☐ When feasible, a *post audit* of the model should be carried out or planned for in the future.

See Footnote 9.

Overall Effectiveness

70 ☐ *Any difficulties encountered in the model application should be documented.

71 ☐ The model application should provide the information being sought by management for decision making.

See Footnote 10.

72 ☐ The model application results should be acceptable to all relevant parties.

73 ☐ The model application should support a timely and effective regulatory decision.

74 ☐ Those aspects of the modeling effort that in hindsight might have been done differently should be documented.

Footnotes

1. For more information on documentation see the Draft ASTM Standard Section D-18.21.10, "Guide for Application of a Ground-Water Flow Model to a Site-Specific Problem" and "Standards For Mathematical Modeling of Ground Water Flow and Contaminant Transport at Hazardous Waste Sites," Chapter 4 of Volume 2 of Scientific and Technical Standards For Hazardous Waste Sites - Draft, Department of Health Services, State of California.

2. For more information on data requirements for conceptual model development see the Draft ASTM Standard Section D-18.21.10, "Guide for Application of a Ground-Water Flow Model to a Site-Specific Problem;" "Standards For Mathematical Modeling of Ground Water Flow and Contaminant Transport at Hazardous Waste Sites," Chapter 4 of Volume 2 of Scientific and Technical Standards For Hazardous Waste Sites - Draft, Department of Health Services, State of California, pg. 4; Ground Water Models, Scientific and Regulatory Applications, Committee on Ground-Water Modeling Assessment, National Research Council, National Academy of Sciences, 1990, pgs. 221 - 230; and Applied Ground Water Modeling: Simulation Of Flow And Advective Transport, Anderson, M. and Woessner, W. W., Academic Press, 1992.

3. For more information on the testing of model codes see Groundwater Modeling: An Overview and Status Report, van der Heijde, P. K., El-Kadi, A. I. and Williams, S. A., International Ground Water Modeling Center, Colorado School of Mines, Golden, Colorado, 1988, pgs. 27 - 33; and "Testing and Validation of Ground Water Models," van der Heijde, P. K., Huyakorn, P.S. and Mercer, J.W., Proceedings, NWWA/IGWMC Conference on Practical Applications of Groundwater Models, Columbus, Ohio, August 19-20, 1985, National Water Well Association, Dublin, Ohio.

4. For more information on the design of the grid see Groundwater Modeling: An Overview and Status Report, van der Heijde, P. K., El-Kadi, A. I. and Williams, S. A., International Ground Water Modeling Center, Colorado School of Mines, Golden, Colorado, 1988, pgs. 45 - 48 and Applied Ground Water Modeling: Simulation Of Flow And Advective Transport, Anderson, M. and Woessner, W. W., Academic Press, 1992.

5. For information on how grid design and time step size can affect the numerical accuracy of a model see Computational Methods in Subsurface Flow, Huyakorn, P. S. and Pinder, G. F., Academic Press, New York, New York, 1983, pgs. 206 and 392; Groundwater Modeling: An Overview and Status Report, van der Heijde, P. K., El-Kadi, A. I. and Williams, S. A., International Ground Water Modeling Center, Colorado School of Mines, Golden, Colorado, 1988, pgs. 45 - 48; and Applied Ground Water Modeling: Simulation Of Flow And Advective Transport, Anderson, M. and Woessner, W. W., Academic Press, 1992.

6. For information on properly locating and representing boundary conditions see Definition of Boundary and Initial Conditions in the Analysis of Saturated Ground-Water Flow Systems - An Introduction, Franke, O. L., T. E. Reilly and G. D. Bennett, Open-File Report 84-458, U. S. Geological Survey, Reston, Virginia, 1984; and Applied Ground Water Modeling; Simulation Of Flow And Advective Transport, Anderson, M. and Woessner, W. W., Academic Press, 1992.

7. For information on model setup, input estimation and criteria for the termination of the calibration process see: Applied Ground Water Modeling; Simulation Of Flow And Advective Transport, Anderson, M. and Woessner, W. W., Academic Press, 1992.

8. For more information on the calibration of ground-water models see: Applied Ground Water Modeling; Simulation Of Flow And Advective Transport, Anderson, M. and Woessner, W. W., Academic Press, 1992; Groundwater Modeling: An Overview and Status Report, van der Heijde, P. K., El-Kadi, A. I. and Williams, S. A., International Ground Water Modeling Center, Colorado School of Mines, Golden, Colorado, 1988; Draft ASTM Standard Section D-18.21.10, "Standard Guide for Comparing Ground-Water Flow Model Simulations to Site-Specific Information;" Subpart 6.5; and "Standards For Mathematical Modeling of Ground Water Flow and Contaminant Transport at Hazardous Waste Sites," Chapter 4 of Volume 2 of Scientific and Technical Standards For Hazardous Waste Sites - Draft, Department of Health Services, State of California, Section 3.3.2.4.

9. For more information on post audits see; "The Role of the Postaudit in Model Validation", Anderson, M. P. and Woessner, W. W., submitted to Advances in Water Resources, October, 1991

10. For more information on decision making under conditions of uncertainty see: "Hydrogeological Decision Analysis: 1. A Framework," Freeze, R. A., Massmann, J., Smith, L., Sperling,T. and James, B., Ground Water 1990, 28(5), 738 - 766.

Glossary of Technical Terms

This glossary provides definitions for some of the technical terms used in Section 2.0, Assessment Framework, of the *Compendium of Modeling Information.* Words appearing in italics are defined elsewhere in the glossary. Numbers in parentheses following each definition correspond to the reference source for the definition. A complete list of references is included on the last page of the glossary.

Analytical model - mathematical expression used to study the behavior of physical processes such as *ground-water flow* and *contaminant transport*. This type of model is generally more economical and simpler than a numerical model, but it requires many simplifying assumptions regarding the geologic setting and hydrologic conditions. In comparison with a numerical model, however, an analytical model provides an exact solution of the governing partial differential equation instead of an approximate solution. (9, 14)

Aquitard - a geologic unit with low values of *hydraulic conductivity* which allows some movement of water through it, but at rates of flow lower than those of adjacent aquifers. An aquitard can transmit significant quantities of water when viewed over a large area and long time periods, but its permeability is not sufficient to justify production wells being placed in it. It may serve as a storage unit, but it does not yield water readily. (1,11,12,15)

Boundary conditions - mathematical expressions specifying the dependent variable (head) or the derivative of the dependent variable (flux) along the boundaries of the problem domain. To solve the ground-water flow equation, specification of boundary conditions, along with the initial conditions is required. Ideally, the boundary of the model should correspond with a physical boundary of the ground-water flow system, such as an impermeable body of rock or a large body of surface water. Many model applications, however, require the use of non-physical boundaries, such as ground-water divides and aquifer underflow. The effect of non-physical boundaries on the modeling results must be tested. (3)

Calibration - a procedure for finding a set of parameters, boundary conditions, and stresses that produces simulated heads and fluxes that match field-measured values within a pre-established range of error. (3)

Capture Zone - steady state: the region surrounding the well that contributes flow to the well and which extends up gradient to the ground-water divide of the drainage basin; travel time related: the region surrounding a well that contributes flow to the well within a specified period of time. (14)

Conceptual model - an interpretation or working description of the characteristics and dynamics of a *physical system*. The purpose of building a conceptual model is to simplify the field problem and organize the field data so the system can be analyzed more readily. (3,9)

Constitutive coefficients and parameters - type of model input that is not directly observable, but, rather, must be inferred from observations of other model variables; for example the distribution of transmissivity, specific storage, porosity, recharge, and evapotraspiration. They are difficult to estimate because they vary and can not be observed, particularly when field measurements are limited. (13)

Containment - action(s) undertaken, such as constructing slurry trenches, installing diversionary booms, earth moving, plugging damaged tank cars, and using chemicals to restrain the spread of the substance, that focus on controlling the source of a discharge or release and minimizing the spread of the hazardous substance or its effects. (18)

Contaminant source, loading and areal extent - the physical location of the source contaminating the aquifer, the rate at which the contaminant is entering the ground-water system, and the surface area of the contaminant source, respectively. In order to model fate and transport of a contaminant, the characteristics of the contaminant source must be known or assumed. (2)

Contaminant transformation - chemical changes and reactions that change the chemical properties of the contaminant. (2)

Contaminant transport - flow and dispersion of contaminants dissolved in ground water in the subsurface environment. (13)

Evapotranspiration - a combined term for water lost as vapor from a soil or open water surfaces, such as lakes and streams (evaporation) and water lost through the intervention of plants, mainly via the stomata (transpiration). Term is used because, in practice, it is difficult to distinguish water vapor from these two sources in water balance and atmospheric studies. Also known as fly-off, total evaporation and water loss. Losses from evapotranspiration can occur at the water table. (1,2)

Field characterization - a review of historical, on- and off-site, as well as surface and sub-surface data, and the collection of new data to meet project objectives. When possible, aerial photographs, contaminant source investigations, soil and aquifer sampling, and the delineation of aquifer head and contaminant concentrations should be reviewed. Field characterization is a necessary prerequisite to the development of a conceptual model. (2)

Finite difference model - a type of *numerical model* that uses a mathematical technique called finite-difference to obtain an approximate solution to the partial differential ground-water flow equation. Aquifer heterogeneity is handled by dividing the aquifer into homogeneous rectangular blocks. An algebraic equation is written for each block, leading to a set of equations which can be input into a matrix and solved numerically. This type of model has difficulty incorporating irregular and uneven boundaries. (2,6,9,10)

Finite element model - a type of *numerical model* that uses the finite-element technique to obtain an approximate solution to the partial differential ground-water flow equation. To handle aquifer heterogeneity, the aquifer can be divided into irregular homogeneous elements, usually triangles. This type of model can incorporate irregular and curved boundaries, sloping soil, and rock layers more easily than a finite difference model for some problem types. This technique, like finite-difference, leads to a set of simultaneous algebraic equations which is input into a matrix and solved numerically. (2,6,9,10)

Fluid potential - mechanical energy per unit mass of fluid at any given point in space and time with regard to an arbitrary state and datum. (6,16)

Forcing terms - type of model input included in most ground-water models to account for *sources and sinks* of water or dissolved contaminants. They may be measured directly (e.g., where and when contaminants are introduced into the subsurface environment), inferred from measurements of more accessible variables, or they may be postulated (e.g., effect of proposed cleanup strategy). (13)

Ground-water divides - ridges in the water table or *potentiometric surface* from which ground water moves away in both directions (14); an imaginary impermeable boundary at the crest or valley bottom of a ground-water flow system across which there is no flow. (6)

Ground-Water flow system - movement of water through, and the collective hydrodynamical and geochemical processes at work in, the interconnected voids in the phreatic zone (the zone of saturation). (1,16)

Hydraulic conductivity - the ability of a rock, sediment, or soil to permit water to flow through it. The scientific definition is the volume of water at the existing kinematic viscosity of the medium that will move in unit time under a unit hydraulic gradient through a unit area measured at right angles to the direction of flow. (14)

Hydraulic properties - those properties of a rock, sediment, or soil that govern the entrance of and the capacity to yield and transmit water (e.g., *porosity, effective porosity, specific yield,* and *hydraulic conductivity*). (2,22)

Hydrologic boundaries - *boundary conditions* which relate to the flow of water in an aquifer system. (2)

Hydrostratigraphy - a sequence of geologic units delimited on the basis of *hydraulic properties*. (5)

Infiltration - flow of water downward from the land surface into and through the upper soil layers. (5)

Kriging - an interpolation procedure for estimating regional distributions of ground-water model inputs from scattered observations. (13)

Model grid - a system of connected nodal points superimposed over the aquifer to spatially discretize the aquifer into cells (*finite difference method*) or elements (*finite element method*) for the purpose of mathematically modeling the aquifer. (21,22)

Model representation - a conceptual, mathematical or physical depiction of a field or laboratory system. A conceptual model describes the present condition of the system. To make predictions of future behavior, it is necessary to develop a dynamic model, such as physical scale models, analog models, or mathematical models. Laboratory sand tanks simulate ground-water flow directly. The flow of ground water can be implied by using an electrical analog model. Mathematical models, including analytical, analytic element, finite difference, and finite element models are more widely used because they are easier to develop and manipulate. (3,5).

Modeling objectives - the purpose of the model application. The objectives should direct model selection and level of effort for the modeling study. (2,3)

Numerical model - a mathematical model that allows the user to let the controlling parameters vary in space and time, enabling detailed replications of the complex geologic and hydrologic conditions existing in the field. Numerical models require fewer restrictive assumptions, and are potentially more realistic and adaptable than analytical models, but provide only approximate solutions for the governing differential equations. (2,10,13)

Peer review - a process by which a panel or individual is charged to review and compare the results of modeling efforts and to assess the importance and nature of any differences which are present. The review may examine, for example, the scientific validity of the model, the mathematical code, hydrogeological/chemical/biological conceptualization, adequacy of data, and the application of the model to a specific site. (2,13)

Performance target - a measure of model accuracy. (2)

Performance testing - determining for the range of expected uses, the efficiency of the model in terms of the accuracy obtained versus the human and computer resources required by comparing model results with predetermined benchmarks. (20)

Porosity - total volume of void space divided by the total volume of porous material. The term, "effective porosity," is related. It is the total volume of interconnected void space divided by the total volume of porous material. Effective porosity is used to compute average linear ground-water velocity. (2,5)

Post audit - comparison of model predictions to the actual outcome measured in the field. Used to determine the success of a model application as well as the acceptability of the model itself. (13)

Potentiometric surface - a surface that represents the level to which water will rise in tightly cased wells. The water table is a particular potentiometric surface for an unconfined aquifer. (5)

Reliability - the probability that a model will satisfactorily perform its intended function under given circumstances. It is the amount of credence placed in a result. (15)

Remediation - long-term action that stops or substantially reduces and prevents future migration of a release or threat of hazardous substances that are a serious but not an immediate threat to public health, welfare, or the environment. (17)

Residuals - the differences between field measurements at calibration points and simulated values. (8)

Sensitivity analysis - process to identify the model inputs that have the most influence on model predictions, at least over a specified range. (2,13)

Sources and Sinks - gain or loss of water or contaminants from the system. In a *ground-water flow system,* typical examples are pumping or injection wells. (2,13)

Specific yield - quantity of water that a unit volume of aquifer, after being saturated, will yield by gravity (expressed as a ratio or percentage of the volume of the aquifer). (15)

Storativity - volume of water given per unit horizontal area of an aquifer and per unit decline of the water table or potentiometric surface. Also known as storage coefficient. (1,6)

Surface water bodies - all bodies of water on the surface of the earth. (15)

Transmissivity - the rate at which ground-water of a prevailing density and viscosity is transmitted through a unit width of an aquifer or confining bed under a unit hydraulic gradient. It is a function of the properties of the liquid, porous media, and the thickness of the porous media. Often expressed as the product of the *hydraulic conductivity* and the full saturated thickness of the aquifer. (1,14)

Uncertainty analysis - the quantification of uncertainty in the spatially distributed values of input hydraulic properties within an aquifer system. (7)

Verification study - consists of the verification of governing equations through laboratory or field tests, the verification of model code through comparison with other models or analytical solutions, and the verification of the model through tests independent of the model calibration data. (3,4,19)

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Section 3.0 - Model Applications

3.0

Model Applications

Introduction

This section provides summary descriptions of the model applications used to test the assessment framework. These descriptions are presented to help the reader understand the variety of model applications that the framework was tested against. These descriptions are not intended to be examples of the application of the framework but simply summaries of the test cases. Each description discusses the:

- Decision objective;
- Regulatory context;
- Site characteristics (e.g., geology, ground-water contamination);
- Modeling activities and results;
- Interesting features of the application; and
- Names of EPA staff to contact for more details about the test case.

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3.1 - Summary Description #1

3.1

Model Applications
Summary Description #1

Decision Objective:

This RCRA site was modeled to determine if the effects of a hydraulic barrier and hydraulic head maintenance system would meet hydraulic gradient performance standards set forth in a Consent Decree. This was an enforcement lead site where contractors for the responsible party performed the modeling. The Region reviewed the modeling effort and results to ensure that the site was modeled as accurately as possible and that the model results indicated that the proposed corrective action would meet the Consent Decree performance standards.

Background:

The site is located in an area of industrial, commercial and warehousing operations on a peninsula in Baltimore Harbor. A significant portion of the perimeter of the site abuts the harbor. Chromium ore was processed at the site from 1845 to 1985. This was a waste intensive operation that generated large quantities of process residuals containing soluble chromium. Historically, these process residuals were used as fill material at the plant site and in other areas around Baltimore Harbor. (See Figure 3.1-1.)

The contamination of soil and ground water with elevated levels of chromium creates the potential for human and environmental exposure. The risk of such exposure, although small, will potentially exist as long as the site remains uncontrolled. To minimize this risk of exposure, a combination of a low permeability cap, a hydraulic barrier and ground-water extraction wells was proposed as a containment strategy.

Remedial investigation and subsequent ground-water modeling of this site began in October 1985, with further site investigations occurring through 1989 as potential remedial actions were evaluated and the ground-water model was refined. The ground-water modeling that is the focus of this case study began with the refinement of the prior model to increase modeling accuracy. This work was performed in 1989 and 1990.

Geologic Summary:

The site is located within the Coastal Plain Physiographic Province, an area that is characterized by an unconsolidated sediment wedge that thickens toward the Atlantic coast. In the vicinity of the site, coastal plain sediments are on the order of 70 ft thick. This site is underlain by artificial fills, recent organic silty clay deposited in the harbor, Pleistocene sediments, lower Cretaceous sediments and bedrock.

The deepest geologic unit investigated consists of gneiss bedrock which is composed of three distinct strata. The lowest stratum is weathered rock composed of fine to medium grained gneiss that is often broken and fractured. Overlaying this lowest stratum is a second stratum with an average thickness of eighteen feet. This stratum consists of fine to coarse sand within a white clay-silt matrix that includes a high feldspar content and a fine to coarse sand containing trace to some silt with a high biotite content. The upper bedrock stratum consists of clayey fine to coarse sand and has an average thickness of ten feet.

Overlaying the bedrock are Lower Cretaceous sediments which vary in thickness from 12 to 40 feet. These sediments range from a silty white sand to white sand and gravel to a white clayey silt. Blanketing the Lower Cretaceous sediments are Pleistocene deposits composed of silty clay, sand, gravel and cobbles which range from 5 to 15 feet in thickness. Above the Pleistocene deposits black organic silty clays and silty fine sand are found along the bulkhead margins of the site. The organic silty clays have an average thickness of 20 feet and the silty fine sand varies between 5 and 10 feet in thickness.

The fill materials, which created the level surface on which the site facilities were built, consist of silty sands, micaceous sandy silts and poorly to well graded sands as well as construction debris, bricks and wood fragments. The fill material occurs at every location across the site and can be as much as 30 feet thick.

Ground-Water Contamination Summary:

The chromium contamination at the site was found to be present in two ground-water yielding layers, one shallow, a water table aquifer, and one deep, a regional aquifer system. The shallow ground water, which lies principally above the low permeability silts near the site perimeter, flows radially off the site through the bulkheads to the north, west and south. The shallow ground-water contamination, which occurs chiefly near major source areas was found to have chromium levels from 0.01 mg/L to 14,500 mg/L.

Deep ground-water contamination within the Cretaceous sands was also highest near the source areas. Regionally, flow in the deep ground water originates from the northwest of the site and flows towards the southeast. Locally, the deep ground water flows radially away from the central portion of the site, with localized small upward and downward flow gradients between the deep and shallow ground water.

Modeling Summary:

The U. S. Geological Survey's three dimensional flow code, MODFLOW, was used to model this site in a steady state. Six model layers, each of which was constructed with variable thicknesses and bottom elevations, were used to simulate the flow of ground water under the site. A 24 row by 24 column finite-difference grid was constructed. (See Figure 3.1-2.) Grid cell dimensions varied between 75 and 150 feet with the smallest cells located directly over the study site. Boundary conditions modeled included the flow directions and gradients of the water table and regional aquifer systems, leakage from the harbor and precipitation recharge.

Horizontal hydraulic conductivity was determined for each layer by averaging hydraulic conductivities from field tests. Vertical hydraulic conductivities were initially assumed to equal the horizontal hydraulic conductivities and were adjusted during calibration of the model.

During the calibration of the model, water levels in the observation wells were used as targets and compared to simulated water levels. The hydraulic parameters were adjusted to provide the best possible match between measured and calculated heads at the calibration targets. Residual analysis was used to measure the effectiveness of the calibration. The residual sum of squares was equal to 32.6 ft^2 and the residual mean was 0.0053 ft.

Additional field testing was performed to refine the calibration of the model. Aquifer tests were used to improve hydraulic conductivity estimates. Additional piezometers were also installed to better understand hydraulic gradients. The model was then recalibrated with these new data.

Three hydraulic barrier scenarios were evaluated through model simulations. All scenarios assumed site closure with the emplacement of a low-permeability cap over the entire site. The first scenario simulated a "deep soil mixing" wall that extended one foot into the uppermost stratum of the bedrock, a clayey fine to coarse sand. This scenario was modeled in combination with ground-water extraction wells and with perimeter trench drains placed at different depths.

The second scenario simulated a shallow slurry wall that extended two feet into the clayey silt stratum of the Lower Cretaceous sediments. This scenario was modeled in combination with alternative configurations of ground-water extraction wells and with perimeter trench drains placed at different depths.

The third scenario simulated only ground-water extraction wells on the site.

<u>Modeling Results Summary:</u>

Model simulations of the first scenario indicated that the use of a deep hydraulic barrier without pumping or trench drains would not meet the head difference performance standards of the Consent Decree. However, the use of 12 extraction wells pumping a total of 2100 gal/day in combination with the wall would meet these performance standards. The model simulations also indicated that perimeter drains in combination with the deep hydraulic barrier would meet the performance standards. When drains were placed at -0.5 ft msl. and 0.0 ft msl. the model simulations indicated that 13,500 gal/day and 3,500 gal/day of ground-water extraction would occur respectively.

Model simulations of the second scenario indicated that the shallow hydraulic barrier without pumping or drains would not meet the head difference performance standards of the Consent Decree. Moreover, the modeling indicated that the use of the shallow hydraulic barrier instead of the deep hydraulic barrier would require significantly increased ground-water extraction. If twelve extraction wells were used a total pumpage of 27,500 gal/day would be needed. If only eight wells were used, the pumpage requirements would increase to 28,000 gal/day. If perimeter trench drains were used in lieu of wells the ground-water extraction rate would vary between 17,440 and 13,500 gal/day depending on the elevation of the drains.

Model simulations of the third scenario indicated that the head difference performance standards of the Consent Decree could be met by pumping alone with no hydraulic barrier. The total pumpage, however, required to meet the performance standard would be 92,580 gal/day distributed over twelve extraction wells.

In summary, model simulations indicated that the Consent Decree hydraulic head difference performance standards could be met by each of the three modeling scenarios. The first scenario, a deep wall and pumping resulted in minimum extraction rates. Pumping wells alone were able to meet the performance standards; however, in the absence of a hydraulic barrier, the amount of pumpage necessary to maintain the performance standards was more than an order of magnitude greater than that of the first scenario.

Strengths And Interesting Features Of This Application:

In this case study, an existing model of a site was refined and recalibrated. The refinement of the model reflected the need for increased simulation accuracy as the regulatory process moved from site characterization, to technology screening, to the design of a specific containment technology and management strategy.

This modeling application was used to predict the performance of alternative corrective actions and the impact of those alternatives upon the hydrogeologic system. It should be noted that the quantity and quality of site field data in this case study are atypical of most sites. These data allowed the development of a model with considerable hydrogeologic specificity.

This application provided the information necessary to justify the need for both a slurry wall and ground-water pumping inside the wall. Originally the responsible party had proposed just a slurry wall with no pumping. This study demonstrated the problems with such an approach and the effectiveness of combining the slurry wall with pumping. For example, this study dramatized that required pumping rates varied by over an order of magnitude with and without the slurry wall. Moreover, this study helped to determine the design capacity of a water treatment system by determining the volume of ground-water extraction for each scenario.

This study demonstrated that the hydrogeologic system would be modified by the proposed corrective action and provided a mechanism for predicting these impacts. The Region noted that they will monitor the effectiveness of the selected corrective action and if necessary the corrective action and/or the model application will be modified as additional information is gained. This type of review, often called a post audit, is strongly encouraged by ground-water modeling experts.

The calibration report provides an example of the use of residual analysis to evaluate the model calibration.

Areas that should be covered in model calibration documentation include:

1. Explicitly establishing and documenting a reasonable range of parameter values to be used in the calibration of the model;
2. Documenting the model residuals and the residual analysis;
3. Documenting the sensitivity of the model to variations in model parameters;
4. Documenting the impact of grid spacing and time step on the numerical accuracy of the model;
5. Documenting the criteria being used to terminate the calibration process; and
6. Documenting the evaluation of the spatial and temporal distribution of residuals.

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Modeling Documents:

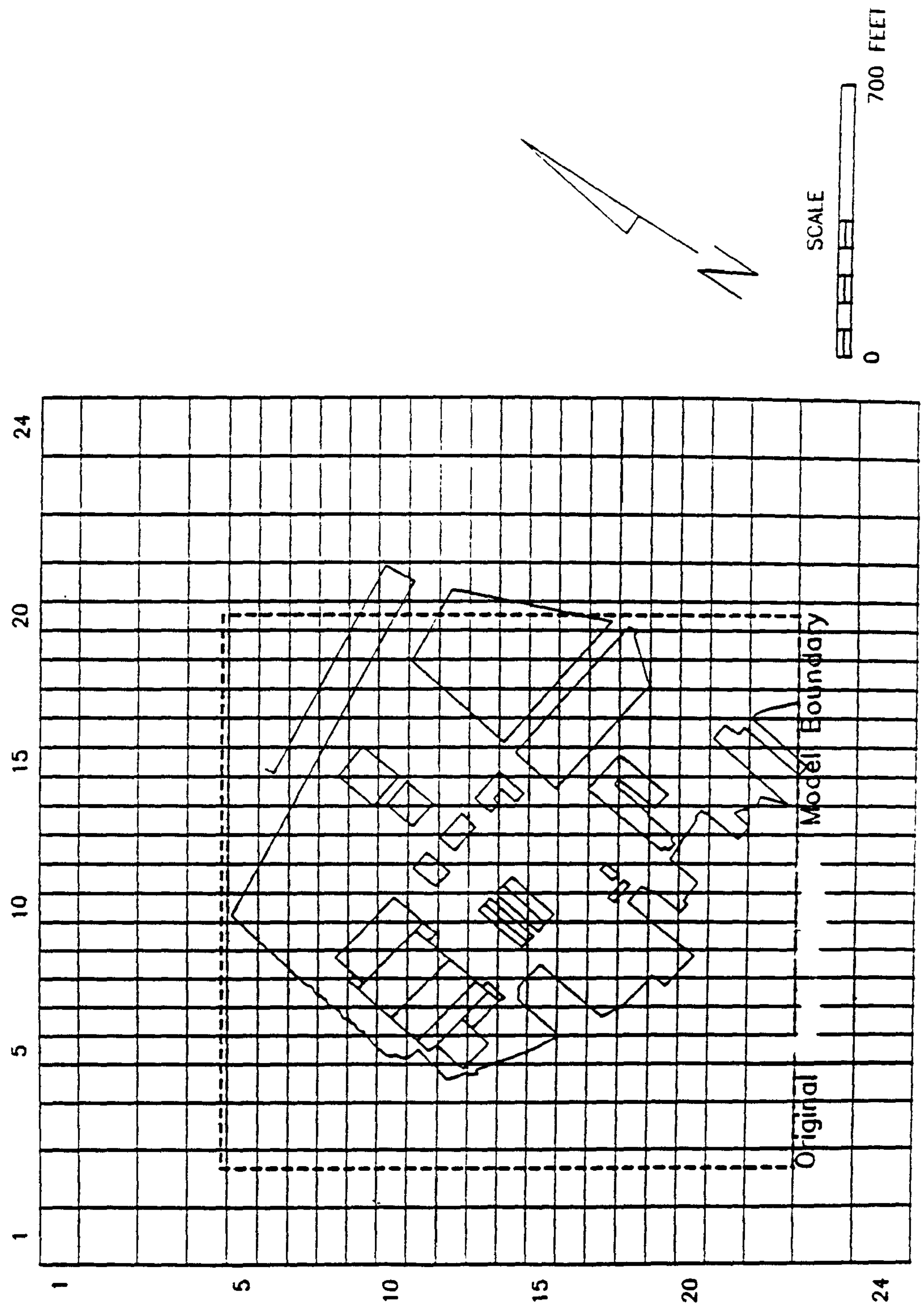
Please contact the above people for specific modeling documents.

Figure 3.1-1

Site Location

Figure 3.1-2

Finite Difference Model Grid



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3.2 - Summary Description #2

3.2

Model Applications
Summary Description #2

Decision Objective:

The United States Army's (Army) Aberdeen Proving Ground O-Field site was modeled in the early phases of a site investigation to assist in screening corrective actions for the site. Specifically, the objective of the modeling was to:

1. Provide a framework for the characterization of contaminant releases and plumes;
2. Determine if contamination was migrating to other aquifers or surrounding surface water bodies; and
3. Predict the probable hydrologic and chemical effects of relevant remedial actions.

This modeling was performed as a requirement of a RCRA permit that EPA issued to the U.S. Department of Army. In turn, the U.S. Army Environmental Management Office of the Aberdeen Proving Ground contracted with the U. S. Geological Survey (USGS) to conduct the modeling that is the focus of this case study. The EPA Region reviewed the modeling results to ensure that the site was modeled as accurately as possible and that the above decision objectives were met.

Background:

O-Field site is a 259 acre area located within the 79,000 acre Aberdeen Proving Ground Army installation and is surrounded by Army testing ranges. O-Field lies on a neck that extends into the Chesapeake Bay and is directly bordered on the west by the Gunpowder River and on the north and east by a tributary of the Gunpowder River, Watson Creek. (See Figures 3.2-1 and 3.2-2.) Watson Creek, which is better described as a pond, discharges into the Gunpowder River through a man-made culvert that restricts tidal flushing and therefore causes high organic loading in the creek. To the south of O-Field lie other Army testing ranges. The site topography is relatively flat with the highest elevation being about 19 feet above sea level.

O-Field includes two sub areas, Old O-Field and New O-Field. Old O-Field was periodically used from the late 1930's into the 1950's for the disposal of munitions and chemical-warfare agents. Disposal at New O-Field began in 1950 and continued for an unspecified period. Disposal materials at New O-Field included ordnance, contaminated material, laboratory quantities of chemical-warfare agents and dead animals. The primary activity in later years at New O-Field was the destruction of material by burning.

At both New and Old O-Field, containerized and uncontainerized material was disposed in unlined and uncovered trenches, pits and directly on the ground. Beginning in 1949, sporadic cleanup efforts were initiated with the goal of destroying some of the explosives. Periodically during the cleanup operations, explosions ruptured container casings and directly exposed contaminants. Today, most of the pits and trenches have been covered with soil.

In 1976, the Army recommended an assessment of the Aberdeen Proving Ground to determine the potential for off-post migration of chemical contaminants. Observation wells installed at O-Field in 1978 showed the presence of arsenic and chlorinated organic solvents in the ground water. Analysis of surface water and soil samples indicated that the ground water was transporting arsenic into Watson Creek. A limited resampling of ground and surface water in 1984 confirmed these findings.

An observation well network was developed in 1985 when eleven existing wells were supplemented with 21 additional wells installed at eight locations. All well drilling was performed using a remote control drill, bombproof shelters and other extraordinary safety and security procedures due to the possibility of encountering buried ordnance or chemical-warfare agents. An additional five wells were installed in 1987 when quarterly sampling indicated the possibility that contaminants might be present beyond the area covered by the original observation well network.

Geologic Summary:

O-Field is located on unconsolidated sand, clay and silt of the Atlantic Coastal Plain. Beneath the Coastal Plain sediments lies a basement complex of Precambrian to Paleozoic crystalline rocks and Mesozoic rift-basin sedimentary rocks. The depth to the pre-Cretaceous basement rocks at O-Field is approximately 650 feet.

The site hydrogeology was investigated to only a 200 hundred foot depth because of the difficulties associated with remote drilling operations and the improbability that contamination had extended to this depth. Four aquifers were discovered but only the upper three were investigated. These three consisted of a water table aquifer and two confined aquifers with the lowest confined aquifer occurring at a depth of 70 to 90 feet. (See Figure 3.2-3.)

The uppermost soils at O-Field are silt to silty lean clay and below this layer lies a low permeability, tan to grey sand with some silt. Lenses of gray clay underlie the sand followed by silty sand where the water table begins. Extensive excavation and explosions have probably destroyed much of the natural strata of the site to a depth of 10 to 12 feet.

The water table aquifer lies 9 to 15 feet below ground surface with an average saturated thickness of ten feet that varies seasonally by as much as three feet. This aquifer is present across the site and is composed of brown to reddish-brown quartz sand interbedded with discontinuous silt and clay layers. The sand is medium grained in the central areas of the site and becomes finer to the east and north and coarser to the northeast. The water table aquifer is underlain by a confining layer composed of highly plastic black to gray or greenish gray clay. The depth of this confining layer is 11 to 30 feet below ground surface and ranges in thickness from 0.5

to 5 feet. The presence of contamination below this layer indicates that the confining layer is either leaky or discontinuous.

The upper confined aquifer is below this confining layer. This aquifer lies 20 to 30 feet below the ground surface with a thickness that varies from 13 feet in the east and south to less than a foot as it nears the Gunpowder River to the west. The aquifer probably remains confined beneath the Watson Creek shoreline but loses its confining bed beneath the deeper parts of the creek. This aquifer is composed of dark grey to brown, medium to coarse-grained sand interbedded with gravel and discontinuous clay lenses. This aquifer is underlain by a confining layer composed of dense, black to dark grey clay. The depth of this confining layer is 20 to 39 feet below ground surface and ranges in thickness from 43 to 60 feet. The extent, thickness and low permeability of this confining bed are probably adequate to prevent contaminant migration or significant water movement from the upper confined aquifer to the lower confined aquifer.

The lower confined aquifer lies approximately 80 feet below ground surface and is 10 to 20 feet thick. There is little information on the extent and lithology of this aquifer. Downhole gamma, spontaneous-potential and resistance logs as well auger behavior during drilling suggests that it is composed of a highly permeable, gravel like material.

Ground-Water Hydrology Summary:

Water flow in the aquifers underlying this site is complex due to the surface-water interactions and lagging tidal cycles in Watson Creek. Ground water in the water-table and upper confined aquifer generally flows from south to north/northeast towards Watson Creek. A ground-water divide that lies to the west of Old O-Field causes a portion of the ground water to bypass Old O-Field and flow into the Gunpowder River. (See Figure 3.2-4.) A gross estimate of the ground-water flow rate is 50 feet/year.

The water-table aquifer derives most of its recharge from vertical infiltration of precipitation. Additional recharge occurs by lateral movement of ground water as discussed above and periodically by Watson Creek, which overflows its banks during periods of high tides. Discharge is primarily to Watson Creek and the Gunpowder River.

Recharge to the upper confined aquifer is by downward leakage from the overlying water-table aquifer. Discharge is by slow upward leakage through the confining bed to the water table aquifer in down gradient areas and by leakage to surface water bodies where the confining bed has eroded.

The hydraulic gradient indicates that the ground water in the lower confined aquifer flows toward the west-northwest, possibly discharging into the Gunpowder River. The heads in this aquifer are typically higher than those in the upper confined aquifer. Thus, in the unlikely event that there are pathways for downward contaminant migration between the upper and lower confined aquifers, the hydraulic gradient would oppose all such flow except for the density driven migration of free product.

Ground-Water And Surface Water Contamination Summary:

The ground water in both the water table and the upper confined aquifer at O-Field contains inorganic and organic contaminants. Inorganic contaminants include arsenic, iron, manganese, zinc, boron, antimony, cadmium and chloride. For example, arsenic concentrations range from 1.96 parts per million (ppm) in the water-table aquifer to 0.0016 ppm in the upper confined aquifer. Dominant organic contaminants are chlorinated aliphatic hydrocarbons, aromatic hydrocarbons and chemical-warfare degradation products which contain sulfur and phosphorus. Concentrations of thiodiglycol, a degradation product, ranged from 1000 ppm to 5 ppm in the water-table aquifer. In general the highest contaminant concentrations are measured in the water-table aquifer, although higher concentrations of boron and 1,1,2,2-tetrachloroethane are present in the upper confined aquifer than in the water-table aquifer. The arsenic and cadmium concentrations found exceed EPA drinking water maximum contaminant levels. The concentrations of chloride, iron, manganese and zinc exceed 1987 EPA secondary maximum contaminant levels.

The distribution of individual dissolved contaminants varies areally in the water table and upper confined aquifer. For example, the concentrations of arsenic and organic contaminants are highest along the northeastern side of Old O-Field. However, iron is present as two distinct plumes, one along the eastern side and one along the northeastern side of Old O-Field. The areal distribution of contaminants at New O-Field could not be evaluated because of the limited number of wells at the site.

Although low concentrations of organic contaminants have been detected in water samples from the lower confined aquifer, hydraulic gradients and the lithology and thickness of the overlying bed make it unlikely that O-Field operations have contaminated the lower confined aquifer.

A surface water quality study in 1985 of Watson and nearby creeks found unusually high organic loading in Watson Creek and dissolved inorganic constituents that exceed EPA chronic toxicity levels for freshwater and saltwater aquatic life. The lateral migration of ground-water contaminants into Watson Creek is thought to be partially responsible for the surface water contamination. Ultimately, this surface water contamination may migrate into the Gunpowder River.

Modeling Summary:

The U. S. Geological Survey's (USGS) three dimensional flow code, MODFLOW, was used to model this site in a quasi three dimensional, steady state mode. Two model layers were used, one layer simulating the water-table aquifer and the second layer simulating the underlying confining layer and the upper confined aquifer. The lower boundary of the second layer coincides with the top of a fifty foot thick layer of dense clay below the upper confined aquifer. The low permeability and continuity of the clay was thought to justify its use as a no-flow boundary for this model application and thus eliminated the need to model the lower confined aquifer. The model was found to be relatively insensitive to this assumption as discussed below.

A 66-row by 61-column finite-difference grid was constructed and aligned with the principal direction of flow. The grid extends to the south and considerably beyond O-Field to coincide with surface water bodies that could be modeled under steady state conditions as constant head boundaries. Grid cell dimensions varied between 20 and 2375 feet with the smallest cells located directly over the areas of interest. Changes in cell size were limited to no more than 1.5 times the size of adjacent cells.

Boundary conditions modeled included surface water bodies, no-flow regions, drains, and leakage between the layers. Vertical hydraulic conductivities were based upon typical values for similar soil types, limited field data and model calibration. The water-table aquifer was bounded at most locations by constant head boundaries which represented the shoreline of surface water bodies. At the two areas where the water-table aquifer extended beyond the modeled area the ground-water flow was parallel to the model boundaries and thus these areas were modeled as no-flow boundaries.

The lateral boundaries of the upper confined aquifer were specified as no-flow boundaries. However, a relatively high vertical hydraulic conductivity was specified for those portions of the overlying confining layer that lay beneath surface water bodies and thus these areas of the modeled layer responded almost as if they had been established as constant head boundaries. Consequently, as the modeled portion of the upper confined aquifer is almost entirely surrounded by surface water bodies this layer was effectively modeled with constant head boundaries with one exception. That exception was determined to be far enough from O-Field that the no-flow boundary had negligible effects on simulations within O-Field.

Preliminary calibration of the steady-state model was achieved by setting average annual recharge constant and adjusting model coefficients, primarily the horizontal hydraulic conductivity of the water-table aquifer and the transmissivity of the upper confined aquifer. These coefficients were adjusted within a range of reasonable values based upon field measurements. The calibration was considered acceptable if the simulated and observed average annual heads agreed within 0.5 feet. The model was then recalibrated against observed head data for a period of elevated ground-water levels. During this second calibration the horizontal hydraulic conductivity and transmissivity values obtained from the first calibration were held constant and recharge was uniformly increased until the predicted heads acceptably matched the observed heads Horizontal hydraulic conductivity and transmissivity were then adjusted slightly to improve the match. These new values were then used to once again calibrate the model against the average annual observed heads. This process was repeated until the model met the calibration criteria under both hydrologic scenarios.

Because of uncertainties about the actual recharge and hydraulic conductivities at O-Field, several alternative solutions to the steady state model were then generated by varying both recharge and hydraulic conductivity. Based upon recharge estimates and field measurements of horizontal hydraulic conductivity, the recharge was varied between 9 and 16 inches per year and the hydraulic conductivity was uniformly adjusted by the same percentage. The resulting head configurations still closely matched the observed heads. These alternative hydrogeologic system representations were used to model the system responses to the remedial alternatives evaluated also. Thus, the impact of hydrogeologic uncertainty upon the results of the remedial alternatives modeled could be quantified.

A sensitivity analysis of the calibrated flow model was performed for a range of recharge, hydraulic conductivity and transmissivity values. This analysis indicated that heads in the water-table aquifer were relatively insensitive to variations in the vertical hydraulic conductivity of the confining layer or transmissivity of the confined aquifer. Heads in the confined aquifer were somewhat more sensitive to these variations. The sensitivity analysis also indicated that simulated heads in both aquifers were very sensitive to changes in the horizontal hydraulic conductivity and recharge of the water-table aquifer.

The assumption that the lower confined aquifer did not need to be modeled was also examined during the sensitivity analysis. Simulations of a modified version of the model that included the lower confined aquifer as a third layer demonstrated that significant head variations in the lower confined aquifer had a minimal impact on the head in the upper two aquifers. This confirmed that simulation of the ground-water system as a two layer system was adequate for the purposes of this modeling effort .

Five remedial actions and a sixth no-action scenario were evaluated. These remedial actions were evaluated on the basis of their ability to lower ground-water levels within the disposal areas and to limit lateral or vertical movement of water through the disposal areas. The remedial actions evaluated included: installation of an impermeable cap; installation of subsurface barriers; installation of a ground-water drain; ground-water pumping to control water levels; ground-water pumping to recover contaminants; and no action. All remedial actions were also simulated with the alternative model configurations described above to quantify the impact of hydrogeologic uncertainty upon each remedial alternative's predicted effectiveness.

The impermeable cap remedial alternative was simulated by establishing areas of no ground-water recharge. The subsurface hydraulic barriers were simulated by reducing horizontal hydraulic conductances in the model cells representing the barriers. These conductances were calculated to represent a 5 foot thick barrier with a horizontal hydraulic conductivity of 0.001 feet per day and accounted for the fact that the barriers did not comprise the entire cell. The ground-water drain was simulated by lowering the surface elevation of an existing natural drain to 1.5 feet above sea level during the period of record.

Ground-water pumping to control water levels was simulated with the addition of three pumping wells upgradient from Old O-Field and two wells upgradient from New O-Field. Each of these wells were simulated at pumping rates of 2,900, 5,800, 10,000 and 21,600 gallons per day (gal/d) but Old O-Field and New Old Field wells were simulated separately. The pumping was simulated with and without impermeable covers. Similarly, ground-water pumping to recover contaminants (pump-and-treat) was simulated with the addition of two wells adjacent to the southeastern side of Old O-Field and two wells adjacent to the northeastern side of New O-Field. Again, each of these wells was pumped at rates of 2,900, 5,800, 10,000 and 21,600 gal/d; Old O-Field and New O-Field wells were simulated separately; and the pumping was simulated with and without impermeable covers on the respective disposal areas.

Modeling Results Summary:

The simulations indicated that covering Old O-Field with an impermeable cap would lower water levels beneath the site by less than 1 foot. An impermeable cap over New O-Field would be even less effective and reduce water levels by only 0.3 feet. Ground-water velocities appear to be sufficient to compensate for the loss of recharge water intercepted by the caps. However, the reduction of precipitation infiltration into the unsaturated zone at the fill could decrease the amount of contaminant leaching.

Subsurface hydraulic barriers upgradient from Old O-Field resulted in water level declines below Old O-Field of about 1 foot but produced increases in water levels at New O-Field. Thus while potentially reducing contaminant leaching at Old O-Field the barriers may also increase leaching at New O-Field. Complete encapsulation of Old O-Field with hydraulic barriers and an impermeable cap was also simulated and was shown to provide short term aquifer protection. However, the concentrations of some contaminants would likely increase in solution and should the encapsulating walls fail at some future point, the concentrations of some contaminants in the ground water would then increase.

The simulation of subsurface barriers at the New Old-Field reduced water levels at the disposal trenches by 2.5 feet but increased water levels by 2 feet on the upgradient side. These reductions increased to 3.5 to 4.5 feet with the addition of an impermeable cap.

The simulation of deepening an existing natural drain lowered water levels in the water table aquifer beneath both Old and New O-Field. In turn, a ground-water divide developed between the drain and Old O-Field and contaminant movement from Old O-Field towards the drain probably would not occur. However, during periods of low ground-water levels or high surface water levels, brackish surface water would enter the drain and recharge parts of the water-table aquifer with brackish surface water.

Pumping to manage water levels at Old O-Field indicated that the water-table aquifer would be drawn down by 0.7 to 1.0 feet when the wells were pumped at 5800 gal/d per well. When an impermeable cap was added the drawdown increased by 0.5 feet. However, some simulations within the range of hydrogeologic uncertainty demonstrated that a pumping rate of 5800 gal/d per well or more could induce contaminants to migrate to previously uncontaminated areas.

Pumping rates of 10,000 and 21,600 gal/d per well were required at New O-Field to reduce ground-water levels by 1.0 and 2.3 to 3.5 feet respectively. However, both rates would produce hydraulic gradient reversals extending to the disposal trenches and thus induce the movement of contaminants toward the wells.

The simulations predicted that pump-and-treat at a rate of 2900 gal/d per well in combination with an impermeable cap would intercept the bulk of ground-water contamination at Old O-Field in the spring, summer and fall. This rate would have to be increased to 5800 gal/d in the winter when ground-water levels are higher. However, this higher rate could induce the movement of water from Watson Creek into the aquifer if it is maintained throughout the year. Pump-and-treat at New O-Field resulted in drawdowns of 1.1 to 1.8 feet for pumpage of 5800 gal/d and 2.2 to 3.5 feet for pumpage of 10,000 gal/d. As little is known about the extent of contamination under New O-Field, no conclusions could be drawn as to whether this would intercept the bulk of the contamination. New O-Field simulations at these rates did not show inducement of infiltration of creek water but the proximity of the hydraulic grade reversal to the creek implies that infiltration would probably be induced if a 5800 gal/d per well pumping rate was maintained during dry summer months.

If no remedial actions are taken at O-Field, the simulations indicated that mobilization and transport of organic and inorganic contaminants will continue, primarily because the seasonal and recharge induced water levels rise above the base of the buried contamination. The ground water contaminants, in turn, will continue to discharge to Watson Creek. If the contaminants in the creek attain sufficient concentrations, then the depletion mechanisms in the creek may be inadequate to prevent contaminant migration from the creek into the Gunpowder River.

Strengths And Interesting Features Of This Study:

In this case study, a model was applied in the early phases of a site investigation to assist in characterizing the contaminant releases and plumes, the future migration of contaminants and to explore and screen potential remedial alternatives. Because of the hazards associated with sampling at this site, only limited hydrogeologic data was available when the modeling began. Perturbations in the ground-water system caused by tidal induced changes in the elevations of the surrounding surface water bodies further complicated the modeling. Nevertheless, data acquired after this modeling was completed confirmed the general flow field and the surface water and ground-water interactions predicted by the model.

A major effort was made to ensure that the model application would accurately predict the system response during both the average and the extreme hydrogeologic conditions found at the site. Specifically, the model was calibrated against two different sets of observed conditions; one representing average annual head observations, the other representing a period of time when significantly higher than average heads were observed. The calibration continued until the model application accurately predicted system response under both sets of conditions.

This modeling effort quantified the impact of the hydrogeologic uncertainty upon the results of the simulations. Alternative solutions to the steady state model application were developed by increasing and decreasing recharge and horizontal hydraulic conductivity within ranges defined by field measurements and professional judgement. These alternative solutions closely matched the observed heads, and therefore, were judged to bound the set of reasonable representations of the ground-water system. In turn, these alternative representations of the system were used to bracket the range of system responses to the remedial alternatives evaluated.

An analysis of the sensitivity of the calibrated model application to changes in hydrogeologic parameters was also performed. As a part of this analysis the sensitivity of the model predictions to modeling the site as a two layer system was investigated. The sensitivity analysis indicated that the two-layer representation was sufficient for the purposes of the study.

The model application provided the EPA Region with the framework for selecting the most appropriate remedial alternative. It provided guidance in determining the goals and objectives of the remediation effort. Based upon the results of the modeling described in this case study, ground-water extraction was selected as the preferred remedial action. The model application was subsequently used to evaluate alternative extraction systems.

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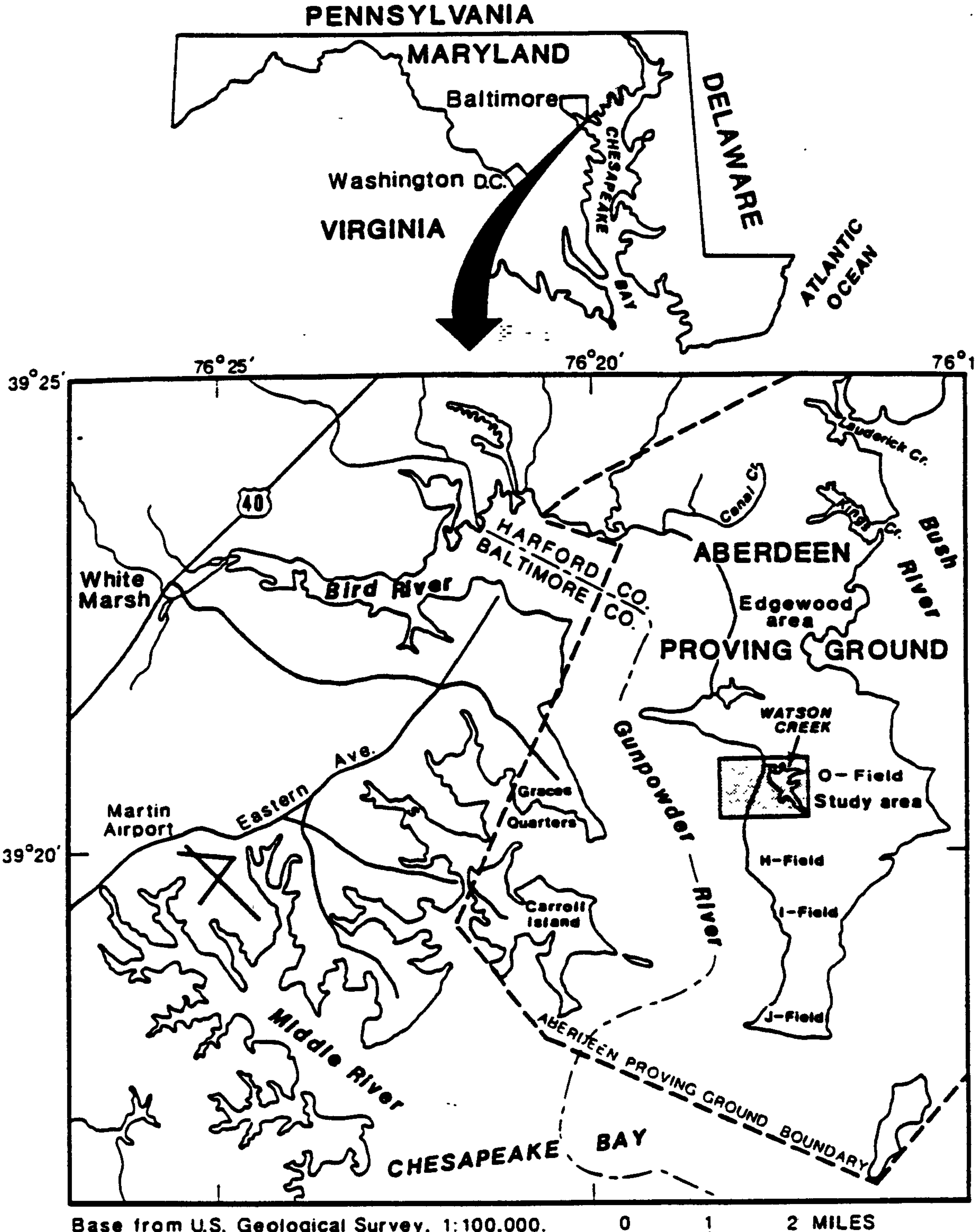
Modeling Documents:

Please contact the above people for specific modeling documents.

Figure 3.2-1

Site Location



Base from U.S. Geological Survey, 1:100,000.

Figure 3.2-2

Detailed Site Location

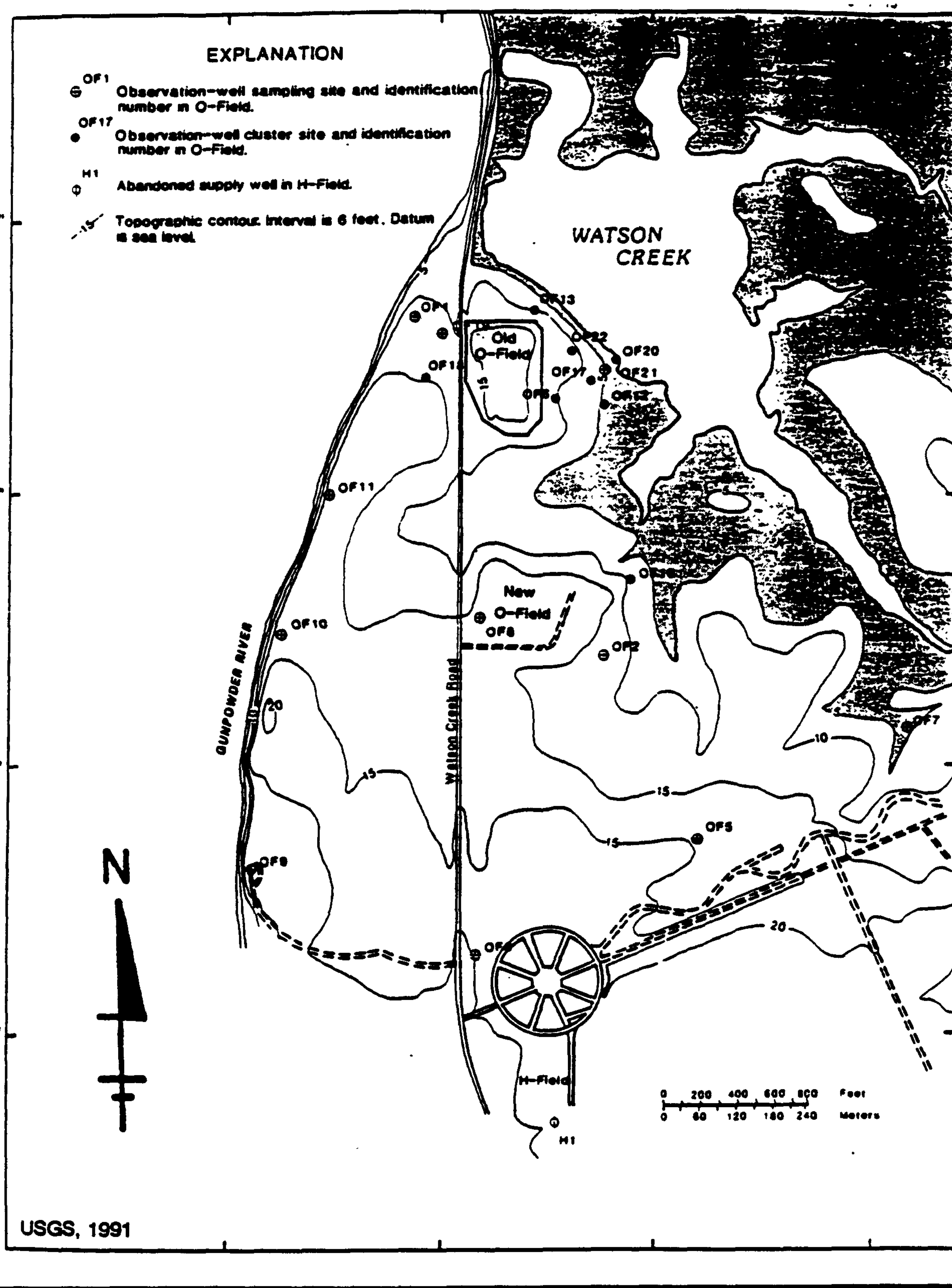
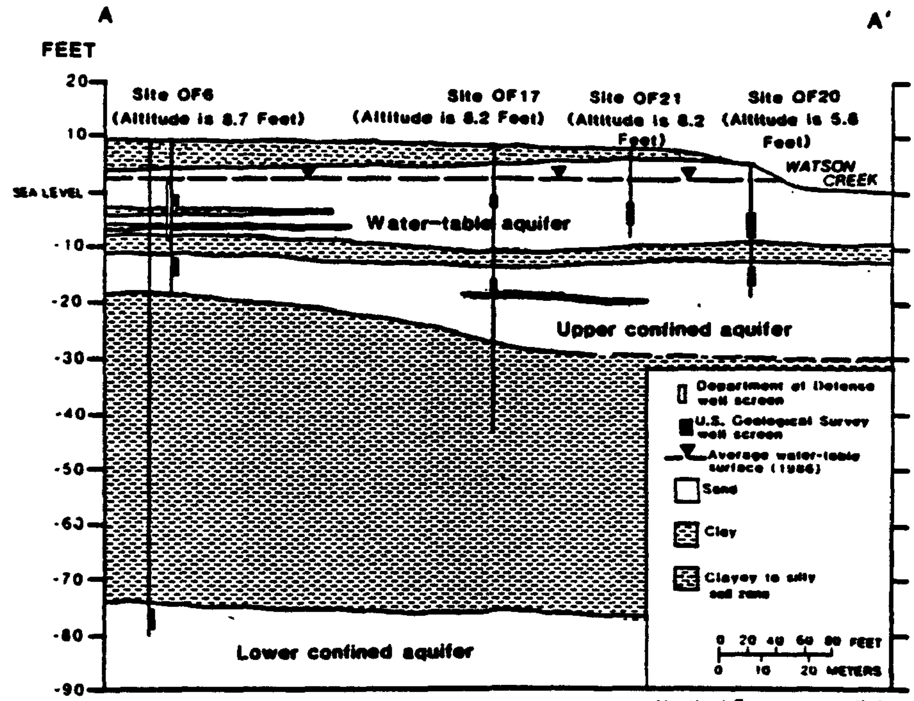
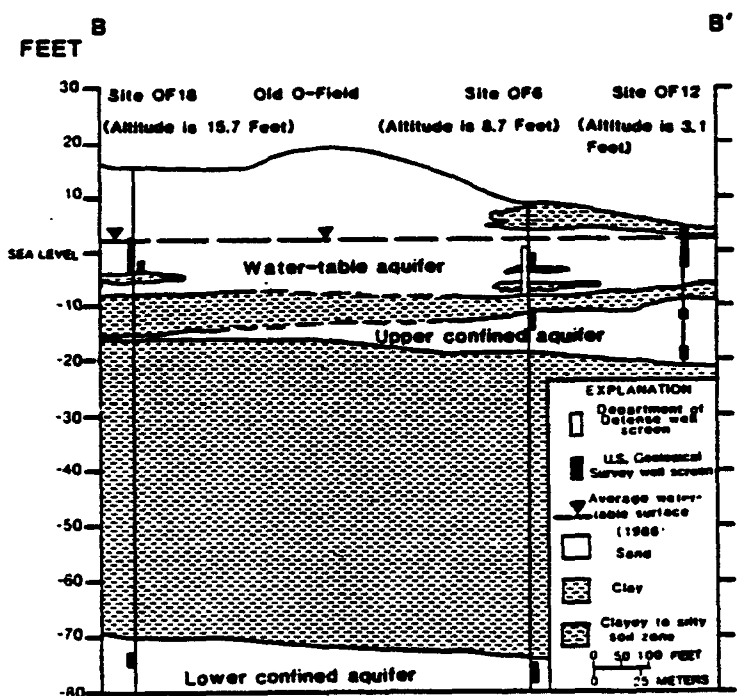


Figure 3.2-3

Sample Hydrogeologic Sections



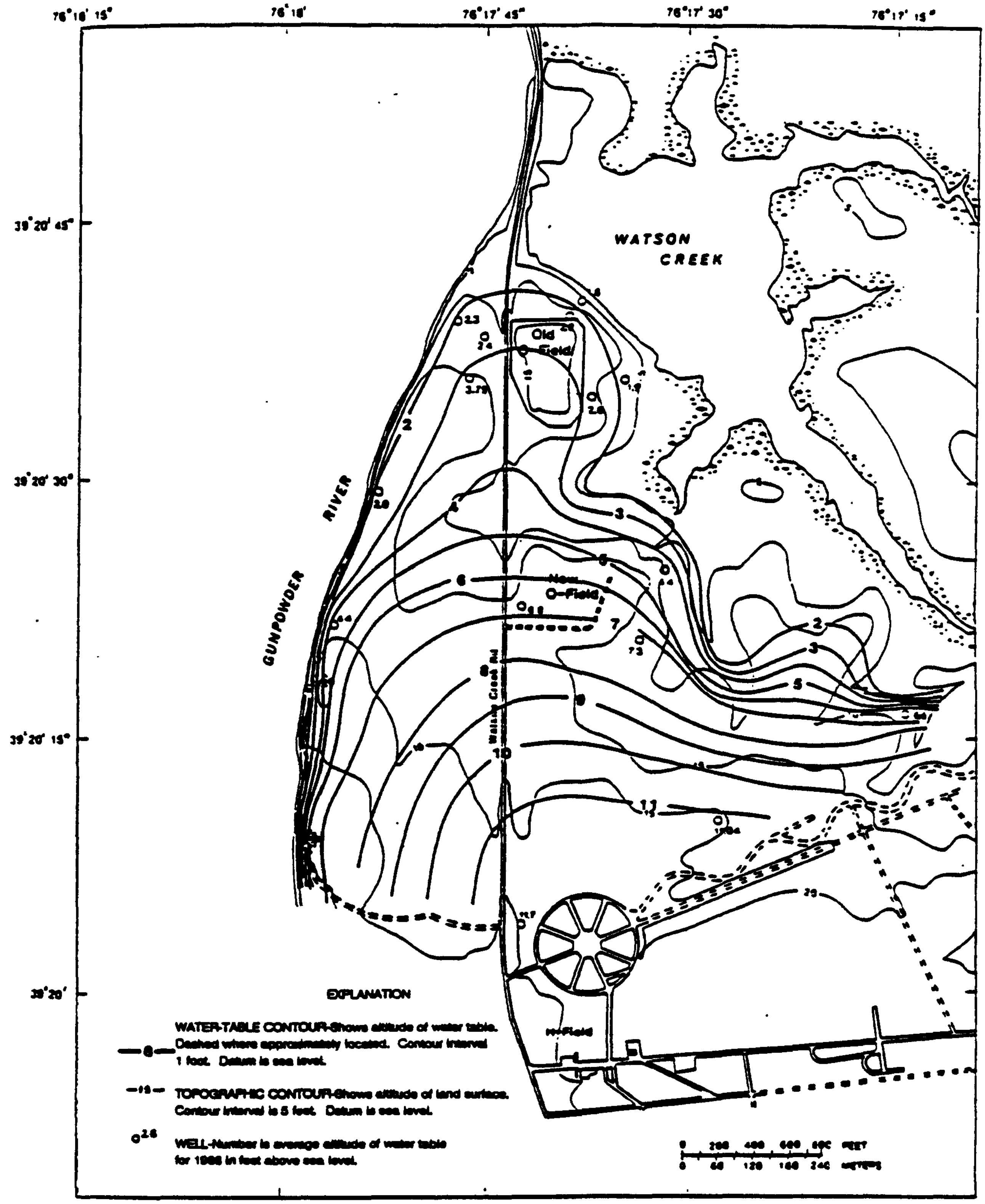
HYDROGEOLOGIC SECTION A-A' Vertical Exaggeration X 4



HYDROGEOLOGIC SECTION B-B' Vertical Exaggeration X 10

Figure 3.2-4

Site Water-Table Contours



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3.3 - Summary Description #3

3.3

Model Applications
Summary Description #3

Decision Objective:

This fund-lead site was modeled during the Remedial Design (RD) to ensure an appropriate design while minimizing design costs. Specifically, additional information on the ground-water flow and contaminant fate and transport was required to design a ground-water extraction and collection system that had been specified in the Record of Decision (ROD). The EPA contractor proposed additional field investigations including an extensive drilling program to obtain the needed design information. EPA suggested that much of the required information could be obtained through the use of ground-water modeling, thus significantly reducing design costs. The contractor agreed to the modeling effort and specific modeling objectives were established. These objectives were to:

1. Delineate the maximum possible extent of the contaminant plume in January 1993, when the pump and treat system is scheduled to begin operation;
2. Estimate the mass of contamination per unit volume of the aquifer;
3. Conceptualize extraction well alignment designs; and
4. Evaluate the design alternatives.

An EPA contractor working under an Alternative Remediation Contracting System contract did the modeling that is the subject of this case study. The EPA project manager reviewed the modeling work.

Background:

This is a six acre site located in a 250 home residential area with homes within 100 feet of the site. (See Figure 3.3-1.) Other land use in the area includes some commercial development along a state highway southeast of the site and agricultural activities southeast of the same highway. The site is an inactive manufacturing facility and is currently used for minor non-production activities, primarily warehousing. Located on the site are process, office and warehouse buildings. (See Figure 3.3-2.) A tank farm and a laboratory have been removed from the site. The site topography is relatively flat but exhibits occasional low rises and gentle depressions. The average annual precipitation is approximately 35 inches and the mean monthly temperatures range from 26° F to 72° F.

This site was used to manufacture and repackage non-lubricating automotive fluids from the early 1960s to 1978. During the facility's operation, a number of releases and a major fire contributed to the site contamination. Undocumented releases of chlorinated hydrocarbons into the vadose zone occurred south of the process buildings. Documented releases of diethyl ether occurred in 1972 when an underground pipeline was ruptured during excavation. Chlorinated organics, benzene and other solvents were released during a two day fire in 1978. During this fire numerous tanks and drums ruptured and their contents were spread onto unpaved areas by the water used to fight the fire. The unsaturated zone soil was thought to be the primary remaining source of contamination at the site.

History of Investigation

The owner of the site installed six on-site monitoring wells in 1972. Contaminant levels detected in these wells and nearby residential wells indicated that the contamination was moving off-site. Consequently, under an agreement with the state agency responsible for environmental protection, the owner began supplying bottled water to homes with contaminated wells in 1973. After the 1978 fire, the owner began removing underground tanks. Then in 1980, 15 more monitoring wells were installed at 9 locations. In 1982, the state agency initiated legal actions against the site owner to force site remediation. The following year the owner began operating a ground-water treatment system.

The site was placed on the National Priorities list (NPL) in 1984 and at that time EPA assumed the lead enforcement role. In 1985, the owner agreed to fund a remedial investigation and feasibility study (RI/FS) under an Administrative Order of Consent. The completion of that study was funded by EPA when the owner filed for bankruptcy in 1986. The state, in 1986, extended a public water supply to the residents in the area near the site. In 1988, the ground-water treatment system was closed down by the site owner due to financial problems.

In 1988, the Record of Decision (ROD) was issued. The ROD specified soil and ground-water remediation including a contaminated soil flushing system, a ground-water extraction and collection system and a ground-water treatment (air stripping) and discharge system. The ROD further specified that the aquifer within the 1.5 parts per billion contaminant concentration isopleth would have to be restored to drinking water standards.

Geologic Summary:

This site is located in an area dominated by glacial sediments deposited in a northeast-southwest trending belt. The two major types of deposits are glacial outwash with post glacial alluvium and ice-contact outwash deposits. Both types of deposits contain fine sand to coarse gravel with occasional large cobbles and are very poorly sorted. Sixteen borings made in the vicinity of this site indicate that the glacial sediments extend to an average depth of 117 feet below the surface. Underlying the site are clay, silty sand, sand and gravel facies which laterally intergrade with one another and result in laterally discontinuous layers.

The uppermost soils at the site consist of a 5 to 10 foot upper layer of fine sand and a lower 115 to 125 foot sand layer. (See Figures 3.3-3 and 3.3-4.) Underlying the lower sand layer is a 20 to 25 foot clay layer and then a layer composed of sands and gravel with occasional minor clay lenses. One boring on the eastern boundary of the site indicated the presence of a five foot silty clay layer just below the upper fine sand layer. This silty clay layer was presumed to be a very small localized lense as no other borings showed evidence of this layer. A large clay lense, however, begins just east of the site 50 feet below the ground surface. This lense extends over 3000 feet to the west and rises to thirty feet below the surface. It reaches a maximum thickness of 20 feet. Several small gravel beds where detected also in the lower parts of the lower sand layer.

Ground-Water Hydrology Summary:

The site hydrogeology is composed of three distinct hydrogeologic units. The uppermost unit is an unconfined aquifer that is encountered at approximately 30 feet below the ground surface with a saturated thickness of 70 to 90 feet in the site area and increasing to a thickness of 135 feet just over a mile and a half to the west. This aquifer corresponds to the lower sand layer discussed previously. The second hydrologic unit, a confining layer of sandy clay that varies between 7 and 22 feet in thickness near the site but thins to a two foot thickness a mile to the west, lies below the aquifer. The third hydrogeologic unit, a confined aquifer, whose confined head is approximately one and one half feet lower than the head of the upper aquifer lies below this confining layer. This lower aquifer corresponds to the layer of sands and gravel with occasional minor clay lenses discussed above. The thickness of this confined aquifer is unknown as none of the borings reached bedrock.

The upper unconfined aquifer is no longer used as a drinking water supply in the immediate site area because of contamination. Two miles to the west of the site are three municipal wells which produce more than a million gallons per day from this aquifer. The cone of depression caused by the operation of these wells may eventually enhance the off-site movement of contaminated ground-water towards the west. The direction of flow in this aquifer is generally west-southwest with a velocity of approximately 0.5 feet per day. Both pump and slug test data were used to estimate the hydraulic properties of this aquifer. The pump test data indicated an average aquifer hydraulic conductivity and transmissivity of 0.0775 cm/sec. and 148,000 gpd/ft, respectively, assuming an average aquifer thickness of 90 feet. The slug test data indicated an average aquifer hydraulic conductivity and transmissivity of 0.0489 cm/sec. and 98,000 gpd/ft, respectively.

The lower confined aquifer was not extensively studied for the purposes of remediating this site because of: (1) the presence of the confining layer above the aquifer, (2) prior sampling which indicated no presence of contamination in the lower aquifer and (3) the relatively small difference in head between the two aquifers.

Ground-Water Contamination Summary:

Eighteen contaminants were found at the site, with ten being selected as indicator compounds. These included 1,1-DCE, 1,1-DCA, 1,1,1-TCA and Benzene. The Remedial Investigation (RI) identified the unsaturated zone underlying two areas of the site as the major sources of contamination. The RI also speculated that there was potentially one other on-site source and several additional off-site sources of contamination based upon the location and discontinuity of the contaminant plume. This plume begins beneath the site and extends west-southwest beyond the site property boundaries. The plume may not be continuous within its boundaries and the thickness of the plume diminishes as it extends off-site. The contaminated zone reaches the bottom of the upper aquifer at the site and at a minimum extends 1500 feet downgradient .

The on-site ground-water contamination was being partially contained by two purge wells that operated from 1983 to the spring of 1988. These wells had a combined pumping rate of 200 gallons per minute which resulted in a maximum drawdown of about one foot. When these wells were operating they apparently contained the plume within the western and northern site boundaries. Since they ceased operation, significant additional contaminant migration has occurred.

Modeling Summary:

Analytic and analytic/numeric models and graphical techniques were used to investigate the site and to evaluate the effectiveness of ground-water extraction alternatives. This approach was chosen after a review of project objectives, the limited quantity and poor quality of the available field data, the modeling budget and project time constraints.

The modeling was divided into three phases. The objective of the Phase One modeling was to determine the maximum extent of contamination in the upper aquifer. An analytical function driven variation of the fate and transport model Random Walk and the analytic transport model PLUME were used in this phase. The objective of the Phase Two modeling was to conceptualize remedial design alternatives. Graphical Javandel type curve analysis procedures were used to determine the minimum number of pumping wells, discharge rates and recovery well locations under different pumping scenarios. Then time related zones of capture for each alternative were determined using the the U.S. EPA Wellhead Protection Area Model (WHPA). Finally, the aquifer drawdown resulting from each alternative was simulated using the analytic ground-water flow model WELFLO. The objective of the Phase Three modeling was to evaluate the most promising remedial design alternatives. Again, Random Walk was used in this phase to: (1) estimate the discharge rates, average concentration and mass of contaminants in the extraction well discharge; (2) evaluate and compare the remedial alternatives and (3) identify areas of uncertainty in design features. This case study will focus on the use of the Random Walk model in phases one and three.

The analytical function driven variation of the Random Walk model was chosen, based on the advice of an outside consultant, to verify the results of the PLUME model. Random Walk was suggested because of the modeling objectives, data limitations and the outside consultant's detailed familiarity with the model. This version of the Random Walk model utilizes an analytic function based upon the Theis equation to generate the flow field. The numeric Random Walk model is applied to simulate the fate and transport of the contaminants.

The simplifying assumptions associated with the analytic flow component of the Random Walk model required that the aquifer be treated as homogeneous, isotropic and infinite in areal extent. Thus, no site-specific boundary conditions or spatial variability in aquifer characteristics could be modeled. Moreover, unidirectional, steady state ground-water flow had to be assumed. The modeling team established a uniform hydraulic conductivity, saturated thickness, transmissivity, hydraulic gradient and aquifer porosity for the modeled area based upon information obtained from the RI report and field data.

For the Phase One modeling, three contaminants were originally selected: the most toxic (1,1-DCE), the most mobile (1,1-DCA) and the most pervasive (1,1,1-TCA). However, initial modeling efforts indicated that insufficient soil and ground-water data were available to develop or calibrate contaminant transport models for 1,1-DCE or 1,1-DCA. As 1,1,1-TCA had migrated and persisted farther downgradient than the other contaminants the modeling team felt that focusing solely on 1,1,1-TCA was valid and appropriately conservative.

The site conceptual model developed by the modeling team hypothesized that the downgradient plume developed primarily through the dissolution of 1,1,1-TCA retained in aquifer pores at residual saturation. This was in contrast to prior studies of the site which suggested that the major contaminant source lay in the unsaturated zone and was percolating into the saturated zone. Initially, the modeling team had accepted this latter hypothesis and developed a batch flushing model to simulate the migration of the contaminant into the saturated zone. However, when the results of the batch flushing model were compared with observed phenomena, there were major discrepancies. For example, only 2 to 4 percent of the contamination in the aquifer could be accounted for under this hypothesis.

After a careful review and some initial skepticism about the validity of the batch flushing model results, the modeling team hypothesized that the source term lay in the saturated zone. They searched peer reviewed ground-water literature for examples of similar conceptual models and found three. Then, additional site sampling including a soil gas survey was initiated. The results of this sampling indicated very limited soil contamination, thus further supporting the new hypothesis that the source term lay in the saturated zone.

The particle tracking component of the Random Walk model was then used to model the 1,1,1-TCA dissolution from the 1,1,1-TCA mass stored at residual saturation in the saturated zone. This included the rate of loading of 1,1,1-TCA from the unsaturated zone by percolation to the ground water, minus the mass removal of 1,1,1-TCA from the ground-water system, during the historic operation of the purge wells described previously. This approach resulted in a source term that varied as a function of time and dropped to zero during the historical operation of the purge wells. The longitudinal and transverse dispersivities, background concentrations, and organic carbon partition coefficients utilized in the model were based upon field data and established EPA methods. All ground-water contamination was assumed to exist in the dissolved phase; and, consequently, dense, nonaqueous phase liquid migration was not simulated. Biodegradation and volatilization was also ignored.

The calibration of the Random Walk model was restricted to the contaminant fate and transport component. This version of Random Walk assumes a unidirectional flow field which can not be directly calibrated against observed piezometric heads. Field data from the RI report was used to establish the flow field parameters. Calibration of the contaminant transport model was achieved by adjusting the flow direction, flow velocity and dispersivity until predicted concentration values matched observed concentrations. These modifications were within reasonable parameter ranges and in the case of the flow direction were based upon additional field data. The source release term was held constant during the calibration process.

The calibration of the model presented a number of challenges. First, the data used to calibrate the model was obtained from prior studies conducted by the site owner's contractors. A review of that data indicated numerous data quality problems including transcription errors, false positive and false negative indications, conflicting sampling dates and surface maps of conflicting scales. Second, data from nested monitoring wells indicated the presence of a vertical contaminant concentration gradient. However, the direction and magnitude of this gradient varied inconsistently from one monitoring location to another.

The modeling team established a two-tier calibration target after analyzing these constraints and the primary model objective, which was to predict the extent of the contaminant plume at the beginning of operation of the extraction system. For those wells where the field data indicated no contamination, the model would have to indicate no contamination. For those wells where field data indicated contamination, the model concentrations would have to be within one half an order of magnitude of the measured values at that location. Furthermore, at nested monitoring wells, the average of the measured values would be used for model calibration. The model was then calibrated against three different sampling events spanning an 8 year period utilizing field data from up to 19 wells.

Recognizing the limitations of the calibration data and in turn the calibration process, the contractor initiated a new round of sampling at 23 monitoring wells under stringent quality assurance procedures. This data was not available until the calibration of the model had been completed. The modeling team, however, was able to use this data to verify the model calibration. The success of this verification surprised the modeling team. With only one exception the model accurately simulated all wells where no contamination was detected. At those wells where field data indicated evidence of contamination, the residuals between the simulated and observed values were much closer than the one half order of magnitude calibration target used. Moreover, at the downgradient monitoring well that lay directly on the center line of the plume, the measured and simulated concentration value varied by only one part per billion.

Modeling Results Summary:

The Phase One modeling results indicated that the 1,1,1-TCA plume will have migrated 625 meters downgradient and 225 meters laterally by 1993. This migration has occurred in spite of the operation of two purge wells from 1983 to 1988. The modeling team was careful to note that they were more confident of the delineation of the plume boundary than the predicted concentrations within the plume because of model and data limitations.

Based upon these results, 15 extraction well alternatives were developed in Phase Two using Javandel type curve analysis, the GPTRAC module of the U.S. EPA Well Head Protection Area Model (WHPA), and the analytic model WELFLO. This analysis indicated that under ideal conditions only one extraction well discharging at 100 gallons per minute would be required. However, recognizing the limitations associated with the Phase One modeling and the models used in this second phase, two additional alternatives utilizing three and five wells respectively were chosen for further consideration in the Phase Three modeling. The location of the capture zone of one alternative is shown in Figure 3.3-5.

The efficiency, flexibility and the mass of contaminants in the extraction well discharges for these three alternative were then evaluated in Phase Three using the Random Walk model. The efficiency of each alternative was defined as a function of the pumping rate, the volume of water requiring treatment and the time required to restore the ground water to clean-up goals. While the pumping rates for the three alternatives were found to be very similar, the five well alternative was found to meet the cleanup goals in one quarter the time of the other two alternatives. The five well alternative, moreover, would significantly reduce the volume of water requiring treatment.

The flexibility of each alternative was defined as the ability of the alternative to operate efficiently when the actual aquifer response to the pumping varied significantly from the response predicted by the modeling. In particular, the modeling team was concerned about the possibility of unmodeled heterogeneity in aquifer properties and the distribution of contaminant concentrations within the plume. The five well alternative was again found to be the preferred alternative because it allowed the operation of each of the five extraction wells to be tailored to the specific characteristics of that part of the plume and aquifer within which the well was located.

EPA has awarded a contract for the construction of the five well ground-water extraction system developed as part of this modeling effort. This system is expected to be in place in early 1993. A ground-water monitoring program has been proposed which will allow the monitoring of the remediation progress and the ongoing validation of this ground-water modeling application.

Strengths And Interesting Features Of This Study:

In this case study, a model was utilized as part of the remedial design process. The modeling was initiated at the suggestion of EPA in order to reduce the magnitude and cost associated with additional site sampling. The model chosen represented a compromise between the level of detail and accuracy desired by the designers, the available data and the modeling budget. In fact, during the development of the modeling objectives, the modeling team attempted to use both a simple analytic and a finite difference contaminant transport model before abandoning the former for its lack of specificity, and the latter because of the limited site data available.

One of the more interesting aspects of this case is that both EPA and the contractor agreed that the modeling reduced the design costs by $450,000. Part of this cost reduction was due to the use of the model to delineate the plume boundary in lieu of locating the boundary by means of an extensive drilling program. The other part of the cost reduction occurred as a result of the modeling process which led to the identification of an error in the source characterization.

Previously it had been hypothesized that the source lay in the unsaturated zone. Consequently, soil flushing had been specified as a remedial action in the ROD. While trying to develop the source term for the model, the modeling team began to question this hypothesis. Based upon the results of a batch flushing model, a search of peer-reviewed literature for similar cases, and additional field sampling, the modeling team determined that the source term most probably lay in the saturated zone. Thus, the need for the design and implementation of the soil flushing system specified in the ROD was eliminated. This resulted in considerable design cost savings and will result in considerable additional construction and operational cost savings.

Another interesting aspect of this modeling was that the Phase One modeling was actually performed twice using two different models. First the site was modeled using PLUME. Then at the suggestion of an outside consultant the site was remodeled using Random Walk. There was a high degree of correlation between the model results. However, such correlation is not necessarily evidence that a site was modeled properly. Rather it demonstrates that for this same conceptual model, these two models produce very similar results.

Both EPA and the contractor noted that this case is another example of how the use of modeling early in the remedial investigation process could have improved the entire remediation effort. Specifically, it was noted that a very simple analytic model could have improved the sampling plan and monitoring well locations in prior site studies. This in turn would have increased the possibility that a more accurate numerical model could have been used during the design process, possibly resulting in a more efficient design.

<u>Contacts:</u>

For further information about this ground-water study please contact:

Bob Whippo	Region 5	Tel. # (312) 886-4759

<u>Modeling Documents:</u>

Please contact the above person for specific modeling documents.

Figure 3.3-1

Site and Contaminant Plume Location

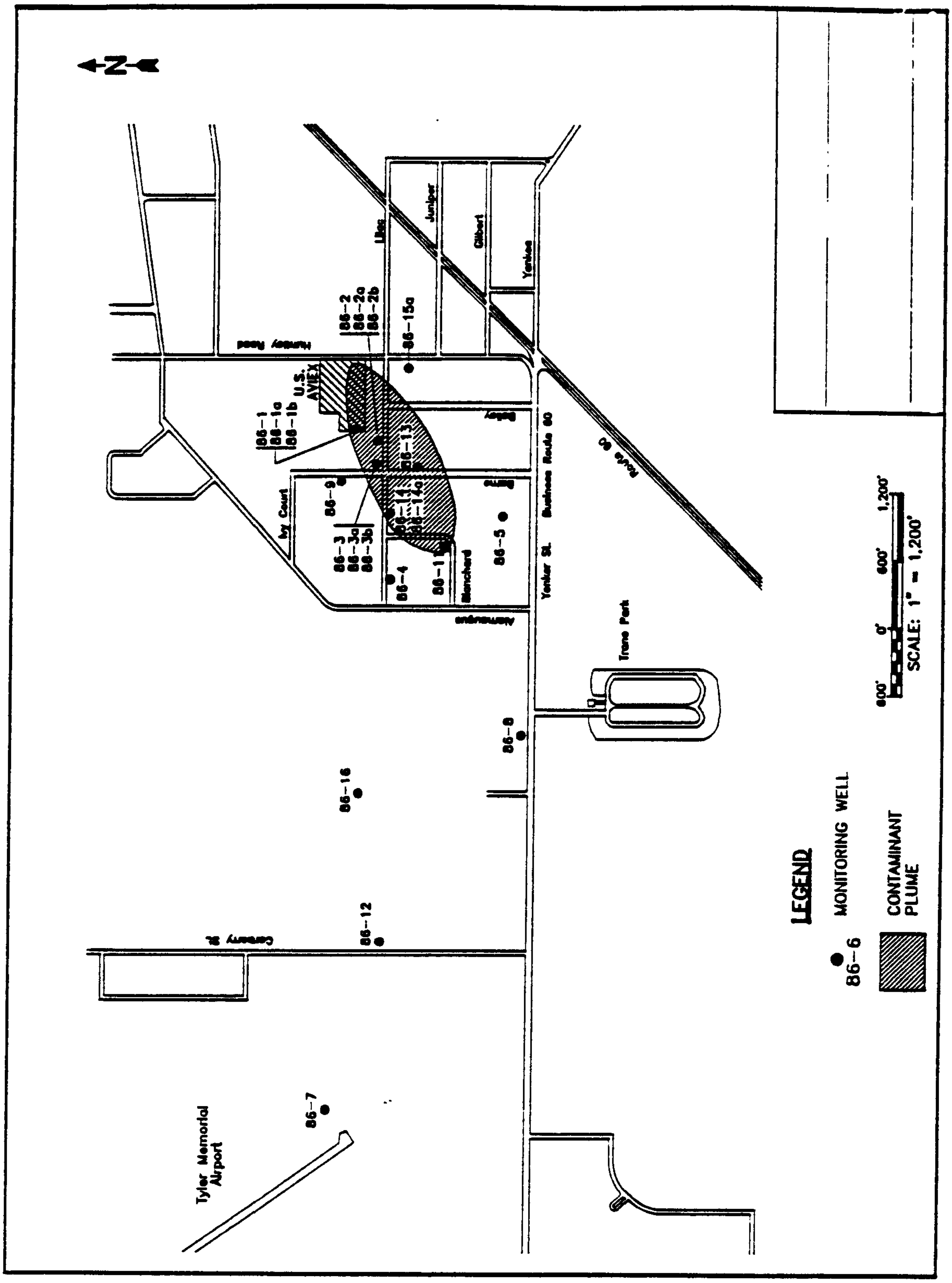


Figure 3.3-2

Detailed Site Location and Monitoring Wells

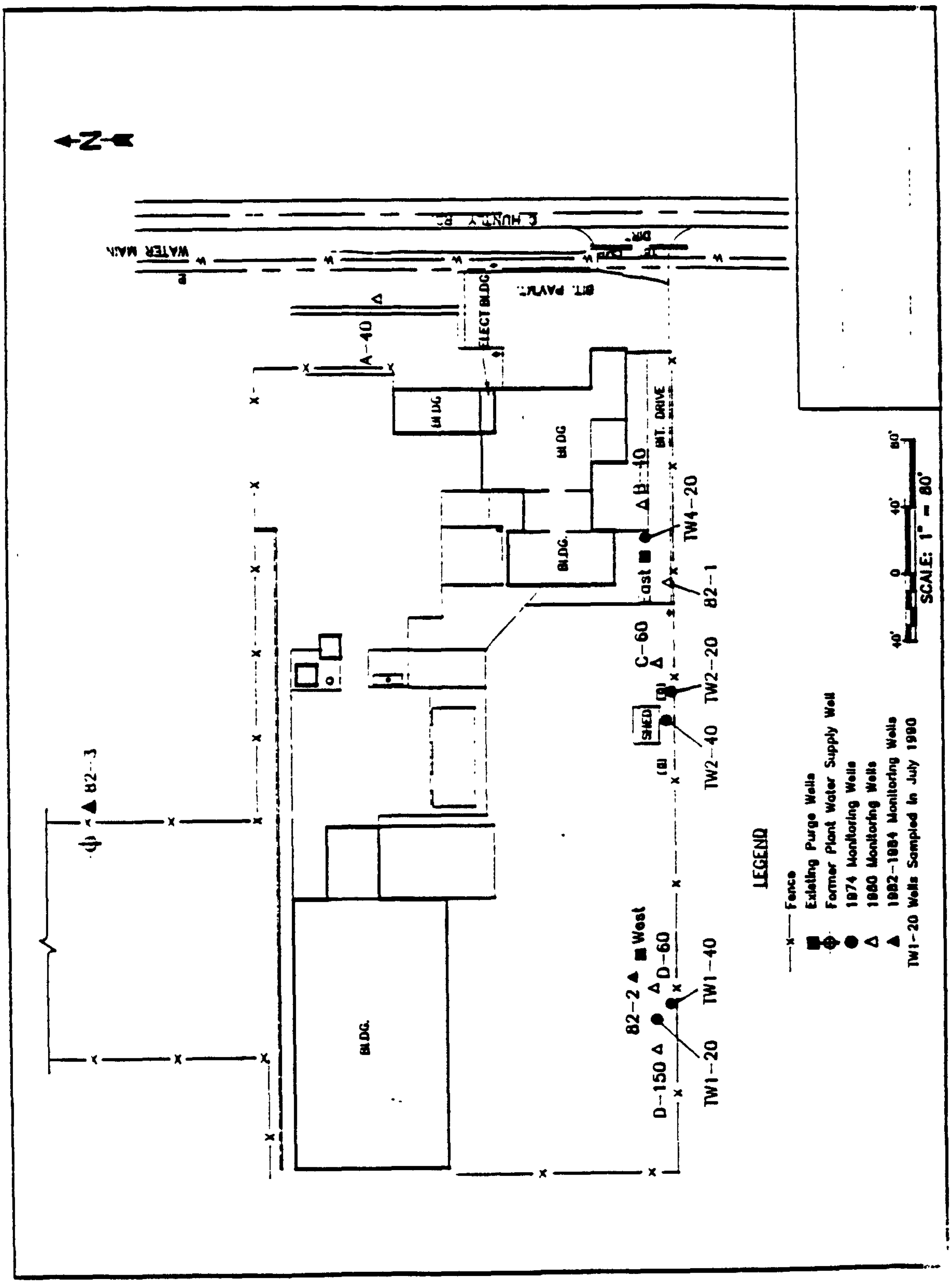


Figure 3.3-3

Sample Hydrogeologic Section

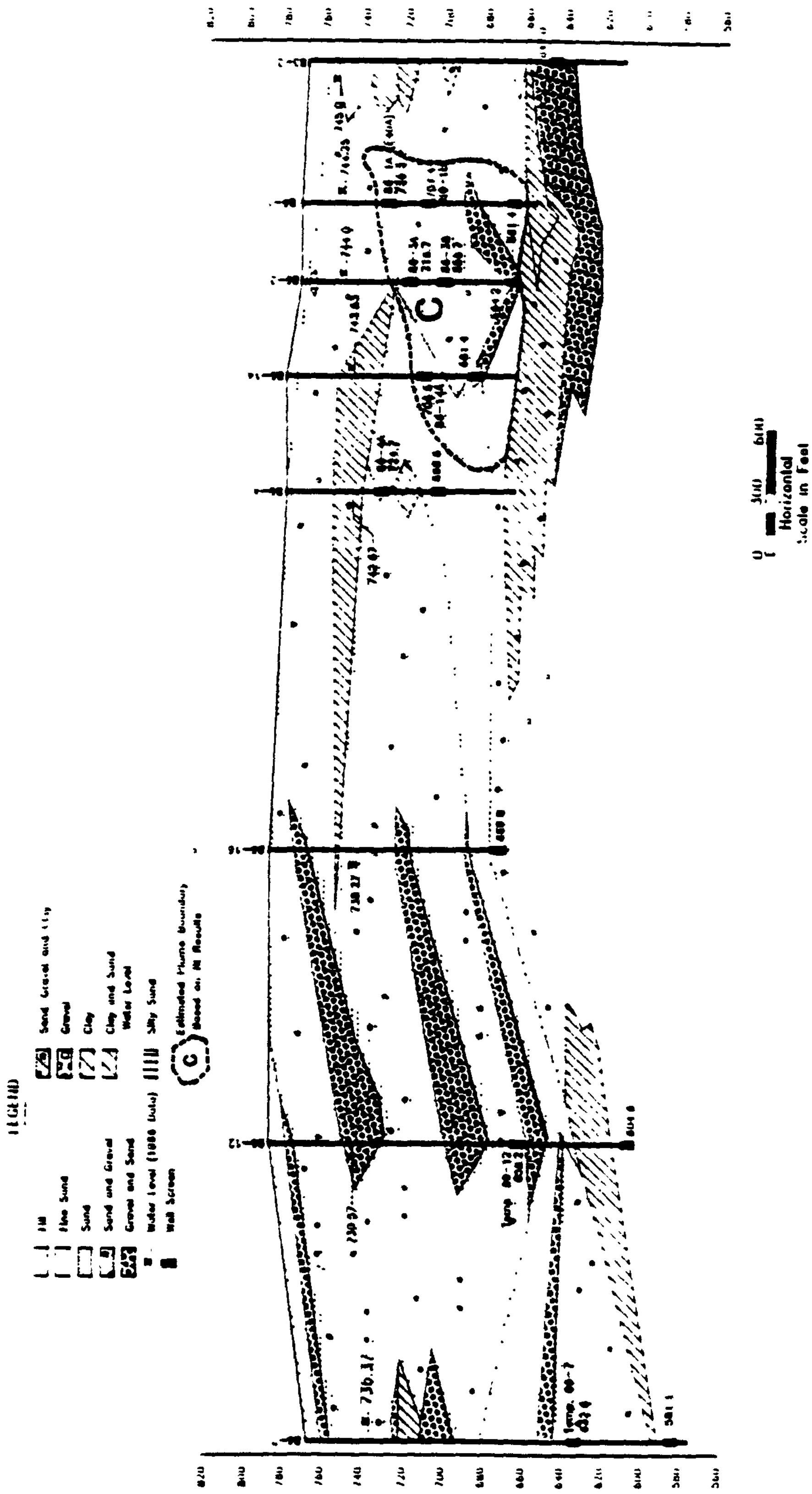


Figure 3.3-4

Location of Sample Hydrogeologic Section

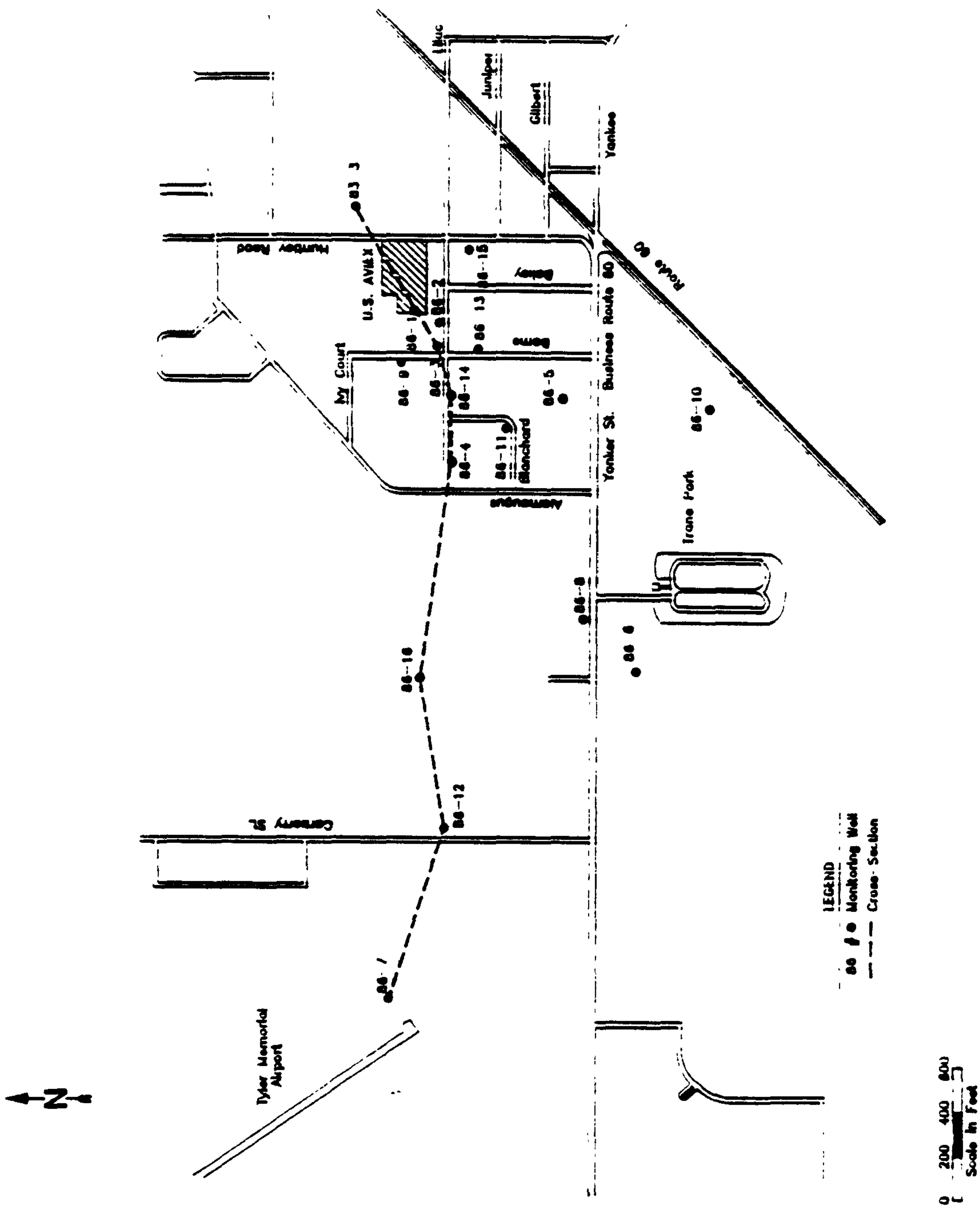
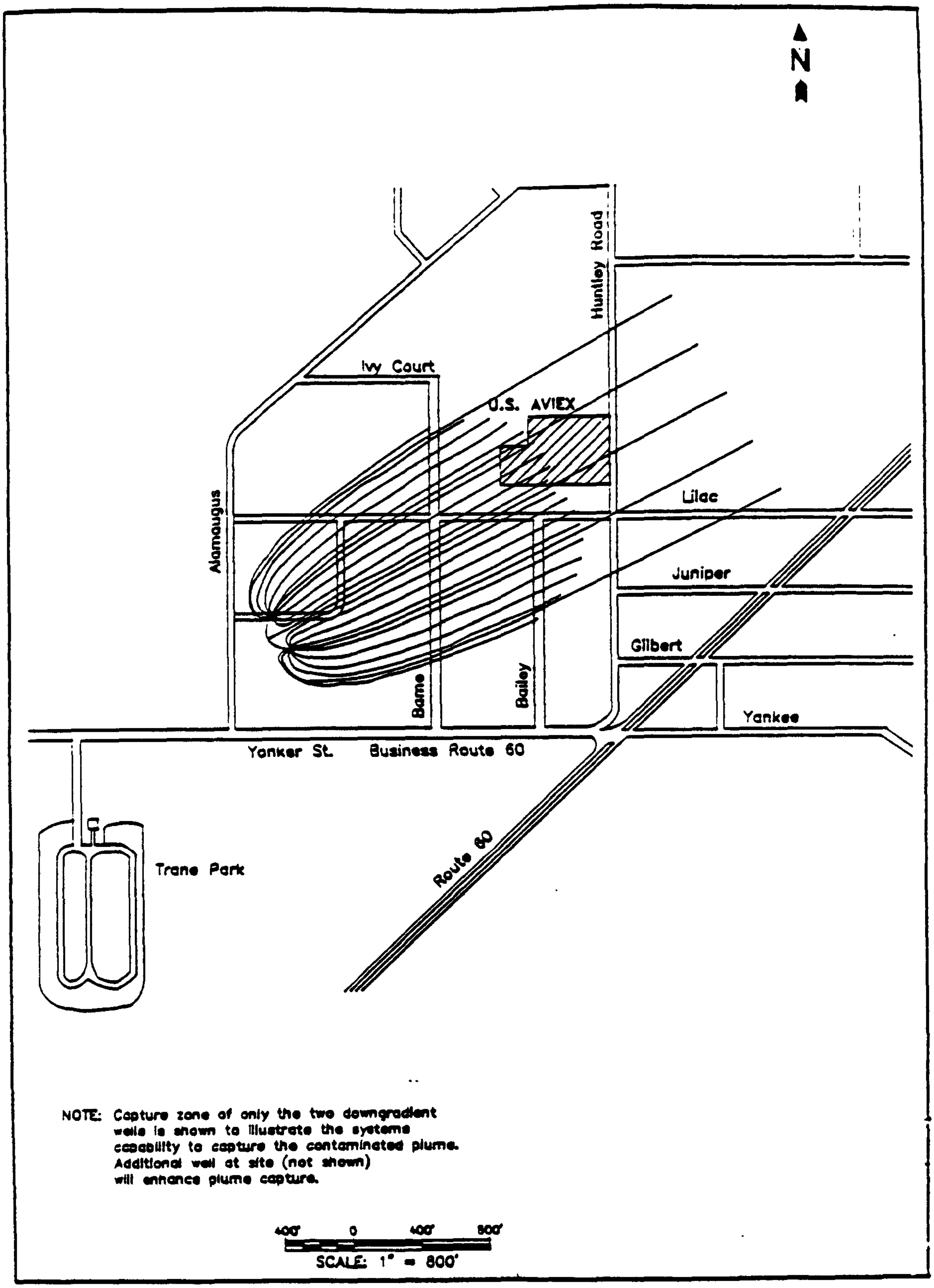


Figure 3.3-5

Capture Zone Analysis



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3.4 - Summary Description #4

3.4

Model Applications
Summary Description #4

Decision Objective:

This enforcement lead site was modeled by EPA during the remedial design (RD) to ensure an appropriate RD and remedial action (RA). Specifically, information on the ground-water flow and contaminant fate and transport was required to support RD and RA negotiations. As this was an enforcement lead site, the objective of EPA in conducting this modeling was to gather sufficient information to be able to review the responsible party's characterization of the nature and extent of contamination at the site and the remedial design.

The modeling was deemed necessary because it was recognized in the Record of Decision (ROD) that the design objectives and remedial action specified in the ROD were based upon incomplete knowledge of both the sources and the actual extent of the contamination and the contaminant plume. Consequently, EPA determined that a limited modeling effort would assist in better understanding the site and the effectiveness of the proposed pump and treat remedial design. In support of these decision objectives the following four modeling objectives were established:

1. Identify potential off-site contaminant migration;
2. Examine the proposed pump and treat extraction well alignment;
3. Improve (if necessary) the extraction well alignment design; and
4. Determine the time required to clean the site.

The modeling that is the subject of this case study was performed by an EPA contractor under a Technical Enforcement Support at Hazardous Waste Sites contract. The modeling work was reviewed by both the EPA project manager and an EPA hydrogeologist.

Background:

This site is comprised of 18 acres located in an industrial corridor adjacent to an interstate in a major western metropolitan area. The site abuts a major railroad line and is surrounded by other small industries. (See Figure 3.4-1.) Located on the site are abandoned and active tank farms and a filled and abandoned sump. There is also a capped evaporation pond, the contents of which are unknown. The site topography is generally flat and low lying with a vacant swampy area to the south. The nearest residential area is within a quarter mile of the site and the total population within a one mile radius of the site is less than 5000.

Operations at the site began in 1957 and included the production of herbicides and pesticides; the production of sodium hypochlorite; refilling and distributing chlorine and ammonia cylinders; and the packaging and distribution of acids, caustics and organic solvents. Information related to the historical operations at the site indicates that the uncontrolled release of contaminates may have begun in the very first year of operation and may have continued through 1989. These releases are believed to have been the result of both disposal practices and spills.

Examples of disposal practises that led to releases include: the use of unlined settlement and evaporation ponds for process wastewater discharge; the discharge of industrial and process waste materials to an on-site septic tank and drain field; and the dumping of wastewater, pesticide and herbicide tank wash water on the ground. Examples of spills included a 4000 to 8000 gallon spill of muriatic acid that occurred during the unloading of a rail tanker and a hydrochloric acid spill due to a tank rupture. Sources of contamination include the former evaporation pond which was filled with earthen materials and capped with concrete in 1980, a process drain system and sump, settlement ponds (location unknown), a leach field, dioxin removal wastes and contaminated soil.

History of Investigation

Beginning in 1980, the site was operated as a RCRA Interim Status Hazardous Waste Storage Facility. Between 1983 and 1989, the owner/operator of the site was cited for several violations by a state agency responsible for RCRA enforcement. In 1984, that agency advised the owner/operator of an alleged release from the property to the environment and then initiated a Preliminary Assessment and a follow-up Site Investigation. Additional field investigations were conducted by the state agency between 1985 and 1987.

In 1986, CERCLA enforcement activities were initiated. This led to an emergency action by EPA later that year to remove drums, cylinders and contaminated material from the site. In 1987, EPA proposed that the site be placed upon the National Priorities List. In 1988, the owner/operator agreed to undertake a Remedial Investigation/Feasibility Study (RI/FS) which was completed in March 1990. In 1989, the owner/operator notified the relevant agencies of its intent to close its RCRA Part A Interim Status Storage Facility. In 1990, additional site sampling was initiated under EPA's "Make Sites Safe" initiative. This sampling found evidence of high levels of dioxin on that part of the site where contaminated materials had been removed as part of EPA's 1986 emergency action. Consequently, actions to stabilize the contaminants on the site pending remediation were initiated.

In March 1991, the Record of Decision (ROD) was issued. In the ROD, EPA with the concurrence of the state, specified soil and ground-water remediation measures at the site but reserved the right to further modify the ground-water remedy because the ground-water contamination had not been fully characterized. The ground-water remedy specified consisted of a pump and treat system utilizing approximately ten wells to capture and treat the contaminant plume. These wells were proposed to be located along the northern and western boundaries of the site and to be operated at an extraction rate of two gallons per minute.

Geologic Summary:

This site is located in a valley that was part of a Pleistocene great basin lake. The surficial geology of the valley is the result of successive expansions and contractions of that great basin lake and glacial surges and retreats. The valley consists of alluvial deposits which overlie and merge with deep, unconsolidated lacustrine sediments. The alluvial deposits typically consist of silt and sand in the first several feet and mostly fine pebble gravel to a depth of 5 feet or more. These deposits are of a deltaic type and are associated with the development of the valley drainage network. The underlying lacustrine deposits consist of clay, silt, sand and gravel facies that laterally intergrade with one another and result in laterally discontinuous layers.

The uppermost soils at the site consist of a 2 to 6 foot layer of mixed fill material and a 2 to 5 foot layer of clay to silty clay material beneath the fill material. Underlying the clay material is a sand to clayey to silty sand layer that extends to a depth of 15 to 18 feet and below this point a clayey layer begins. Two borings to depths of 27 and 50 feet indicated that this clayey layer extends to at least a depth of 50 feet and exhibits interfingering (clay, silt and sand) characteristic of the general geology of the valley. A fluvial paleochannel consisting of fine to coarse grained sand appears to meander across the center of most of the site. The top of this channel lies 7 to 9 feet below the surface of the site and the channel is approximately 6 to 8 feet deep.

Ground-Water Hydrology Summary:

There is some disagreement regarding the ground-water hydrology. Prior studies by the responsible party's consultants indicated that the site hydrogeology is consistent with the regional hydrogeology and is composed of three distinct hydrogeologic units. These studies indicated that the uppermost unit is a shallow unconfined aquifer that begins 3 to 5 feet beneath the site and extends to a depth of 15 to 18 feet. This aquifer corresponds to the sand to clayey to silty sand layer discussed in the above paragraph. Below this shallow aquifer lies the second hydrogeologic unit, a relatively impermeable confining layer which acts as a single confining bed that ranges from approximately 40 to 100 feet in thickness. This unit corresponds to the clayey layer described in the above paragraph. Below this confining unit lies a confined aquifer that consists of Quaternary deposits of clay, silt, sand and gravel. The maximum thickness of this aquifer is greater than 1000 feet.

The state agency responsible for environmental enforcement disagrees with the concept that there are two completely distinct aquifers underneath the site. They take the position that the second hydrologic unit is not truly impermeable as there are interfingerings of sand and silt in the clay layer. Consequently, they believe that there is communication between the upper and lower hydrologic unit and all three units should be considered as one aquifer with shallow and deep portions. The modeling team did not feel it was necessary to resolve this discrepancy in the conceptual model given EPA's decision objectives and the fact that the modeling focused solely on the upper 13.5 feet of the shallow aquifer.

The shallow unconfined aquifer is not used as a drinking water supply because of its poor quality (e.g. high total dissolved solids, sulfide and chloride) and the low yields to wells. The direction of flow in this aquifer is generally to the west-northwest, which is consistent with the regional flow direction. In the late summer there are several localized deviations in the flow pattern as several ground-water mounds build and dissipate. The transmissivity of this aquifer is estimated to be 77 ft^2 per day. The recharge to this aquifer is primarily from upward flow through the confining layer from the underlying confined aquifer and infiltration from irrigation, precipitation and a nearby drainage ditch. This drainage ditch which runs adjacent to the site is hydraulically connected to the shallow unconfined aquifer. In the spring this ditch appears to recharge the aquifer while during the summer that portion of the aquifer underlying the site appears to contribute 1.1 to 1.4 gallons per minute to the flow in the ditch.

The deep confined aquifer is a primary source of drinking water for the surrounding metropolitan area. Pumping tests from other studies indicate that the transmissivity of this aquifer ranges from 4000 to 10,000 ft^2. This aquifer was not extensively studied for the purposes of managing this site because of the presence of a thick confining layer above the aquifer and the upward movement of water from this aquifer to the shallow aquifer.

Ground-Water Contamination Summary:

A wide variety of contaminants was found at the site including VOCs, SVOCs, Pesticides, Herbicides, Dioxins and Furans. The major sources of contamination on the site include a process drain system, a former evaporation pond, a yard drain system and a septic system. The primary contaminants of concern in the ground water are the indicator chemicals TCE, PCE, PCP and 2,4-D. Ground-water samples from monitoring wells indicated that these contaminants exceed maximum contaminant levels (MCLS) as established under the Safe Drinking Water Act by up to three orders of magnitude. These contaminants are widely dispersed horizontally and vertically in the shallow aquifer underlying the site. (See Figure 3.4-1.) However, ground-water samples from monitoring wells below the shallow aquifer do not indicate that the contamination has extended into the confining layer separating the shallow aquifer from the deep confining aquifer.

At the time the ROD was issued, the extent and origin of the contaminated water found on the northern portion of the site had not been fully characterized. The ROD anticipated that further investigations and subsequent ground-water remediation decisions would have to be made prior to the initiation of remedial actions.

Modeling Summary:

A series of analytic and analytic/numeric models were used to investigate the site. An analytic modeling approach was chosen as a function of EPA's decision objectives and resource constraints. As this was an enforcement lead site, EPA's responsibility was to review the responsible party's remediation plan and activities to ensure they met regulatory and legal requirements. Thus, EPA's objective in conducting this modeling was not to develop a definitive remedial design but to gather sufficient information to be able to review the responsible party's characterization of the site and the RD.

New information, received since the issuance of the ROD, suggested the need for the RD/RA to address ground-water contamination not previously thought to be connected with the site. Evidence suggested that the plume in the shallow aquifer may have migrated off-site. EPA desired to explore this possibility and to examine its impact upon the proposed remedial design. As these were review and not design objectives, these decision objectives were not considered sufficient to warrant the costs associated with a full fledged numerical modeling effort at this stage in the remediation process. Moreover, EPA and their contractor believed that current data on the site was not sufficient to support a numerical model. Consequently, an analytic modeling approach was chosen.

The modeling was divided into two phases. The objective of the phase one modeling was to determine the maximum extent of chloride and TCE contamination in the shallow aquifer. An analytical function-driven variation of the fate and transport model Random Walk was used in this phase. The objective of the phase two modeling was to examine the effectiveness of proposed and alternative extraction well designs. Two models were used in this phase. The analytic flow model THWELLS was used to determine well field drawdown. Then the capture zones for the ground-water remedial alternatives were estimated using the particle tracking module of the U.S. EPA Wellhead Protection Area (WHPA) model called GPTRAC. This case study will focus on phase one of the modeling which is the use of the Random Walk model to delineate the contaminate plume and potential sources.

The analytical function-driven variation of the Random Walk model was chosen for the phase one modeling because of its relative simplicity, prior contractor experience and prior contractor verification of the model through a comparison of its results with that of another well-respected model. This version of the Random Walk model utilizes an analytic function based upon the Theis equation to generate the flow field. Then the numeric Random Walk model is applied to simulate the fate and transport of the contaminants.

The simplifying assumptions associated with the analytic flow component of the Random Walk model required that the aquifer be treated as homogeneous, isotropic and infinite in areal extent. Thus, no site specific boundary conditions or spatial variability in aquifer characteristics could be modeled. Moreover, unidirectional, steady state ground-water flow had to be assumed. The modeling team established a uniform hydraulic conductivity, saturated thickness, transmissivity, hydraulic gradient and aquifer porosity for the modeled area based upon information obtained from the RI report and the ROD. They assumed that there was no precipitation recharge to the aquifer.

Chloride was chosen as one of the two contaminants to be modeled because it is mobile and non-retarded. Thus, its plume would represent the outermost limits of the plumes of the other contaminants of interest. Moreover, since chloride is a conservative substance, it was hypothesized that the successful replication in the model of the existing chloride plume would be evidence that the simplifying assumptions of the analytic flow model did not unduly compromise the model results given EPA's decision objectives. TCE was selected as the other contaminant to be modeled because it is relatively toxic and ubiquitous to the site.

The particle tracking component of the Random Walk model was used to model the chloride releases as slugs that began in 1982 at four potential sources. The TCE releases were modeled as continuous releases that began in 1957 at eight potential sources. The location of the sources and the timing of the releases were inferred from soil and ground-water chemistry, information in the RI and the ROD and model calibration. The longitudinal and transverse dispersivities, background concentrations and organic carbon partition coefficients were based upon field data and established EPA methods. All ground-water contamination was assumed to exist in the dissolved phase and consequently dense, nonaqueous phase liquid migration was not simulated. Biodegradation and volatilization were also ignored.

The calibration of the Random Walk model was restricted to the contaminant fate and transport component. This version of Random Walk assumes a unidirectional flow field which can not be directly calibrated against observed piezometric heads. Field data from the RI report was used to establish the flow field parameters. Moreover, as was noted above, it was thought that the successful calibration of the chloride plume would serve as an indication of the appropriateness of the assumed flow field. Calibration of the contaminant transport model was achieved by adjusting the number, location and release terms of the sources until simulated concentrations matched field observations for twelve on-site monitoring wells. The calibration process was terminated when:

- The mean model error and standard deviation of errors were less than 10 percent of the largest observed field concentration;
- The regression analyses of field data versus model results yielded a correlation coefficient squared (r^2) value greater than 0.90, (an r^2 value of 1.0 indicates perfect correlation between the field data and the model data); and
- The shapes of the simulated plumes approximated the shapes of the plumes observed in the field.

The calibration of the contaminant transport model required that the grid nodes in the model be close to the physical location of the monitoring wells on the site. Considerable effort was made to do this, but in order to determine the predicted contamination concentrations at the monitoring wells, linear interpolation routines ultimately had to be developed In retrospect, the modeling team realized that by varying the location of the origin of the model grid, the grid nodes could have been located precisely over the monitoring well locations thus eliminating the need to interpolate the contaminate concentrations and possibly improving the calibration. It was noted, however, by the modeling team that the shifting of the grid would become very time consuming with a large number of wells.

Difficulties were encountered calibrating the model. These difficulties caused the modeling team to explore the possibility of the existence of undocumented on and off-site sources. In an iterative fashion, sources were added to the model until all calibration targets were met, the simulated plumes approximated the field observable plumes and r^2 values of 0.92 and 0.99 were obtained for the chloride and TCE models respectively. (See Figures 3.4-2 and 3.4-3.) The reasonableness of the location of these hypothetical contaminate sources was examined using site information and aerial photographs of the site taken in the 1960's and 1980's.

Interestingly, these photographs had not been available to the modeling team during the calibration process, yet wherever a hypothetical source had been introduced into the model in order to effect a better calibration, the aerial photographs provided confirming evidence of the existence of a potential source at that location.

Because of budget limitations a sensitivity analysis was not performed to determine the potential variations in the results as a function of changes in key parameters or the removal of hypothetical sources. In retrospect, the modeling team felt additional resources should have been requested to perform a sensitivity analysis.

Modeling Results Summary:

The phase one modeling results indicated that the ground-water contamination moved much further off-site than was estimated in the ROD. Moreover, the model simulations suggested the possibility of off-site sources of chloride and TCE contamination. (See Figure 3.4-4.) Specifically, the model indicated that the plume had migrated almost 450 feet north and a 150 feet west of the site and covered a surface area over 1/3 larger than the contaminant plume defined in the ROD.

Four potential chloride sources and eight potential TCE sources were identified. One of the chloride sources and three of the TCE sources were located off-site. None of these potential off-site sources had been identified in the ROD. Consequently, EPA's concerns about the completeness of the field characterization were supported by the modeling results.

The phase one results were then used to evaluate the proposed and alternative pump and treat extraction well designs. This evaluation (not part of this case study) determined that the proposed design of the pump and treat extraction wells would not fully capture the contaminant plume because the plume had migrated so far off-site. Moreover, it was determined that the proposed pumping rate would de-water the aquifer.

Based upon the information developed in this modeling effort, EPA directed the Responsible Party to initiate further site characterization including a search for additional off-site sources. The Agency also requested that the design of the extraction wells be reviewed. However, the Agency and the modeling team were careful to not assign certitude to the model results. As was stated in the modeling report, the simplifications associated with the use of analytic models and the limited field data available required that the results of this modeling effort be used with great care. Thus the Agency limited the use of the model results to:

1. Estimate the maximum downgradient and lateral extent of ground-water contamination;
2. Focus future field activities;
3. Provide insight into the location of additional potential sources; and

4. Provide preliminary ideas regarding the conceptual design of pump and treat alternatives.

Strengths And Interesting Features Of This Study:

In this case study, a model was applied late in the remedial process to review the completeness and accuracy of the site characterization and remedial design specified in the ROD. The decision and modeling objectives of this model application were carefully limited so as not to exceed the limitations of the model and available data.

Perhaps the most striking aspect of this case was that the entire modeling effort required only 180 hours. This was possible because the decision objectives of the modeling effort were limited in such a way that relatively simple models and simplifying assumptions could be used. Nonetheless, the information gained from the modeling could be used to guide field characterization activities and to raise significant concerns about the characterization of the site and the design of the proposed extraction wells. The ultimate consequences may be a considerable cost savings through the implementation of a more appropriate remedial design.

Another interesting aspect of this study was the use of the model to identify the location of previously undocumented potential sources of contamination and the post modeling corroboration through the use of aerial photographs. This is an example of the power of relatively simple models when they are carefully used as preliminary investigation tools.

In retrospect, the Region noted that it might have been useful to conduct this type of modeling during the RI/FS phase of the cleanup. The Region also noted that additional modeling might be required later, once the additional site characterization activities are completed. The Region suspected that should additional modeling be performed, the level of certainty they would then require would necessitate the use of a more sophisticated model and significantly more data.

Contacts:

For further information about this ground-water study please contact:

Bert Garcia Region 8 Tel. # (303) 293-1526

Modeling Documents:

Please contact the above person for specific modeling documents.

Figure 3.4-1

Chloride Concentrations

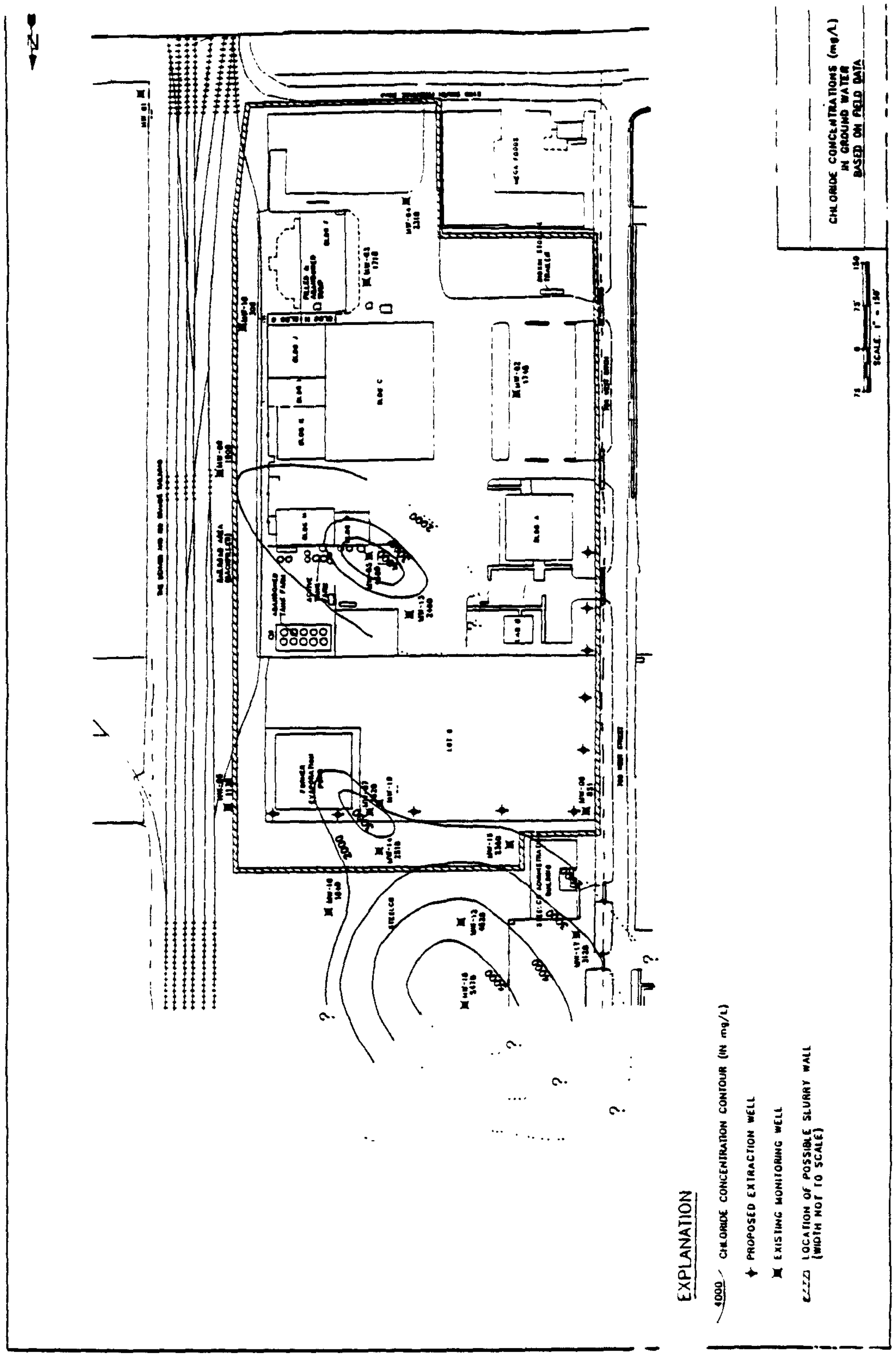


Figure 3.4-2

Location of Suspected Chloride Sources

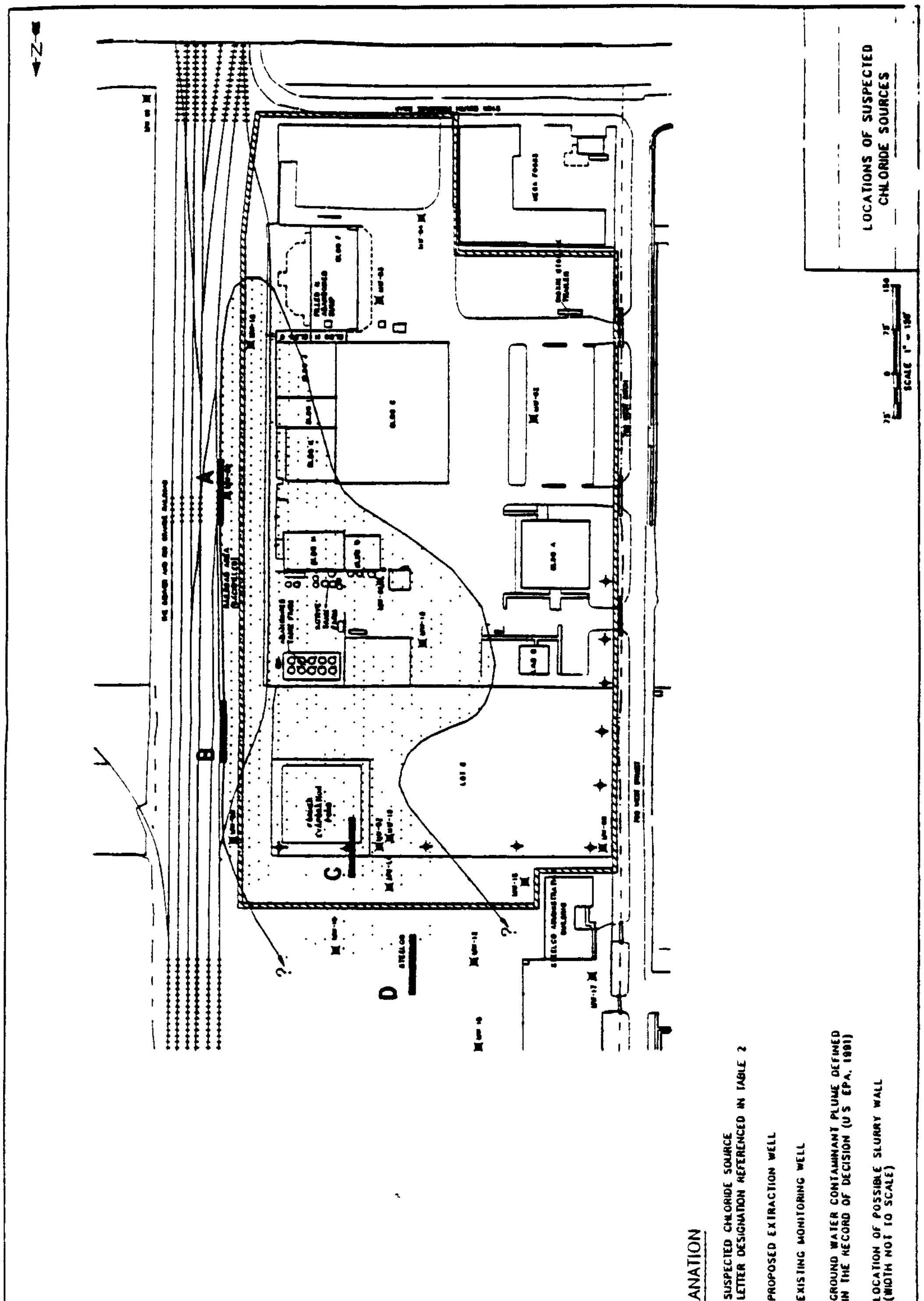


Figure 3.4-3

Model Calibration - Chloride

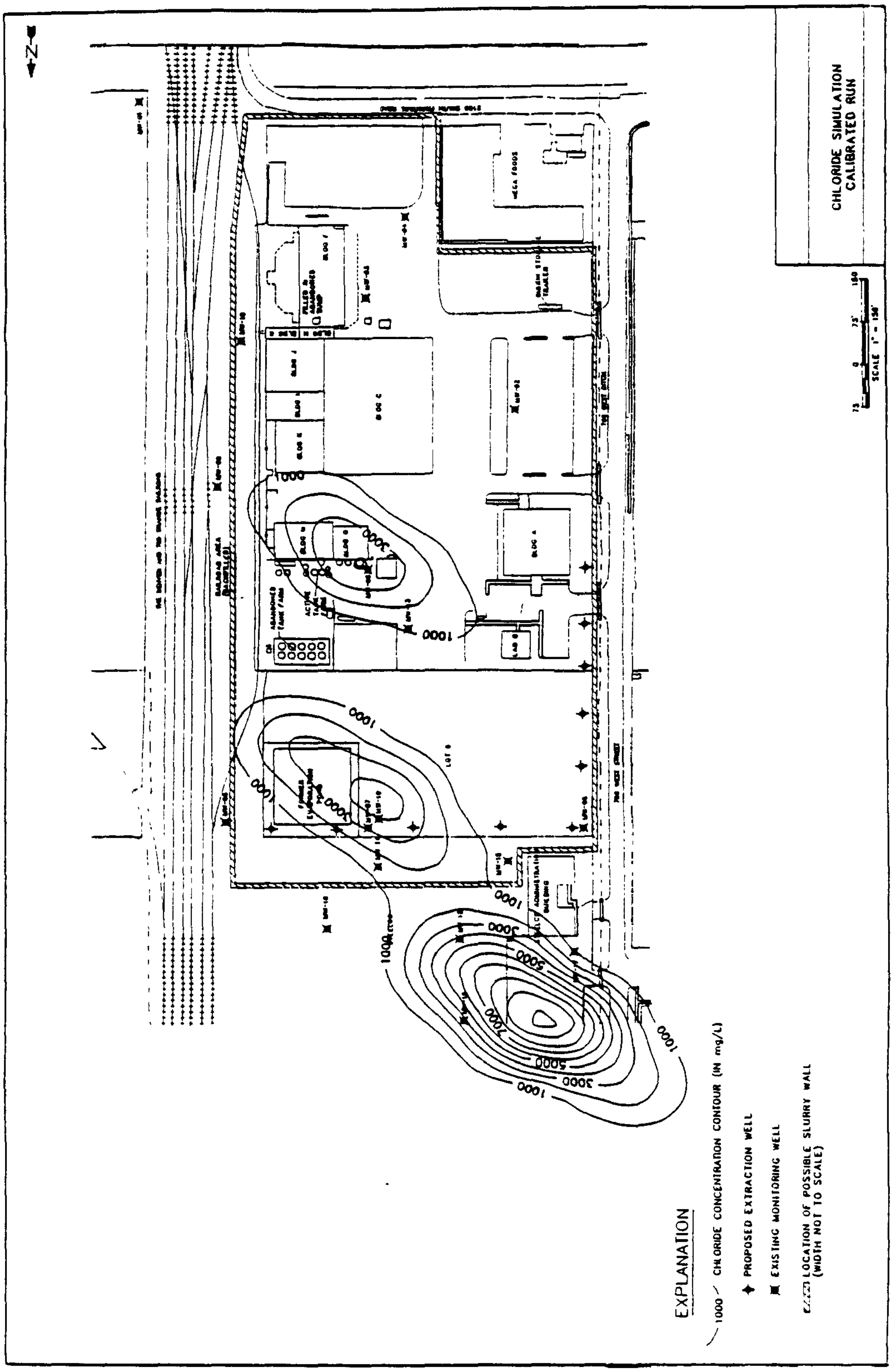
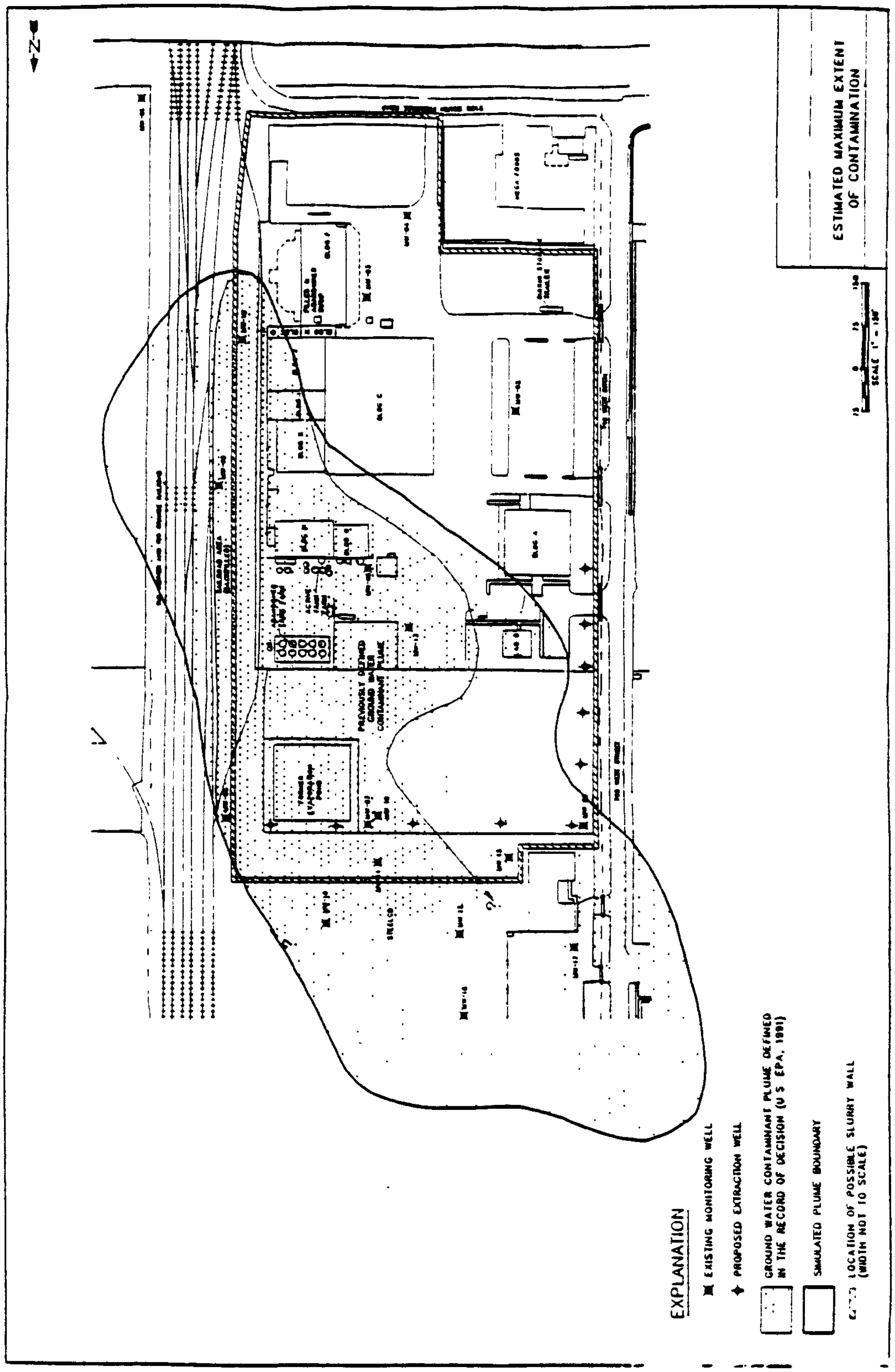


Figure 3.4-4

Estimated Maximum Extent of Contamination



Section 4.0 - Model Descriptions

4.0

Model Descriptions

Introduction

This section provides summary and detailed descriptions for four ground-water models that were selected as the initial set of models to be considered as part of this pilot project. The four models are:

- ❐ MOC
- ❐ MODFLOW
- ❐ RANDOM WALK
- ❐ PLASM

While these models are generally well known and have been used often in EPA programs, the inclusion of them in the *Compendium* does not represent an endorsement of them by OSWER for any specific purpose. In the future, OSWER may develop guidelines for application of models under certain conditions or for specified types of analyses, and add other models to the *Compendium*. At this time, the descriptions are provided as general reference information only.

Fact Sheets

The beginning of this section contains a two-sided Fact Sheet for each of the models. These were developed based on comments received from EPA Regional office staff, who identified a need to have quick access to some key model descriptors. The Fact Sheets are designed to provide an "at a glance" overview of the models' characteristics, scope, and applicability, as well as the name of a contact for technical support and more information.

Model Descriptions

The latter part of this section contains more detailed information on the same set of four models. This information was extracted from a computerized database maintained by the International Ground Water Modeling Center (IGWMC) in Golden, Colorado. The information has been re-formatted, and in some cases, sub-sections have been re-numbered and re-ordered, but the information itself has been modified only slightly. IGWMC's database contains information on many more ground-water models. Using data that comes directly from the IGWMC database will maintain the integrity of the information, if for example, OSWER wishes to expand this portion of the *Compendium* in the future by taking larger extracts from the IGWMC database.

Modeling Data Requirements

There is often confusion about how modeling data requirements are determined and the relationship between data requirements and the model (code). It is important to understand that the determination of a modeling application's general data requirements should precede the selection of a model. Furthermore, the determination of the type, quantity, and accuracy of the data required for the modeling application can be complex because it is dependent upon:

1. *Management's reasons for performing the modeling and the subsequent accuracy and level of detail required of the modeling results.* For example, a preliminary screening of alternative remedial technologies conducted as part of a remedial investigation and feasibility study can usually be modeled with less detail than a remedial design being modeled as part of the remedial design phase.

2. *The physical processes and the characteristics of the site being modeled.* For example, chemical fate and transport processes often require considerably more types of data than flow processes. Moreover, the quantity and the accuracy required of the data are often a function of the types of chemicals being modeled or the level of heterogeneity of the site.

3. *The engineering objectives of the modeling.* For example, the types and quantity of data required to determine the effectiveness of a deep hydraulic barrier design are often different from the data required to analyze a network of ground-water extraction wells.

Once the data requirements have been determined, a model can be selected which will support these data requirements and provide management with the information they need to make informed decisions. Thus, the decision objectives, process and site characteristics, and engineering objectives are the factors which primarily determine a model application's data requirements and, in turn, govern the selection of a particular model.

To determine if a model will support an application's data requirements, the reader is referred to the model descriptions that follow and the model documentation that is usually available from the model's authors or the International Ground Water Modeling Center.

Model Fact Sheets For

- MOC
- MODFLOW
- PLASM
- RANDOM WALK

SOURCE:
INTERNATIONAL GROUND WATER MODELING CENTER
(IGWMC)

Model Type: Solute Transport

MOC
(USGS-2D-TRANSPORT, KONBRED)
Version 3.0
Release Date: 11/89

Summary Updated 5/29/92

MOC is a ground-water flow and mass transport model. It provides capabilities for two dimensional simulation of non-conservative solute transport in heterogeneous, anisotropic aquifers. It computes changes in time in the spatial concentration distribution caused by convective transport, hydrodynamic dispersions, mixing or dilution from recharge, and chemical reactions. The chemical reactions include first-order sorption irreversible rate reaction (e.g. radioactive decay), equilibrium-controlled sorption with linear, Freundlich or Langmuir isotherms, and monovalent and/or divalent ion-exchange reactions. MOC solves the finite difference approximation of the ground-water flow equation using iterative ADI and SIP. It uses the method of characteristics followed by an explicit procedure to solve the transport equation. MOC uses a subgrid of the flow grid for simulation of containment transport.

Note: A version of MOC called MOC Dense simulates two dimensional density dependent flow and transport in a crossectional plane. The specific characteristics of MOC Dense are not incorporated in this summary.

Technical Assistance:

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Robert S. Kerr Environmental Research Laboratory (RSKERL)
U.S. Environmental Protection Agency
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Ada, OK 74820
(405) 332-8800

Availability

Usability						Reliability			
Public Domain	Documentation	User Support	Preprocessors	Postprocessors	Mult. Hardware Platforms	Verification	Peer Review	Previous EPA Use	Case Studies
✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

Distributed By:

International Ground Water Modeling Center
Colorado School of Mines
Golden, CO 80401, USA
(303) 273-3103

U.S. Geological Survey
WRD WGS - Mail Stop 433
National Center
Reston, Virginia 22092

Scientific Software Group
P.O. Box 23041
Washington D.C. 20026-3041
(703) 620-9214

Geraghty & Miller, Inc.
Modeling Group
1895 Preston Drive, Suite 301
Reston, Virginia 22091
(703) 476-0335

Scope

Remedial Design Feature

Capping, Grinding & Revegetation	Groundwater Pumping	Wastewater Injection	Interceptor Trenches	Impermeable Barriers	Subsurface Draining	Solution Mining	Excavation
○	●	◐	◐	◐	◐	●	○

Contaminant Source Type

Solid Waste Disposal				Liquid Waste Disposal					Leakage				
Uncontrolled Dumps	Sani. & Secured Landfills	Deep Subsurface Burial	Leachate	Wastewater Impound.	Deep Subsurface Injection	Land Spraying	Discharge To Surf. Water	Ind. Sewage Disposal	Surface Storage Facilities	Subsurface Storage Faci.	Subsurface Transport Sys.	Subsurface Disposal Faci.	Surface Spills
◐	◐	○	○	◐	○	◐	◐	◐	◐	○	◐	○	◐

Key

Likely ●
Possibly ◐
Not Likely ○
Not Applicable N/A

Technical Characteristics

Model Processes			Flow System				Aquifer Type		Flow Characteristics (Saturated)			Transport Processes			Fate & Transfer Processes		Flow Solution Technique			Parameter Representation			
Flow	Transport	Transfer	Single Aquifer	Multiple Aquifer	Saturated Zone	Unsaturated Zone	Confined	Unconfined	Dimension	Steady State	Transient	Advection	Diffusion	Dispersion	Fate	Transfer	Analytic	Finite Difference	Finite Element	Homogeneous	Heterogeneous	Isotropic	Anisotropic
✓	✓	✓	✓		✓		✓		2	✓	✓	✓	✓	✓	✓	✓		✓		✓	✓	✓	✓

Flow Boundary Conditions			Transport Boundary Conditions			Flow Output			Transport Output					Output Format				
Specified Value	Specified Flux	Value Dependent Flux	Specified Value	Specified Flux	Value Dependent Flux	Head/Pressure/Potential	Fluxes/Velocities	Water Budget	Conc. in Aquifer/Soil	Concentrations in Well	Velocities	Mass Balance		ASCII File	Contours	Flow Lines	Particle Paths	Plots
✓	✓	✓	✓	✓		✓	✓	✓	✓			✓		B	P	P	P	P

Key

Model
M

Pre or Post Processor
P

Both
B

Neither
X

Definitions

Boundary Conditions

Specified Value - Values of head, concentration or temperature are specified along the boundary. (Dirichlet Condition)
Specified Flux - Flow rate of water, contaminent mass or energy is specified along the boundary. (Neumann Condition)
Value Dependent Flux - A specified flux is given for a specified value. (Cauchy Condition)

Hardware Platforms: Prime, DEC VAX, IBM PC/XT/AT, IBM 80386/486, Apple Macintosh

Preprocessors: PREMOC, MODELCAD

Postprocessors: POSTMOC, MOCGRAF

Detailed information on this model, sources of distribution, and postprocessors and preprocessors is available in *The Ground-Water Modeling Compendium.*

MODFLOW

Version 3.2
Release Date: 10/89

MODFLOW is a modular, block-centered finite difference model for the simulation of two dimensional and quasi- or fully-three-dimensional, transient ground-water flow in anisotropic, heterogeneous, layered aquifer systems. It calculates piezometric head distributions, flow rates and water balances. The model includes modules of flow towards wells, through riverbeds, and into drains. Other modules handle evapotranspiration and recharge. Various textual and graphic pre-and postprocessors are available.

Note: Several particle tracking programs including ModPath utilize Modflow output to simulate contaminant transport. The specific characteristics of these particle tracking programs are not incorporated in this summary.

Technical Assistance:

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Availability

Usability						Reliability			
Public Domain	Documentation	User Support	Preprocessors	Postprocessors	Mult. Hardware Platforms	Verification	Peer Review	Previous EPA Use	Case Studies
✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

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(703) 620-9214

Geraghty & Miller, Inc.
Modeling Group
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Reston, Virginia 22091
(703) 476-0335

Scope

Remedial Design Feature

Capping, Grinding & Revegetation	Groundwater Pumping	Wastewater Injection	Interceptor Trenches	Impermeable Barriers	Subsurface Draining	Solution Mining	Excavation
○	●	◐	●	●	●	◐	◐

Contaminant Source Type

Solid Waste Disposal				Liquid Waste Disposal					Leakage				
Uncontrolled Dumps	Sani. & Secured Landfills	Deep Subsurface Burial	Leachate	Wastewater Impound.	Deep Subsurface Injection	Land Spraying	Discharge To Surf. Water	Ind. Sewage Disposal	Surface Storage Facilities	Subsurface Storage Faci.	Subsurface Transport Sys.	Subsurface Disposal Faci.	Surface Spills
N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A

Key

Likely ●
Possibly ◐
Not Likely ○
Not Applicable N/A

Technical Characteristics

Model Processes			Flow System				Aquifer Type		Flow Characteristics (Saturated)			Transport Processes			Fate & Transfer Processes		Flow Solution Technique			Parameter Representation			
Flow	Transport	Transfer	Single Aquifer	Multiple Aquifer	Saturated Zone	Unsaturated Zone	Confined	Unconfined	Dimension	Steady State	Transient	Advection	Diffusion	Dispersion	Fate	Transfer	Analytic	Finite Difference	Finite Element	Homogeneous	Heterogeneous	Isotropic	Anisotropic
✓			✓	✓	✓		✓	✓	3	✓	✓							✓		✓	✓	✓	✓

Flow Boundary Conditions			Transport Boundary Conditions			Flow Output			Transport Output					Output Format				
Specified Value	Specified Flux	Value Dependent Flux	Specified Value	Specified Flux	Value Dependent Flux	Head/Pressure/Potential	Fluxes/Velocities	Water Budget	Conc. in Aquifer/Soil	Concentrations in Well	Velocities	Mass Balance		ASCII File	Contours	Flow Lines	Particle Paths	Plots
✓	✓	✓				✓	✓	✓						B	P	P	X	P

Key

Model
M

Pre or Post Processor
P

Both
B

Neither
X

Definitions

Boundary Conditions

Specified Value - Values of head, concentration or temperature are specified along the boundary. (Dirichlet Condition)
Specified Flux - Flow rate of water, contaminent mass or energy is specified along the boundary. (Neumann Condition)
Value Dependent Flux - A specified flux is given for a specified value. (Cauchy Condition)

Hardware Platforms: DEC VAX 11/780, IBM PC/XT/AT, PRIME 750, IBM 80386/486, Apple Macintosh, Intel 80386/80486

Preprocessors: PREMOD, MODELCAD

Postprocessors: POSTMOD

Detailed information on this model, sources of distribution, and postprocessors and preprocessors is available in *The Ground-Water Modeling Compendium.*

Model Type: Saturated Flow

Summary Updated: 5/29/92

PLASM

Version - Illinois State Water Survey
Release Date: 1985

PLASM (Prickett Lonnquist Aquifer Simulation Model) is a finite difference model for simulation of transient, two-dimensional or quasi-three-dimensional flow in a single or multi-layered, heterogeneous, anistropic aquifer system. The original model of 1971 consisted of a series of separate programs for various combinations of simulation options. Later versions combined most of the options in a single code, including variable pumping rates, leaky confined aquifer conditions, induced infiltration from a shallow aquifer or a stream, storage coefficient conversion between confined and waterable conditions, and evapotranspiration as a function of depth to watertable. The model uses the iterative alternating implicit method (IADI) to solve the matrix equation.

Technical Assistance:

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Availability

Usability						Reliability			
Public Domain	Documentation	User Support	Preprocessors	Postprocessors	Mult. Hardware Platforms	Verification	Peer Review	Previous EPA Use	Case Studies
✓	✓	✓	✓		✓	✓	✓	✓	✓

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Geraghty & Miller, Inc., Modeling Group
1895 Preston Drive, Suite 301
Reston, Virginia 22091
(703) 476-0335

Scope

Remedial Design Feature								Contaminant Source Type: Solid Waste Disposal				Contaminant Source Type: Liquid Waste Disposal					Contaminant Source Type: Leakage				
Capping, Grinding & Revegetation	Groundwater Pumping	Wastewater Injection	Interceptor Trenches	Impermeable Barriers	Subsurface Draining	Solution Mining	Excavation	Uncontrolled Dumps	Sani. & Secured Landfills	Deep Subsurface Burial	Leachate	Wastewater Impound.	Deep Subsurface Injection	Land Spraying	Discharge To Surf. Water	Ind. Sewage Disposal	Surface Storage Facilities	Subsurface Storage Faci.	Subsurface Transport Sys.	Subsurface Disposal Faci.	Surface Spills
○	●	◐	●	●	◐	◐	◐	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A

Key

Likely ●

Possibly ◐

Not Likely ○

Not Applicable N/A

Technical Characteristics

Model Processes			Flow System				Aquifer Type		Flow Characteristics (Saturated)			Transport Processes			Fate & Transfer Processes		Flow Solution Technique			Parameter Representation			
Flow	Transport	Transfer	Single Aquifer	Multiple Aquifer	Saturated Zone	Unsaturated Zone	Confined	Unconfined	Dimension	Steady State	Transient	Advection	Diffusion	Dispersion	Fate	Transfer	Analytic	Finite Difference	Finite Element	Homogeneous	Heterogeneous	Isotropic	Anisotropic
✓			✓	✓	✓		✓	✓	3	✓	✓							✓		✓	✓	✓	✓

Flow Boundary Conditions			Transport Boundary Conditions			Flow Output			Transport Output					Output Format				
Specified Value	Specified Flux	Value Dependent Flux	Specified Value	Specified Flux	Value Dependent Flux	Head/Pressure/Potential	Fluxes/Velocities	Water Budget	Conc. in Aquifer/Soil	Concentrations in Well	Velocities	Mass Balance		ASCII File	Contours	Flow Lines	Particle Paths	Plots
✓	✓	✓				✓		✓						M	X	X	X	X

Key

Model M

Pre or Post Processor P

Both B

Neither X

Definitions

Boundary Conditions

Specified Value - Values of head, concentration or temperature are specified along the boundary. (Dirichlet Condition)

Specified Flux - Flow rate of water, contaminent mass or energy is specified along the boundary. (Neumann Condition)

Value Dependent Flux - A specified flux is given for a specified value. (Cauchy Condition)

Hardware Platforms: DEC VAX, IBM PC/XT/AT, IBM 360, 370

Preprocessors: PREPLASM, MODELCAD

Postprocessors: None

Detailed information on this model, sources of distribution, and postprocessors and preprocessors is available in *The Ground-Water Modeling Compendium.*

Model Type: Solute Transport

Summary Updated: 5/29/92

RANDOM WALK

Version - Illinois State Water Survey
Release Date: 7/81

RANDOM WALK/TRANS is a numerical model to simulate two-dimensional steady or transient flow and transport problems in heterogeneous aquifers under water table and/or confined or leaky confined conditions. The flow is solved using a finite difference approach and the iterative alternating direction implicit method. The advective transport is solved with a particle-in-cell method, while the dispersion is analyzed with the random walk method.

Note: A number of other versions of Random Walk including analytical function driven versions are available. The specific characteristics of these other versions including output capababilities vary considerably.

Technical Assistance:

Dr. David S. Burden, Director
Center for Subsurface Modeling Support (CSMoS)
Robert S. Kerr Environmental Research Laboratory (RSKERL)
U.S. Environmental Protection Agency
P.O. Box 1198
Ada, OK 74820
(405) 332-8800

Availability

Usability						Reliability			
Public Domain	Documentation	User Support	Preprocessors	Postprocessors	Mult. Hardware Platforms	Verification	Peer Review	Previous EPA Use	Case Studies
✓	✓	✓	✓		✓	✓	✓	✓	✓

Distributed By:

International Ground Water Modeling Center
Colorado School of Mines
Golden, CO 80401, USA
(303) 273-3103

Thomas A. Prickett
6 G. H. Baker Drive
Urbana, IL 61801
(217) 384-0615

Bob Sinclair, Director of Computer Service
Illinois State Water Survey
Box 5050, Station A
Champaign, IL 61820
(217) 333-4952

Geraghty & Miller, Inc., Modeling Group
1895 Preston Drive, Suite 301
Reston, Virginia 22091
(703) 476-0335

Scope

Remedial Design Feature								Contaminant Source Type: Solid Waste Disposal				Contaminant Source Type: Liquid Waste Disposal					Contaminant Source Type: Leakage				
Capping, Grinding & Revegetation	Groundwater Pumping	Wastewater Injection	Interceptor Trenches	Impermeable Barriers	Subsurface Draining	Solution Mining	Excavation	Uncontrolled Dumps	Sani. & Secured Landfills	Deep Subsurface Burial	Leachate	Wastewater Impound.	Deep Subsurface Injection	Land Spraying	Discharge To Surf. Water	Ind. Sewage Disposal	Surface Storage Facilities	Subsurface Storage Faci.	Subsurface Transport Sys.	Subsurface Disposal Faci.	Surface Spills
○	●	◐	●	●	◐	◐	◐	◐	◐	○	○	◐	○	◐	◐	◐	◐	○	◐	○	◐

Key

Likely ●

Possibly ◐

Not Likely ○

Not Applicable N/A

Technical Characteristics

Model Processes			Flow System				Aquifer Type		Flow Characteristics (Saturated)			Transport Processes			Fate & Transfer Processes		Flow Solution Technique			Parameter Representation			
Flow	Transport	Transfer	Single Aquifer	Multiple Aquifer	Saturated Zone	Unsaturated Zone	Confined	Unconfined	Dimension	Steady State	Transient	Advection	Diffusion	Dispersion	Fate	Transfer	Analytic	Finite Difference	Finite Element	Homogeneous	Heterogeneous	Isotropic	Anisotropic
✓	✓		✓		✓		✓	✓	2	✓	✓	✓	✓	✓	✓	✓		✓		✓	✓	✓	✓

Flow Boundary Conditions			Transport Boundary Conditions			Flow Output			Transport Output					Output Format				
Specified Value	Specified Flux	Value Dependent Flux	Specified Value	Specified Flux	Value Dependent Flux	Head/Pressure/Potential	Fluxes/Velocities	Water Budget	Conc. in Aquifer/Soil	Concentrations in Well	Velocities	Mass Balance		ASCII File	Contours	Flow Lines	Particle Paths	Plots
✓	✓	✓	✓	✓		✓	✓	✓	✓	✓	✓	✓		B	X	X	X	X

Key

Key	
Model	M
Pre or Post Processor	P
Both	B
Neither	X

Definitions

Boundary Conditions

Specified Value - Values of head, concentration or temperature are specified along the boundary. (Dirichlet Condition)
Specified Flux - Flow rate of water, contaminent mass or energy is specified along the boundary. (Neumann Condition)
Value Dependent Flux - A specified flux is given for a specified value. (Cauchy Condition)

Hardware Platforms: Cyber 175, VAX 11/780, IBM PC/XT/AT

Preprocessors: PREWALK, MODELCAD

Postprocessors: POSTWALK

Detailed information on this model, sources of distribution, and postprocessors and preprocessors is available in *The Ground-Water Modeling Compendium.*

Detailed Model Descriptions For

- ***MOC***
- ***MODFLOW***
- ***PLASM***
- ***RANDOM WALK***

SOURCE:
INTERNATIONAL GROUND WATER MODELING CENTER (IGWMC)

Model Description For

MOC
(USGS-2D-TRANSPORT/KONBRED)

SOURCE:
INTERNATIONAL GROUND WATER MODELING CENTER (IGWMC)

Table of Contents

MOC

1. Model Identification

1.1. Model Name(s)
- USGS-2D-TRANSPORT
- MOC
- KONBRED

1.2. Date of First Release
- 11/76

1.3. Current Version
- 3.0

1.4. Current Release Date
- 11/89

1.5. Author
- 1. Konikow, L.F.
- 2. Bredehoeft, J.D.

2. Model Information

2.1. Model Category
- ground-water flow
- mass transport

2.2. Model Developed For
- general use (e.g. in field applications)

2.3. Units of Measurement Used
- SI system
- metric units
- US customary units
- any consistent system

2.4. Abstract

MOC is a two-dimensional model for the simulation of non-conservative solute transport in heterogeneous, anisotropic aquifers. It computes changes in time in the spatial concentration distribution caused by convective transport, hydrodynamic dispersion, mixing or dilution from recharge, and chemical reactions. The chemical reactions include first-order irreversible rate reaction (e.g. radioactive decay), equilibrium-controlled sorption with linear, Freundlich or Langmuir isotherms, and monovalent and/or divalent ion-exchange reactions. MOC solves the finite difference approximation of the ground-water flow equation using iterative ADI and SIP. It uses the method of characteristics followed by an explicit procedure to solve the transport equation.

2.5. Data Input Requirements:
Data input requirements are provided in the model documentation and are discussed in the introduction to Section 4.0 of the *Compendium*.

2.6. Versions Exist For The Following Computer Systems
- minicomputer
- workstations
- mainframe
- microcomputer

- Make/Model
  -- Prime
  -- DEC VAX
  -- IBM PC/XT/AT
    - operating system
      MS DOS
  -- IBM 80386/486
    - operating system
      MS DOS
      OS/2
      Unix
  -- Apple Macintosh

2.7. System Requirements
- core memory (RAM) for execution (bytes)
  -- 640Kb (standard IBM PC version)
- mass storage (disk space in bytes)
  -- at least 2Mb for data files
- numeric/math coprocessor
  -- (for micro computers)
- compiler required
  -- (for mainframe)

2.8. Graphics Requirements
- none

2.9. Program Information
- programming language/level
  -- Fortran 77
- number of program statements (total)
  -- 2000

3. General Model Capabilities

3.1. Parameter Discretization
- distributed

3.2. Coupling
- none

3.3. Spatial Orientation
- saturated flow
- 2D-horizontal
- 2D-vertical

3.4. Types of Possible Updates
- parameter values
- boundary conditions

3.5. Geostatistics and Stochastic Approach
- none

3.6. Comments
- This model has restart capability

4. Flow Characteristics

4.1. Flow System Characterization
- Saturated Zone

- System
  - single aquifer

- Aquifer Type(s)
  - confined
  - semi-confined (leaky-confined)

- Medium
  - porous media

- Parameter Representation
  - homogeneous
  - heterogeneous
  - isotropic
  - anisotropic

- Flow Characteristics (Saturated Zone)
  - laminar flow
  - linear (Darcian flow)
  - steady-state
  - transient

- Flow Processes Included
  - areal recharge
  - induced recharge (from river)

- Changing aquifer conditions
  - in space
  - variable thickness

- Well Characteristics
  - none

- Unsaturated Zone
  - none

4.2. Fluid Conditions
- Single Fluid Flow
  - water

- Flow of Multiple Fluids
  - none

- Fluid Properties
  - constant in time/space

4.3. Boundary Conditions
- First Type - Dirichlet
  - head/pressure

- Second type - Neumann (Prescribed Flux)
  - injection/production wells
  - no flow boundary
  - areal boundary flux
  - ground-water recharge

- Third Type - Cauchy
  - head/pressure-dependent flux

4.4. Solution Methods for Flow
- General Method
  - Numerical

- Spatial Approximation
  - finite difference method
  - block-centered

- Time-Stepping Scheme
  - Crank-Nicholson

- Matrix-Solving Technique
  - SIP
  - iterative ADIP

4.5. Grid Design

- Cell/Element Characteristic
  - constant cell size
  - variable cell size

- Possible Cell Shapes
  - 2D-square
  - 2D-rectangular

- Maximum Number of Nodes
  - 2000

4.6. Flow Output Characteristics

- Simulation Results
  - Head/Pressure/Potential
    - ASCII file (areal values)
    - ASCII file (hydrograph)

- Water Budget Components
  - ASCII file (global total area)

5. Mass Transport Characteristics

5.1. Water Quality Constituents

- any component(s)
- single component
- total dissolved solids (TDS)
- inorganics
- organics
- radionuclides

5.2. Processes Included

- (Conservative) Transport
  - advection
  - dispersion (isotropic; anisotropic)
  - diffusion

- Phase Transfers
  - Solid <-> Liquid
    - sorption equilibrium isotherm
    - linear
    - Langmuir
    - Freundlich

- Fate
  - first-order radioactive decay (single mother/daughter decay)
  - first-order chemical decay
  - first-order microbial decay

5.3. Boundary Conditions

- First Type - Dirichlet
  - Chemical processes embedded in transport equation
  - concentration

- Second Type - Neumann (Prescribed Solute Flux)
  - areal boundaries
  - injection wells
  - point sources
  - line sources
  - areal sources

5.4. Solution Methods for Transport

- General Method
  - numerical
  - uncoupled flow and transport equation

- Spatial Approximation
  - finite difference method
  - block-centered
  - particle-tracking

- Time-Stepping Scheme
  - fully explicit

- Matrix-solving Technique
  - method of characteristics

5.5. Output Characteristics for Transport

- Simulation Results
  - Concentration in Aquifer/Soil
    - ASCII file (areal values)
    - ASCII file (time series)

- Mass Balance Components
  - ASCII file (global total area)

6. Evaluation

6.1. Verification/Validation

- verification (analytic solutions)
- laboratory data sets
- field datasets (validation)
- synthetic datasets
- code intercomparison

6.2. Internal Code Documentation (Comment Statements)

- incidental

6.3. <u>Peer (Independent) Review</u>

- concepts
- theory (math)
- coding
- accuracy

7. Documentation and Support

7.1. <u>Documentation Includes</u>

- model theory
- user's instructions
- example problems
- code listing

7.2. <u>Support Needs</u>

- Can be used without support
- Support is available
  - from author
  - from third parties

7.3. <u>Level of Support</u>

- limited
- support agreement available

8. Availability

8.1. <u>Terms</u>

- available
- public domain
- proprietary

8.2. <u>Form</u>

- source code only (tape/disk)
- source and compiled code
- compiled code only

9. Pre and Post Processors

9.1. Data Preprocessing

- name: PREMOC
  - separate (optional) program
  - generic (can be used for various models)
  - textual data entry/editing

- name: MODELCAD
  - separate (optional) program
  - generic (can be used for various models)
  - textual data entry/editing
  - graphic data entry/modification (e.g manual grid design, arrays)
  - data reformatting (e.g. for GIS)
  - error-checking
  - help screens

9.2. Data Postprocessing

- name: POSTMOC
- separate (optional) program
- reformatting (e.g. to standard formats)

10. Institution of Model Development

10.1. Name

- U.S. Geological Survey

10.2. Address

- National Center
  Reston, Virginia

10.3. Type of Institution

- federal/national government

11. Remarks

The MOC package distributed by the International Ground Water Modeling Center includes a preprocessor (PREMOC) to prepare input files, a postprocessor (POSTMOC) to reformat parts of the output file to allow the import the results in graphic display programs, and two versions of the MOC simulation program, MOCADI and MOCSIP. MOCADI and MOCSIP are identical apart from the methods used to solve the finite difference flow equations. The IGWMC distributes both IBM-PC and mainframe versions.

Contact the International Ground Water Modeling Center for latest information:

IGWMC USA: Inst. for Ground-Water Res. and Educ.,
Colorado School of Mines,
Golden, CO 80401, USA.

IGWMC Europe: TNO Institute of Applied Geoscience,
P.O. Box 6012, 2600JA Delft,
The Netherlands.

IBM-PC, Macintosh and mainframe versions of the MOC code are also available from:

Scientific Software Group
P.O. Box 23041
Washington, D.C. 20026-3041
(703) 620-9214

MOCGRAF is a program developed by TECSOFT, Inc. to provide graphics capability to MOC. It uses the output from MOC to contour heads and concentrations and to plot velocity vectors. It supports a variety of graphic screen formats, printers and plotters. MOCGRAF requires TECSOFT's TRANSLATE program. MOCGRAF is available from Scientific Software Group

MACMOC is the implementation of the USGS Method of Characteristics Solute Transport Model (MOC) for the Apple Macintosh. The data input editor, simulation code and output postprocessor are integrated in a single application. Graphic output includes head and concentration contouring, and velocity vector plotting. It requires a Macintosh Plus with System 6.02 and Finder 6.1 or higher and at least 2Mb RAM. MACMOC is available from the Scientific Software Group.

Notes on computer program updates have been published by the USGS, Reston, Virginia, on the following dates:

1. May 16, 1979	7. Jul. 26, 1985	13. Oct. 20, 1986
2. Mar. 26, 1980	8. Jul. 31, 1985	14. Mar. 2, 1987
3. Dec. 4, 1980	9. Aug. 2, 1985	15. Mar. 5, 1987
4. Aug. 26, 1981	10. Aug. 8, 1985	16. Jan. 29, 1988
5. Oct. 12, 1983	11. Aug. 12, 1985	17. Nov. 21, 1988
6. Jun. 10, 1985	12. Jul. 2, 1986	18. Jul. 20, 1989

A modification of this model to track representative water of tracer particles initially loaded along specific lines has been developed by Garabedian and Konikow (1983):

TRACK (see IGWMC key # 0741).

The code has been modified by Hutchinson to allow head-dependent flux as a boundary condition:

Hutchinson, C.B. et al. 1981. Hydrogeology of Well-field Areas near Tampa, Florida. USGS Open-File Report 81-630.

A modification to allow linear and non-linear sorption isotherms and first-order decay was introduced in 1982:

Tracy, J.V. 1982. Users Guide and Documentation for Adsorption and Decay Modifications of the USGS Solute Transport Model. NUREG/CR-2502, Div. of Waste Management, Off. of Nuclear Material Safety and Safeguard, U.S. Nuclear Regulatory Comm., Washington, D.C.

MODELCAD is a graphical oriented, model-independent preprocessor to prepare and edit input files for two- and three-dimensional ground-water models, including aquifer properties, boundary conditions, and grid dimensions. The program prepares input files for MODFLOW, MOC, PLASM and RANDOM WALK, among others. File formatting routines for other models are available upon request. Contact:

Geraghty & Miller Modeling Group
1895 Preston White Drive
Suite 301, Reston, VA 22091
(703) 476-0335

Strecker,E.W., W-S. Chu, and D. P. Lettenmaier. 1985. Evaluation of Data Requirements for Groundwater Contaminant Transport Modeling. Water Resources Series, Techn. Rept. 94, Univ. of Washington, Seattle, Wash.

In this study a parameter identification algorithm was used together with the USGS-MOC code and applied to two synthetic aquifers, evaluating the effects of data availability and uncertainty on ground-water contaminant transport prediction. The parameter identification algorithm is based on constrained least-squares minimization.

Also:

Strecker, E.W., and W-s. Chu. 1986. Parameter Identification of a Ground-Water Contaminant Transport Model. Ground Water, Vol. 24(1), pp. 56-62.

A modified version of the 1978 version of the USGS MOC model has been presented by Kent et Al. (1983; see references). Modifications include water-table option for flow and non-linear sorption. The same authors developed a menu-driven, preprocessor for their version of MOC. For more information contact Dr. Douglas C. Kent, School of Geol., Oklahoma State University, Stillwater, Oklahoma.

A stochastics-based analysis of the performance of the MOC model in remedial action simulations is discussed in:

El-Kadi, A.I. 1988. Applying the USGS Mass-Transport Model (MOC) to Remedial Actions by Recovery Wells. Ground Water, Vol. 26(3), pp. 281-288.

An IBM PC/386 extended memory version of this model is also available from:

Geraghty & Miller, Inc.
Modeling Group
1895 Preston Drive, Suite 301
Reston, VA 22091
tel.: 703/476-0335
fax: 703/476-6372

12. References

Pinder, G.F. and H.H. Cooper. 1970. A Numerical Technique for Calculating the Transient Position of the Saltwater Front. Water Resources Research, Vol. 6(3), pp. 875-882.

Bredehoeft, J.D., and G.F. Pinder. 1973. Mass Transport in Flowing Groundwater. Water Resources Research, Vol. 9(1), pp. 194-210.

Konikow, L.F., and J.D. Bredehoeft. 1974. Modeling Flow and Chemical Quality Changes in an Irrigated Stream-Aquifer System. Water Resources Research, Vol. 10(3), pp. 546-562.

Konikow, L.F., and J.D. Bredehoeft. 1978. Computer Model of Two-Dimensional Transport and Dispersion in Ground Water. USGS Techniques of Water Resources Investigations, Book 7, Chapter 2, U.S. Geological Survey, Reston, Virginia.

Kent, D.C., J. Alexander, L. LeMaster, and J. Wagner. 1983. Interactive Preprocessor Program for the U.S.G.S. Konikow Solute Transport Model. Oklahoma State University, School of Geology, Stillwater, Oklahoma.

Kent, D.C., M.M. Hoque, L. LeMaster, and J. Wagner. 1983. Modifications to the U.S.G.S. Solute Transport Model. School of Geology, Oklahoma State University, Stillwater, Oklahoma.

Goode, D.J., and L.F. Konikow. 1989. Modification of a Method-of-Characteristics Solute Transport Model to Incorporate Decay and Equilibrium-Controlled Sorption or Ion Exchange. USGS Water Resources Investigations Report 89-4030, U.S. Geological Survey, Reston, Virginia.

13. Users

Spinazola, J.M., J.B. Gillespie, and R.J. Hart. Ground-Water Flow and Solute Transport in the Equus Beds Area, South Central Kansas, 1940-79. Water-Resources Investig. Rept. 85-4336, Lawrence, Kansas.

The transport model was used to study the movement of chloride in the past and under the various proposed pumping development schemes. The sources of the chloride is oilfield brine moving towards the wellfields and the Arkansas river.

Robertson, J.B. 1974. Digital Modeling of Radioactive and Chemical Waste Transport in the Snake River Plain Aquifer at the National Reactor Testing Station, Idaho. USGS Open-File Report IDO-22054. U.S. Geological Survey, Boise, Idaho.

Konikow, L.F. 1977. Modeling Chloride Movement in the Alluvial Aquifer at the Rocky Mountain Arsenal, Colorado. USGS Water Supply Paper 2044, U.S. Geological Survey, Denver, Colorado.

Sohrabi, T. 1980. Digital Transport Model Study of Potential Nitrate Contamination from Sceptic Tank Systems near Edmond, Oklahoma. Rept. 80-38, National Center for Ground Water Research, University of Oklahoma, Norman, Okla.

Sophocleous, M.A. 1984. Groundwater Flow Parameter Estimation and Quality Modeling of the Equus Beds Aquifer in Kansas, USA. Journ. of Hydrology, Vol. 69, pp. 197-222.

In an accompanying Technical Completion Report of the Kansas Water Resources Research Institute at the University of Kansas, Lawrence, Sohocleous et al. compares the MOC code with Pinder's ISOQUAD-4 code and Grove's finite difference solute transport code.

Freeberg, K.M. 1985. Ground Water Contaminant Modeling Applied to Plume Delineation and Aquifer Restoration at an Industrial Site. M.Sc. Thesis, Dept. of Env. Sciences and Eng., Rice Univ., Houston, Texas.

Groschen, G.E. 1985. Simulated Effects of Projected Pumping on the Availability of Fresh Water in the Evangeline Aquifer in an Area Southwest of Corpus Christi, Texas. USGS Water Resources Investigations Report 85-4182, Austin, Texas.

Chapelle, F.H. 1986. A Solute Transport Simulation of Brackish Water Intrusion near Baltimore, Maryland. Ground Water, Vol. 24(3), pp 304-311.

The model was used to estimate the future movement of the brackish-water plume in the coarse sands and gravels of the Patuxent Formation based on alternative strategies of aquifer use. (see also Maryland Geological Survey Report of Investig. 43 (1986)).

Davis, A.D. 1986. Deterministic Modeling of Dispersion in Heterogeneous Permeable Media. Ground Water, Vol. 24(5), pp. 609-615.

Perez, R. 1986. Potential for Updip Movement of Saline Water in the Edwards Aquifer, San Antonio, Texas. USGS Water Resources Investigations Report 86-4032, U.S. Geological Survey, Austin, Texas.

Bond, L.D., and J.D. Bredehoeft. 1987. Origins of Seawater Intrusion in a Coastal Aquifer--A Case Study of the Pajaro Valley, California. Journ. of Hydrology, Vol. 92, pp.363-388.

Mixon, F.O., A.S. Damle, R.S. Truesdale, and C.C. Allen. 1987. Effect of Capillarity and Soil Structure on Flow in Low permability Saturated Soils at Disposal Facilities. EPA/600/2-87/029, Hazardous Waste Eng. Research Lab., U.S. Environmental Protection Agency, Cincinnati, Ohio.

Patterson, C-V. 1987. Risk Analysis of Annular Disposal of Oil and Gas Well Brines. M.Sc. Thesis, Dept. of Systems Eng., Case Western Reserve University, Cleveland, Ohio.

Al-Layla, R., H. Yazicigil, and R. de Jong. 1988. Numerical Modeling of Solute Transport Patterns in the Damman Aquifer. Water Resources Bulletin, Vol. 24(1), pp. 77-85.

Used to predict the extent of the saline intrusion in this carbonate rock aquifer in the Kingdom of Saudi Arabia and studying the effects of changes in the hydrologic regime on TDS concentration. The model was modified to include the effects of salt gradients resulting from vertical leakage into the host aquifer.

Satkin, R.L., and P.b. Bedient. 1988. Effectiveness of Various Aquifer Restoration Schemes under Variable Hydrogeologic Conditions. Ground Water, Vol. 26(4), pp. 488-498.

Yager, R.M. and M.P. Bergeron. 1988. Nitrogen Transport in a Shallow Outwash Aquifer at Olean, Cattaraugus County, New York. Water-Resources Investigations Report 87-4043, U.S. Geological Survey, Ithaca, New York.

Model Description For

MODFLOW

SOURCE:
INTERNATIONAL GROUND WATER
MODELING CENTER
(IGWMC)

Table of Contents

PAGE

MODFLOW

1. Model Identification

1.1. Model Name(s)
- MODFLOW

1.2. Date of First Release
- 6/83

1.3. Current Version #
- 3.2

1.4. Current Release Date
- 10/89

1.5. Authors
- 1. McDonald, M.G.
- 2. Harbaugh, A.W.

2. Model Information

2.1. Model Category
- ground-water flow

2.2. Model Developed For
- general use (e.g. in field applications)
- research (e.g. hypothesis/theory testing)
- demonstration/education

2.3. Units of Measurement Used
- SI system
- metric units
- any consistent system

2.4. Abstract

MODFLOW is a modular, block-centered finite difference model for the simulation of two-dimensional and quasi- or fully-three-dimensional, transient ground-water flow in anisotropic, heterogeneous, layered aquifer systems. It calculates piezometric head distributions, flow rates and water balances. The model includes modules for flow towards wells, through riverbeds, and into drains. Other modules handle evapotranspiration and recharge. Various textual and graphic pre- and postprocessors are available.

2.5. Data Input Requirements:

Data input requirements are provided in the model documentation and are discussed in the introduction to Section 4.0 of the *Compendium*.

2.6. Versions Exist for the Following Computer Systems

- supercomputer
- minicomputer
- workstations
- mainframe
- microcomputer

- Make/Model
  - IBM-PC/XT/AT
    - operating system DOS 2.1 or later
  - DEC VAX 11/780
  - PRIME 750
  - Macintosh
  - Intel 80386/80486 based computers

2.7. System Requirements

- core memory (RAM) for execution (bytes)
  - 640Kb (standard IBM PC version)
- mass storage (disk space in bytes)
  - at least 2Mb for data files
- numeric/math coprocessor
  - (for micro computers)
- compiler require
  - (for mainframe)

2.8. Graphics Requirements

- none

2.9. Program Information

- programming language/level
  - Fortran 77
- number of program statements (total)
  - 5000 lines
- size of runtime (compiled) version (bytes)
  - 580Kb (IBM-PC version)

3. General Model Capabilities

3.1. Parameter Discretization

- distributed

3.2. Coupling

- N.A.

3.3. Spatial Orientation

- saturated flow
- 2D-horizontal
- 2D-vertical
- 3D-layered (quasi 3D)

3.4. Types of Possible Updates
- parameter values
- boundary conditions

3.5. Geostatistics and Stochastic Approach
- optional

3.6. Comments
- This model has restart capability.

4. Flow Characteristics

4.1. Flow System Characterization
- Saturated Zone

- System:
  - single aquifer
  - single aquifer/aquitard system
  - multiple aquifer/aquitard systems

- Aquifer Type(s)
  - confined
  - semi-confined (leaky-confined)
  - unconfined (phreatic)

- Medium:
  - porous media

- Parameter Representation
  - homogeneous
  - heterogeneous
  - isotropic
  - anisotropic

- Flow Characteristics (Saturated Zone)
  - laminar flow
  - linear (Darcian flow)
  - steady-state
  - transient

- Flow Processes Included
  - areal recharge
  - induced recharge (from river)
  - evapotranspiration

- Changing Aquifer Conditions
  - in space
    - variable thickness
    - confined/unconfined
    - pitching aquitard

- in time
    - desaturation(saturated/unsat.)
    - confined/unconfined
    - resaturation of dry cells

- Well Characteristics
    - partial penetration

4.2. Fluid Conditions

- Single Fluid Flow
    - water

- Flow of Multiple Fluids
    - N.A.

- Fluid Properties
    - constant in time/space

4.3. Boundary Conditions

- First Type - Dirichlet
    - head/pressure

- Second Type - Neumann (Prescribed Flux)
    - injection/production wells
    - no flow boundary
    - areal boundary flux
    - ground-water recharge
    - seepage face
    - springs
    - induced infiltration

- Third Type - Cauchy
    - head/pressure-dependent flux
    - free surface (steady-state; movable)

4.4. Solution Methods for Flow

- General Method
    - Numerical

- Spatial Approximation
    - finite difference method
    - block-centered

- Time-Stepping Scheme
    - fully implicit

- Matrix-Solving Technique
    - Iterative
    - SIP
    - LSOR

4.5. Grid Design

- Cell/Element Characteristic
  - constant cell size
  - variable cell size
  - 3D-hexahedral

- Possible Cell Shapes
  - 2D-square
  - 2D-rectangular
  - 3D-cubic

- Maximum Number of Nodes
  - 9999

4.6. Flow Output Characteristics

- Simulation Results
  - Head/Pressure/Potential
    - binary file (areal values)
    - ASCII file (areal values)
    - binary file (hydrograph)
    - ASCII file (hydrograph)
  - Fluxes/Velocities
    - binary file (areal values)
    - ASCII file (areal values)
    - binary file (temporal values)
    - ASCII file (temporal values)
  - Water Budget Components
    - ASCII file (cell-by-cell values)
    - ASCII file (global total area)

5. Evaluation

5.1. Verification/Validation

- verification (analytical solutions)
- synthetic datasets
- code intercomparison

5.2. Internal Code Documentation (Comment Statements)

- sufficient

5.3. Peer (Independent) Review

- concepts
- theory (math)
- coding
- accuracy
- documentation
- usability

6. Documentation and Support

6.1. Documentation Includes
- model theory
- user's instructions
- example problems
- code listing
- program structure and development
- verification/validation

6.2. Support Needs
- Can be used without support
- Support is available
  - from author
  - from third parties

6.3. Level of Support
- limited
- support agreement available

7. Availability

7.1. Terms
- available
- public domain
- proprietary

7.2. Form
- source code only (tape/disk)
- source and compiled code
- compiled code only
- paper listing of source code

8. Pre and Post Processors

8.1. Data Preprocessing
- name: MODELCAD
  - separate (optional) program
  - graphic data entry/modification (e.g manual grid design, arrays)
  - (semi-) automatic grid generation
  - data reformatting (e.g. for GIS)
  - error-checking
  - help screens

- name: PREMOD
  - part of model package (dedicated)
  - textual data entry/editing

8.2. Data Postprocessing
- name: POSTMOD
  - part of model package (dedicated)
  - textual data display on screen/printer
  - reformatting (e.g. to standard formats)

9. Institution of Model Development

9.1 Name
U.S. Geological Survey

9.2. Address
Ground Water Branch
WRD WGS - Mail Stop 433
National Center
Reston, Virginia 22092

9.3. Type of Institution
- federal/national government

10. Remarks

The code is available from the U.S.G.S. on tape ($40). Contact Arlen Harbaugh (see contact address). The documentation (paper copy $69.95, microfiche $3.50) is available from:

U.S. Geological Survey
Open-File Service Section
Branch of Distribution
Box 25425, Federal Center
Denver, CO 80225

Various MODFLOW implementations for IBM-PC and main frame systems are also available from the International Ground Water Modeling Center (see also MARS # 3983, 3984, 3985, and 3986), including MODFLOW PC for IBM PC/XT/AT (640K), and MODFLOW PC/EXT for extended memory Intel 80386/80486 based computers (2Meg,4Meg) which includes a preconditioned conjugate gradient solver and a stream-flow routing package.

IGWMC USA: Inst. for Ground-Water Res. and Educ.,
Colorado School of Mines,
Golden, CO 80401, USA.

IGWMC Europe: TNO Institute of Applied Geoscience,
P.O. Box 6012, 2600JA Delft,
The Netherlands.

Wagner, Heindel and Noyes Inc. has implemented MODFLOW on a Hewlett-Packard microcomputer (series 200). Contact Jeffrey E. Noyes, Geologist:

Wagner, Heindel and Noyes, Inc.
285 North St.
Burlington, Vermont 05401
phone: (802) 658-0820.

Various implementations of MODFLOW are available from:

Scientific Publications Co.
P.O. Box 23041
Washington, DC 20026-3041
phone: 703/620-9214
fax: 703/620-6793.

Versions included:

MODFLOW/PC for IBM PC/XT/AT (640K)

MODFLOW/EM for extended memory Intel 80386/80486 based computers (2Meg,4Meg) which includes a preconditioned conjugate gradient solver and a stream-flow routing package.

MOCGRAF is a program developed by TECSOFT, Inc. to provide graphics capability to MODFLOW. The menu-driven MODGRAF program uses the output from MODFLOW to automatically contour heads and drawdowns from each layer, stress period and time step and superpose velocity vectors on the head contour plots. The program requires TECSOFT's TRANSLATE program. A special 80386/486 version is available. Contact:

Scientific Software Group
P.O. Box 23041
Washington, D.C. 20026-3041
phone 703/620-9214.

MODPATH: a particle-tracking program developed by the USGS for use with the MODFLOW model. MODPATH calculates the path a particle would take in a steady-state three-dimensional flow field in a given amount of time. It operates as a post-processor for MODFLOW using heads, cell-by-cell flow terms and porosity to move each particle through the flow field. The program handles both forward and backward particle tracking. (See also IGWMC Key 3984).

MODPATH-PLOT: a graphic display program for use with MODPATH-PC. It uses the Graphical Kernal System (GKS) to produce graphical output on a wide range of commonly used printers and plotters. MODPATH-PLOT comes with MODPATH.

MACMODFLOW: this is the Macintosh implementation of the MODFLOW model. It supports the standard Macintosh user-interface. The simulation code is integrated with the input data editor and the graphic post-processor. Extensive data-checking is employed and simulation stops are trapped with control returning to the program. Graphic functions include contouring of heads, drawdowns, hydraulic conductivity, transmissivity, and plots of the finite difference grid. This version of MODFLOW is available from Scientific Software Group.

PATH3D is a general particle tracking program for calculating ground-water paths and travel times. The program uses the head solution of the USGS modular finite difference model MODFLOW. The program is available from:

S.S. Papadopulos and Assoc., Inc
12250 Rockville Pike
Suite 290
Rockville , Maryland 20852

MODELCAD is a graphical oriented, model-independent pre- processor to prepare and edit input files for two- and three-dimensional ground-water models, including aquifer properties, boundary conditions, and grid dimensions. The program prepares input files for MODFLOW, MOC, PLASM and RANDOM WALK, among others. File formatting routines for other models are available upon request. Contact:

Geraghty & Miller Modeling Group
1895 Preston White Drive
Suite 301
Reston, VA 22091
Phone: (703) 476-0335.

A related program contains a preconditioned conjugate gradient method for the solution of the finite difference approximating equations generated by MODFLOW (Kuiper 1987; see references). Five preconditioning types may be chosen: three different types of incomplete Choleski, point Jacobi or block Jacobi. Either a head change or residual error criteria may be used as an indication of solution accuracy and interation termination. A later version of this solver is included in the extended memory PC version from IGWMC, Scientific Software and Geraghty & Miller Modeling Group.

A computer program to summarize the data input and output from MODFLOW is described by Scott (1990; see references). This program, the Modular Model Statistical Processor, provides capabilities to easily read data input to and output from MODFLOW, calculate descriptive statistics, generate histograms, perform logical tests using relational operators, calculate data arrays using arithmic operators, and calculate flow vectors for use in a graphical display program. The program is written in Fortran 77 and tested on a Prime 1/model 9955-II.

A computer program for simulating aquifer-system compaction resulting from ground-water storage changes in compressible beds has been published by Leake and Prudic (1988; see references). This program can be incorporated in MODFLOW as the INTERBED-STORAGE-PACKAGE. (see also MARS 3985).

STR1 is a computer program written for use in MODFLOW to account for the amount of flow in streams and to simulate stream-aquifer interaction. The program is known as the Streamflow Routing Package (Prudic 1989; see references.) (see also MARS 3896).

PCG2 (Hill 1990; see references) is a numerical code to be used with the USGS MODFLOW model. It uses the preconditioned conjugate-gradient method to solve the equations produced by the MODFLOW model. Both linear and nonlinear flow conditions may be simulated. PCG2 includes two preconditioning options: modified Cholesky preconditioning and polynomial preconditioning. Convergence of the solver is determined using both head-change and residual criteria. Non linear problems are solved using Picard iterations. This solver is included in various extended memory PC versions.

An IBM PC/386 extended memory version of this model is also available from:

Geraghty & Miller, Inc.
Modeling Group
1895 Preston Drive
Suite 301
Reston, VA 22091
tel.: 703/476-0335
fax: 703/476-6372

11. References

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12. Users

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Model Description For

PLASM

SOURCE:
INTERNATIONAL GROUND WATER
MODELING CENTER
(IGWMC)

Table of Contents

PAGE

PAGE

PLASM

1. Model Identification

1.1. Model Name(s)
- PLASM

1.2. Date of First Release
- 1971

1.3. Current Release Date
- 1985

1.4. Authors
- 1. Prickett, T.A.
- 2. Lonnquist, C.G.

2. Model Information

2.1. Model Category
- ground-water flow

2.2. Model Developed For
- general use (e.g. in field applications)
- research (e.g. hypothesis/theory testing)
- demonstration/education

2.3. Units of Measurement Used
- SI system
- metric units
- US customary units
- any consistent system

2.4. Abstract

PLASM (Prickett Lonnquist Aquifer Simulation Model) is a finite difference model for simulation of transient, two-dimensional or quasi-three-dimensional flow in a single or multi-layered, heterogeneous, anisotropic aquifer system. The original model of 1971 consisted of a series of separate programs for various combinations of simulation options. Later versions combined most of the options in a single code, including variable pumping rates, leaky confined aquifer conditions, induced infiltration from a shallow aquifer or a stream, storage coefficient conversion between confined and watertable conditions, and evapotranspiration as a function of depth to water table. The model uses the iterative alternating implicit method (IADI) to solve the matrix equation.

2.5. Data Input Requirements:
Data input requirements are provided in the model documentation and are discussed in the introduction to Section 4.0 of the *Compendium.*

2.6. Versions Exist for the Following Computer Systems
- minicomputer
- workstations
- mainframe
- microcomputer

- make/model
  - IBM 360,370
  - DEC VAX
  - IBM PC/XT/AT

2.7. System Requirements
- core memory (RAM) for execution (bytes)
  - 640K (for IBM PC version)
- mass storage (disk space in bytes)
  - 1M
- numeric/math coprocessor
  - (for micro computers)
- compiler required
  - (for mainframe)

2.8. Graphics Requirements
- none

2.9. Program Information
- programming language/level
  - Fortran IV

3. General Model Capabilities

3.1. Parameter Discretization
- distributed

3.2. Spatial Orientation
- saturated flow
- 2D-horizontal
- 3D-layered

3.3. Types of Possible Updates
- parameter values
- boundary conditions

3.4. Geostatistics and Stochastic Approach
- none

3.5. Comments
- This model has restart capability.

4. Flow Characteristics

4.1. Flow System Characterization
- Saturated Zone

- System
  - single aquifer
  - single aquifer/aquitard system
  - multiple aquifer/aquitard systems

- Aquifer Type(s)
  - confined
  - semi-confined (leaky-confined)
  - unconfined (phreatic)

- Medium
  - porous media

- Parameter representation
  - homogeneous
  - heterogeneous
  - isotropic
  - anisotropic

- Flow characteristics (saturated zone)
  - laminar flow
  - linear (Darcian flow)
  - steady-state
  - transient

- Flow processes included
  - areal recharge
  - induced recharge (from river)
  - evapotranspiration

- Changing aquifer conditions
  - in space
    - variable thickness
    - confined/unconfined

  - in time
    - confined/unconfined

- Well characteristics
  - none

4.2. Fluid Conditions

- Single Fluid Flow
  - water
- Flow of Multiple Fluids
  - N.A.
- Fluid Properties
  - constant in time/space

4.3. Boundary Conditions

- First Type - Dirichlet
  - head/pressure
- Second Type - Neumann (Prescribed Flux)
  - injection/production wells
  - no flow boundary
  - areal boundary flux
  - ground-water recharge
  - induced infiltration
- Third Type - Cauchy
  - head/pressure-dependent flux

4.4. Solution Methods for Flow

- General Method
  - Numerical
- Spatial Approximation
  - finite difference method
  - node-centered
- Time-Stepping Scheme
  - fully implicit
- Matrix-Solving Technique
  - Iterative
  - iterative ADIP
  - Direct
  - Gauss elimination

4.5. Grid Design

- Cell/Element Characteristic
  - constant cell size
  - variable cell size
- Possible Cell Shapes
  - 2D-square
  - 2D-rectangular

- Maximum Number of Nodes
  - 5000

4.6. Flow Output Characteristics
- Simulation Results
  - head/pressure/potential
    - ASCII file (areal values)
    - ASCII file (hydrograph)
  - water budget components
    - ASCII file (cell-by-cell values)
    - ASCII file (global total area)

5. Evaluation

5.1. Verification/Validation
- verification (analytical solutions)
- field datasets (validation)
- synthetic datasets
- code intercomparison

5.2. Internal Code Documentation (Comment Statements)
- incidental

5.3. Peer (Independent) Review
- concepts
- theory (math)
- coding
- accuracy
- documentation
- usability
- efficiency

6. Documentation and Support

6.1. Documentation Includes
- model theory
- user's instructions
- example problems
- code listing
- program structure and development
- verification/validation

6.2. Support Needs
- Can be used without support
- Support is available
  - from author
  - from third parties

6.3. Level of Support
- limited

7. Availability

7.1. Terms
- available
- public domain
- proprietary
- restricted public domain
- purchase
- license

7.2. Form
- source code only (tape/disk)
- source and compiled code
- compiled code only
- paper listing of source code
- (depends on version)

8. Pre and Post Processors

8.1. Data Preprocessing
- name: PREPLASM
  - part of model package (e.g. under a shell; dedicated)
  - textual data entry/editing
  - error-checking

- name: MODELCAD
  - separate (optional) program
  - graphic data entry/modification (e.g manual grid design, -- arrays)
  - (semi-) automatic grid generation
  - data reformatting (e.g. for GIS)
  - error-checking
  - help screens

9. Institution of Model Development

9.1. Name
Illinois State Water Survey

9.2. Address
P.O. Box 232
Urbana, Illinois 61801

9.3. Type of Institution
state/provincial government

10. Remarks

A modified version of PLASM to analyze hydrologic impacts of mining is documented in in a report of the U.S. Office of Surface Mining (1981; see user references).

An extended and updated single aquifer version of PLASM for the IBM-PC is available from:

T.A. Prickett
6 G.H. Baker Drive
Urbana, IL 61801
phone: 217/384-0615.

This version is the same as published in Bulletin 55, except for the multi-layered option and the confined/unconfined storage conversion.

The IGWMC distributes a mainframe version of PLASM running on the DEC/VAX 11 series. The Center distributes also an IBM-PC version. This latter version comes as a program package including separate codes for confined (CONPLASM) and watertable (UNCPLASM) conditions and a textual preprocessor for input data preparation (PREPLASM). Contact:

IGWMC USA:	International Ground Water Modeling Center, Colorado School of Mines, Golden, Colorado, USA, or TNO Inst. of Applied Geoscience, P.O. Box 6012, 2600JA Delft, The Netherlands.
IGWMC Europe:	TNO Institute of Applied Geoscience, P.O. Box 6012, 2600JA Delft, The Netherlands.

For earlier microcomputer versions of PLASM see IGWMC Key # 6010 and 6011 (MARS historic data base).

MODELCAD is a graphical oriented, model-independent pre-processor to prepare and edit input files for two- and three-dimensional ground-water models, including aquifer properties, boundary conditions, and grid dimensions. The program prepares input files for MODFLOW, MOC, PLASM and RANDOM WALK, among others. File formatting routines for other models are available upon request. Contact:

Geraghty & Miller Modeling Group
1895 Preston White Drive
Suite 301
Reston, VA 22091
Phone: (703) 476-0335.

The IBM-PC version of this program is also available from:

National Water Well Association
Ground Water Bookstore
P.O. Box 182039
Dept. 017
Columbus, Ohio 43218
Tel. (614) 761-1711

The version available from the National Water Well Association runs on IBM PC or compatible and has been prepared by Koch and Associates and includes interactive data preparation. The code is directly available from Koch and Associates. Contact:

Ann Koch
2921 Greenway Drive
Ellicot City, Maryland 21043
tel. 301/461-6869.

11. References

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12. Users

T.R. Knowles developed two models based on PLASM for the Texas Dept. of Water Resources, Austin, Texas. See models GWSIM (IGWMC key # 0681) and GWSIM II (IGWMC key # 0680).

Beltran, J.M.A., L.L. Garcia, and M.R.L. Madurga. 1973. Estudio de la Explotacion de los Aquiferos del Llano de Palma de Mallorca Mediante un Modelo Digital Simplificado. Boletin 38, Dirrecion General de Obras Hidraulicas, Ministerio de Obras Publicas, Madrid, Spain.

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Naymik, T.G. 1979. The Application of Digital Model for Evaluating the Bedrock Water Resources of the Maumee River Basin, Northwestern Ohio. Lawrence Livermore Laboratory. University of California. Livermore, California.

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Kalinski, R.J. 1985. Investigation and Computer Simulation of Stream-Aquifer Relationship at Elm Creek, Nebraska. In: Proceed. Practical Applications of Ground Water Models, Columbus, Ohio, pp. 146-161. Nat. Water Well Assoc., Dublin, Ohio.

Song, S. and A.O. Akan. 1985. Ground Water Management by Linear Programming with Sample Applications to the Eastern Shore of Virginia Aquifer. In: Proceed. Conf. on Practical Applications of Ground Water Models, Columbus, Ohio, pp. 90-107. Nat. Water Well Assoc., Dublin, Ohio.

Contractor, D.N., S.M.A. El-Didy, and A.S. Ansary. 1986. Numerical Modeling of Groundwater Flow and Water Quality at Underground Coal Gasification Sites. DOE/ LC/11053-2151. Office of Fossil Energy, U.S. Dept. of Energy, Laramie, Wyoming. (pp.7-50).

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Model Description For

RANDOM WALK

SOURCE:
INTERNATIONAL GROUND WATER
MODELING CENTER
(IGWMC)

Table of Contents

RANDOM WALK

1. Model Identification

1.1. Model Name(s)
- RANDOM WALK

1.2. Date of first release
- 7/81

1.3. Current Release date
- 7/81

1.4. Authors
- Prickett, T.A.
- Naymik, T.G.
- Lonnquist, C.G.

2. Model Information

2.1. Model Category
- ground-water flow
- mass transport

2.2. Model Developed For
- general use (e.g. in field applications)
- research (e.g. hypothesis/theory testing)
- demonstration/education

2.3. Units of Measurement Used
- metric units
- US customary units
- any consistent system

2.4. Abstract

RANDOM WALK/TRANS is a numerical model to simulate two-dimensional steady or transient flow and transport problems in heterogeneous aquifers under water table and/or confined or leaky confined conditions. The flow is solved using a finite difference approach and the iterative alternating direction implicit method. The advective transport is solved with a particle-in-a-cell method, while the dispersion is analyzed with the random walk method.

2.5. Data Input Requirements

Data input requirements are provided in the model documentation and are discussed in the introduction to Section 4.0 of the *Compendium.*

2.6. Versions Exist for the Following Computer Systems
- minicomputer
- workstations
- mainframe
- microcomputer
  - make/model
    - Cyber 175
    - VAX 11/780
    - IBM PC/XT/AT or compatible

2.7. System Requirements
- core memory (RAM) for execution (bytes)
  - 640K (for IBM PC version)
- mass storage (disk space in bytes)
  - at least 2Mb for data files
- numeric/math coprocessor
  - (for micro computers)
- compiler required
  - (for mainframe)

2.8. Graphics Requirements
- none

2.9. Program Information
- programming language/level
  - Fortran IV

3. General Model Capabilities

3.1. Parameter Discretization
- distributed

3.2. Coupling
- none

3.3. Spatial Orientation
- saturated flow
- 2D-horizontal

3.4. Geostatistics and Stochastic Approach
- random walk

4. Flow Characteristics

4.1. Flow System Characterization
- Saturated Zone

- System
  - single aquifer
  - single aquifer/aquitard system

- Aquifer Type(s)
  - confined
  - semi-confined (leaky-confined)
  - unconfined (phreatic)

- Medium
  - porous media

- Parameter representation
  - homogeneous
  - heterogeneous
  - isotropic
  - anisotropic

- Flow characteristics (saturated zone)
  - laminar flow
  - linear (Darcian flow)
  - steady-state
  - transient

- Flow processes included
  - areal recharge
  - induced recharge (from river)
  - evapotranspiration

- Changing aquifer conditions
  - in space
    - variable thickness
    - confined/unconfined

  - in time
    - confined/unconfined

- Well characteristics
  - none

4.2. <u>Fluid Conditions</u>

- Single Fluid Flow
  - water

- Flow of Multiple Fluids
  - N.A.

- Fluid Properties
  - constant in time/space

4.3. Boundary Conditions

- First Type - Dirichlet
  - head/pressure

- Second Type - Neumann (Prescribed Flux)
  - injection/production wells
  - no flow boundary
  - areal boundary flux
  - ground-water recharge
  - springs
  - induced infiltration

- Third Type - Cauchy
  - head/pressure-dependent flux

4.4. Solution Methods for Flow

- General Method
  - Numerical

- Spatial Approximation
  - finite difference method
  - node-centered

- Time-Stepping Scheme
  - fully implicit

- Matrix-Solving Technique
  - Iterative
  - iterative ADIP
  - Direct
  - Gauss elimination

4.5. Grid Design

- Cell/Element Characteristic
  - constant cell size
  - variable cell size

- Possible Cell Shapes
  - 2D-square
  - 2D-rectangular

- Maximum Number of Nodes
  - 5000

4.6. Flow Output Characteristics
- Simulation Results
  - head/pressure/potential
    - ASCII file (areal values)
    - ASCII file (hydrograph)
  - fluxes/velocities
    - ASCII file (areal values)
  - water budget components
    - ASCII file (cell-by-cell values)
    - ASCII file (global total area)

5. Mass Transport Characteristics

5.1. Water Quality Constituents
- any component(s)
- single component
- total dissolved solids (TDS)
- inorganics
- organics
- radionuclides

5.2. Processes Included
- (Conservative) Transport
  - advection
  - dispersion
  - isotropic
  - anisotropic
  - diffusion
- Phase Transfers
  - equilibrium
  - isotherm
- Fate
  - first-order radioactive decay (single mother/daughter decay)
  - first-order chemical decay

5.3. Boundary Conditions
- First Type - Dirichlet
  - Chemical processes embedded in transport equation
  - concentration

- Second Type - Neumann (Prescribed Solute Flux)
  - areal boundaries
  - injection wells
  - point sources
  - line sources
  - areal sources

5.4. Solution Methods for Transport
- General Method
  - numerical
  - uncoupled flow and transport equation
- Spatial Approximation
  - finite difference method
  - node-centered
  - particle-tracking
- Time-Stepping Scheme
  - fully implicit
- Matrix-Solving Technique
  - Random Walk
  - direct
  - Gauss elimination

5.5. Output Characteristics for Transport
- Simulation Results
  - concentration in aquifer/soil
    - ASCII file (areal values)
    - ASCII file (time series)
  - concentration in well
    - ASCII file (time series)
  - velocities (from given heads)
    - ASCII file (areal values)
  - mass balance components
    - ASCII file (cell-by-cell values)
    - ASCII file (global total area)

6. Evaluation

6.1. Verification/Validation
- verification (analytic solutions)
- code intercomparison

6.2. Internal Code Documentation (Comment Statements)
- incidental

6.3. Peer (Independent) Review
- concepts
- theory (math)

7. Documentation and Support

7.1. Documentation Includes
- model theory
- user's instructions
- example problems
- program structure and development
- code listing
- verification/validation

7.2. Support Needs
- Can be used without support
- Support is available
  - from author
  - from third parties

7.3. Level of Support
- limited

8. Availability

8.1. Terms
- available
- public domain
- proprietary
- purchase

8.2. Form
- source code only (tape/disk)
- source and compiled code
- compiled code only
- paper listing of source code

9. Pre and Post Processors

9.1. Data Preprocessing
- name: PREWALK (IGWMC)
  - separate (optional) program
  - textual data entry/editing
  - data reformatting
  - error-checking

- name: MODELCAD
  - separate (optional) program
  - generic (can be used for various models)
  - textual data entry/editing
  - graphic data entry/modification (e.g manual grid design, arrays)
  - data reformatting (e.g. for GIS)
  - error-checking
  - help screens

9.2. Data Postprocessing

- name: POSTWALK (IGWMC)
  - separate (optional) program
  - textual data display on screen/printer
  - reformatting (e.g. to standard formats)

10. Institution of Model Development

10.1. Name

Illinois State Water Survey

10.2. Address

P.O. Box 5050
Sta.A
Urbana, IL 61820

10.3. Type of Institution

- state/provincial government

11. Remarks

Various microcomputer versions are available among others from the International Ground Water Modeling Center:

IGWMC USA: Inst. for Ground-Water Res. and Educ.,
Colorado School of Mines,
Golden, CO 80401, USA.

IGWMC Europe: TNO Institute of Applied Geoscience,
P.O. Box 6012
2600JA Delft
The Netherlands.

Code is available from:
Bob Sinclair
Director of Computer Service
Illinois State Water Survey
Box 5050
Station A
Champaign, IL 61820
telephone (217) 333-4952
at cost of magnetic tape, copying and postage.

Code is also available from:
Thomas A. Prickett
6 G.H. Baker Drive
Urbana, IL 61801
Phone 217/384-0615

A modified version of PLASM and RANDOM WALK to analyze hydrologic impacts of mining is documented in U.S. Office of Surface Mining (1981; see user references). Program codes are available through Boeing Computer Network.

MODELCAD is a graphical oriented, model-independent pre-processor to prepare and edit input files for two- and three-dimensional ground-water models, including aquifer properties, boundary conditions, and grid dimensions. The program prepares input files for MODFLOW, MOC, PLASM and RANDOM WALK, among others. File formatting routines for other models are available upon request. Contact:

Geraghty & Miller Modeling Group
1895 Preston White Drive
Suite 301, Reston, VA 22091
(703) 476-0335

12. References

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13. Users

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