Groundwater Modeling
Using Geographical Information Systems

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To Phyllis
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The purpose of this book is to present elements of the art of groundwater flow and transport modeling using tools generally identified with geographical information systems (GISs). The book is the outgrowth of notes I prepared for teaching a course in groundwater flow and transport modeling while I was teaching at Princeton University. The concept of employing GIS as an integral part of the modeling course was added during my tenure at the University of Vermont.

The motivation for introducing a GIS format in the course stems from the realization that from the outset, groundwater modeling has entailed the organization, quantification, and interpretation of large quantities of geohydrological data. Early work in groundwater modeling required the translation and transfer of information on maps, charts, and tables into computer-readable form. The work was lengthy, tedious, and error prone. Changes that were required in the data sets in the course of calibrating the models often involved sifting through thousands of numbers to make what often turned out to be minor modifications to the input-data sets.

The specification of hydrological information such as rainfall, parametric information such as hydraulic conductivity, design parameter specifications such as well locations and discharge values, and auxiliary conditions such as boundary conditions all involve the organization and manipulation of enormous quantities of data. Virtually all of this information is spatially, and in some instances temporally, distributed. Much of it is available in computerized databases either as maps in bitmap or vector image format or as data tables. Due to advances in computer-graphical technology, the information in such databases is now accessed most efficiently through GIS systems.

The resulting groundwater model-building tools generally incorporate a Windows-based, user-friendly, graphically oriented, functionally integrated, data-input, analysis, and postprocessing system. I have used two such systems in this book to facilitate
presentation of the basic concepts of groundwater flow and transport modeling. In
each instance the system consists of the Argus ONE Geographic Information Mod-
eling (GIM) environment, a groundwater flow and transport model, and a plug-in
extension (PIE) that interfaces Argus ONE and the model.

The Princeton Transport Code (PTC), MODFLOW, and MT3D are the ground-
water flow and transport models discussed in this book. These three models were
selected from a universe of possible candidates because (1) they are widely used in
practical application; (2) collectively, they represent both the finite-difference and
finite-element numerical-modeling approaches; and (3) plug-in extensions (PIEs)
have been developed and are available at http://www.argusint.com.

Using the GIS approach, the analyst works with the original spatial information:
for example, information provided on maps. Such information is generally accessible
and is normally cataloged and presented in commonly understood terminology rather
than in the more specialized vocabulary of the groundwater-modeling professional.
A visually based, computer-graphical approach, this method of data organization and
analysis is much more intuitive than cumbersome utilization of numerical arrays. I
refer to the above-described GIS approach as the geographic modeling approach
(GMA).

The book consists of three parts. Part 1 is dedicated to groundwater-flow model-
ing, Part 2 to groundwater-transport modeling, and Part 3 is a model-development
tutorial that considers both finite-difference- and finite-element-based approaches. A
comparison of these two approaches is also provided in this part.

The PTC used extensively in the preparation of this manuscript was developed
over a period of approximately 20 years. Among those besides myself who have
contributed to its development are D. P. Ahlfeld, D. K. Babu, L. R. Bentley, E. O.
Frind, J. F. Guarnaccia, G. P. Karatzas, A. Niemi, R. H. Page, M. P. Papadopoulou,
A. A. Spiliotopoulos, S. A. Stothoff, and K. Yamada. The MODFLOW and MT3D
computer codes employed in this text are provided by the U.S. Geological Sur-
vey. The Argus ONE site (http://www.argusint.com) provides links to these mod-
els and their associated PIEs. The PIE for PTC was created by J. L. Olivares. PTC,
its documentation, and the PIE interface to Argus ONE can be downloaded from

I am indebted to those who provided helpful criticisms and contributions during
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1.1 INTRODUCTION

Over the past three decades, groundwater-flow and transport modeling has evolved from a scientific curiosity to a widely used design and analysis technology. At the outset, groundwater modeling focused on the evaluation of groundwater supplies from the perspective of quantity, but more recent applications have addressed issues of water quality. Groundwater resource issues involving primarily water quantity are largely addressed by groundwater-flow models. Groundwater-transport models, however, are often needed when the problem to be addressed involves groundwater quality. A groundwater-flow model is a necessary precursor to the development of a groundwater-transport model. The groundwater velocity needed in the transport model is obtained from the flow model.

Groundwater flow models have a long history and come in many forms. Early flow models were based primarily on the finite-difference method of approximation of the governing field equations. Simple in concept and computationally efficient, finite-difference models found broad acceptance by the groundwater community. Later model development focused on the finite-element approach, which was more mathematically abstract and more difficult to code. The finite-element approach had the advantage of being able to represent irregular aquifer geometries more accurately because unlike the broadly used version of the finite-difference model which relied on rectangular meshes,\textsuperscript{1} finite-element models could accommodate triangular and even deformed rectangular meshes. Both finite-difference and finite-element models

\textsuperscript{1}Early finite-difference models were also available that could accommodate polygonal meshes, but they were not widely used.
are currently used routinely in groundwater hydrology and groundwater-contaminant hydrology to predict groundwater-reservoir behavior.

In this chapter we provide, through a field example, the conceptualization, formulation, and construction of a groundwater-flow model. Model construction, whether based on finite-difference or finite-element methods of approximation, involves a number of well-defined steps. In summary, these steps are as follows:

1. Establish the minimum area to be represented by the model;
2. Determine the hydrological features that can serve as boundaries to the model.
3. Compile the geological information.
4. Compile the hydrological information.
5. Determine the number of physical dimensions needed for the model.
6. Define the size of the model.
7. Define the model discretization.
8. Input the model boundary conditions.
9. Input the model parameters.
10. Input the model stresses.
11. Run the model.
12. Output the calculated hydraulic heads.
13. Calibrate the model.
14. Make the production runs.

To clarify the various aspects of modeling, we will introduce a field site located in Tucson, Arizona. Using the Argus ONE modeling environment, we will illustrate each of the steps listed above. In this example we focus on the contaminant trichloroethylene (TCE), the major contaminant of concern (COC) at this site.

**Tucson Example**

As an introduction to the Tucson site, we provide the following description recorded by one of the groundwater professionals who investigated the area (Rampe [4])

Groundwater pollution in the vicinity of the Tucson, Arizona, International Airport has been known or suspected since the early 1950’s. At that time, although some drinking water wells had been affected, the full extent of the pollution was not investigated. In some measure this appears to have been due to efforts on the part of government and industry to control the effects of groundwater pollution by controlling the above-ground pollution sources and by providing alternate supplies to those affected. It is also possible that the implications for the presence of very low levels of organic pollutants in drinking water were not fully appreciated by those involved at the time. In 1981, extensive

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2 Argus ONE is a commercially available program. It is a programmable interface that allows one to access the PTC groundwater code as well as other groundwater modeling codes in a Windows environment.
INTRODUCTION

and Veatch [10].

groundwater contamination by volatile organic compounds (VOCs) was discovered. The most abundant pollutant found was trichloroethylene (TCE), which has since been shown to occur in an area roughly extending from the Hughes Aircraft Company facility (HAC) in a northwesterly direction to Irvington Road (Figures 1.1 and 1.2). Other contaminants have also been found in the plume. These include chromium, isomers of dichloroethylene (DCE), benzene, chloroform, and other organic compounds. TCE is a compound suspected of being a carcinogen by the National Research Council, and has been placed on the Environmental Protection Agency’s (EPA) list of Priority Pollutants [5]. The Arizona Department of Health Services (ADHS) adopted an action limit of 5 ppb\(^3\) (parts per billion) for TCE in drinking water supplies.

The extent and severity of the contamination prompted action from Federal agencies. The U.S. Air Force began investigations of groundwater conditions in 1981, and in 1982 embarked upon a program of aquifer restoration south of Los Reales Road. The

\[^3\] ppb is the acronym for parts per billion, which is the weight in grams of a compound per billion grams of solution.
Tucson Airport Area (TAA) was placed in Superfund’s original National Priority List in 1982. EPA began investigations under Superfund to investigate further the sources and occurrence of groundwater contamination north of Los Reales Road. ADHS applied for and received funding from EPA under a Superfund cooperative agreement, and was named lead agency for the TAA.

After an extensive discussion of the scope, goals, and objectives of the investigation as well as the methodology employed, Rampe [4] provides the following conclusions:

Several potential sources of groundwater contamination exist in the vicinity of the Tucson International Airport. These are summarized in Table 1.1. Based on evidence gath-
<table>
<thead>
<tr>
<th>Facility</th>
<th>Years Operated</th>
<th>Number of Employees</th>
<th>TCE Use</th>
<th>Chromium Use</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Consolidated Aircraft</td>
<td>4–6</td>
<td>Unknown</td>
<td>Possible, unquantified</td>
<td>Possible, unquantified</td>
<td>Nature of activities appears to make widespread Cr and TCE use unlikely</td>
</tr>
<tr>
<td>Grand Central Aircraft</td>
<td>4</td>
<td>Up to 4700; varied</td>
<td>1200–4800 gal/yr (est.)</td>
<td>129 lb/yr (est.) from TURCO products; plating known but use of Cr unquantified</td>
<td>Widespread use of additional chemicals; probable source of groundwater contamination in early 1950s</td>
</tr>
<tr>
<td>Douglas Aircraft</td>
<td>4</td>
<td>1500</td>
<td>None, according to former workers</td>
<td>None, according to former workers</td>
<td>Despite former employee accounts, nature of activities makes some TCE use likely, although quantities were probably relatively small</td>
</tr>
<tr>
<td>Tucson Aviation Center</td>
<td>15</td>
<td>Unknown, possibly several hundred</td>
<td>300 gallons documented; est. waste = 192 gal/yr</td>
<td>Negligible use documented in §3007 letter responses</td>
<td>Aggregate of numerous small businesses</td>
</tr>
<tr>
<td>Burr-Brown</td>
<td>20</td>
<td></td>
<td>267–10,000 kg/yr</td>
<td>Up to 132 lb/yr</td>
<td>Waste disposal practices highly suspect</td>
</tr>
<tr>
<td>West-Cap of Arizona</td>
<td>22</td>
<td>Unknown</td>
<td>2000 gal/yr</td>
<td>None documented</td>
<td>Poor accounting of waste TCE; improper disposal</td>
</tr>
<tr>
<td>Hughes Aircraft Co./Air Force Plant 44</td>
<td>34</td>
<td>Up to 6000</td>
<td>3000 gal/yr (est.)</td>
<td>6800 lb/yr (1959 est.)</td>
<td>Documented poor chemical handling and disposal practices; multiple potential source areas on-site</td>
</tr>
</tbody>
</table>
erred in this and previous investigations, the following conclusions were reached regarding possible sources of groundwater contamination:

1. **Air Force Plant #44** is an acknowledged source of chromium and TCE contamination. Use of chromium at the plant was the largest documented in the area; TCE use estimates were among the largest. The duration of large-scale use of chromium and TCE was longer at this plant than at any other potential source, including aggregate use at the Tucson airport hangar area. The site has had a number of potential sources, including pits in which spent chemical and sludges were disposed of and a wastewater discharge which was not retained on-site until 1961. Historic documents indicate careless chemical handling in areas where drainage systems allowed chemicals to flow directly to open washes, in some cases bypassing the plant’s wastewater treatment systems. Historic analyses of Tucson well SC-7 show that the plant’s effluent was probably responsible for elevation of chromium levels in groundwater as early as 1958. Analyses of soils and perched groundwater indicate that disposal pits and the historic wastewater were both probable means whereby contaminants, including TCE, entered the regional groundwater system. The available data appear to be consistent with the hypothesis that Air Force Plant #44 is the most significant source of groundwater contamination in the vicinity of the Tucson International Airport.

2. The **Grand Central Aircraft Company** almost certainly caused the contamination of local wells through the improper disposal of wastewater. While this wastewater probably contained chromium and TCE, these were probably relatively minor constituents compared to other chemicals known to have been supplied to the plant by TURCO Products, Inc. These other chemicals are known to be capable of causing groundwater pollution but are not now found in local groundwater. Chromium plating took place to some degree at Grand Central, although no estimates of usage were discovered, nor was a means of disposal for plating wastes generated. Use of TURCO products may have accounted for approximately 130 pounds of chromium per year. TCE use at Grand Central may have been as great as 4,800 gallons per year. Waste TCE from Grand Central was disposed of primarily at the Tucson Airport Authority landfill, which may have received as much as 2,400 gallons of TCE per year according to reliable witnesses. While activity at Grand Central was intense and corresponding estimates of TCE use were large, the duration of such activity at the plant was brief, lasting for probably little more than two years of the company’s four-year tenancy. Primarily for this reason, Grand Central’s potential for contribution of TCE to groundwater, although highly likely, appears to have been much smaller than that of Air Force Plant #44. Indications of chromium use at Grand Central comparable to that which took place at Air Force Plant #44 have not been discovered.

3. Information on the activities of **Consolidated Aircraft** at the hangars is very limited, but allows for the possibility that this facility contributed to groundwater pollution. Neither the existence nor the improper disposal of chromium or TCE have been reliably demonstrated at Consolidated. This facility’s role as a new-aircraft modification center engaged primarily in assembly and installation would seem to preclude use of TCE or chromium on as large a scale as at Air Force Plant #44 or Grand Central Aircraft.
4. **Douglas Aircraft** does not appear to have been a significant source of groundwater contamination during the tenancy at the hangars based on an analysis of work performed there and information supplied by former employees. No TCE or chromium use or disposal was documented at Douglas, although the nature of work performed there allows for the possibility that some use of TCE or similar solvent occurred.

5. The **U.S. Air Force** occupied the Tucson Airport Authority hangars for approximately one month in 1968–69, and reportedly disposed of hundreds of gallons of liquids, including JP-4 jet fuel and TCE, in the desert south of the hangars. Subsequent EPA intermediate depth soil borings at the reported disposal sites failed to show evidence of vadose zone contamination, however.

6. Recent operators at the Tucson Airport Authority hangars include **small businesses** such as aircraft modification/repair companies of a type known to generate waste solvents. The largest reported use of TCE by any of these businesses is approximately 50 gallons per year. Using figures gathered for similar Maricopa County businesses, the aggregate waste solvent generated by the aircraft modification firms currently in residence at the hangars was estimated at approximately 200 gallons per year. While such figures leave open the possibility of groundwater contamination emanating from small businesses at the hangars, they are small in comparison with figures derived for other potential sources. The contaminant contribution of recent activities (that is, post-1970) thus appears to be minor.

7. Intermediate depth **soil sampling** performed by EPA in the vicinity of the airport hangars failed to find evidence of **vadose zone** contamination. Shallow soil samples taken near the hangars by ADHS did indicate disposal there of TCE and, in one instance, chromium. High levels of DCE, a volatile compound, in one of these samples may be indicative of recent disposal activities. Certain aspects of these sampling results, in particular the predominance of DCE over TCE, do not correspond well to conditions in underlying groundwater. Neither did the high chromium level found in one sample near the entrance to the hangars correspond well to known disposal practices there. In general, the presence of contaminants in shallow soil samples could not be conclusively traced to individual tenants or specific disposal activities at the hangars.

8. Three landfills were evaluated as to their probable groundwater pollution potential. Of these, only the old **Tucson Airport Authority landfill** appears to have received hazardous materials. TCE from Grand Central was dumped in the TAA landfill, along with other waste chemicals. While this is the only known dumping of TCE there, the possibility that other dumping of hazardous materials took place over the landfill’s long history cannot be eliminated. Deep **soil borings** contained TCE, possibly indicative of historic dumping. The TAA landfill appears to have had the potential to contribute TCE to local groundwater.

9. **Burr-Brown Research Corporation** is a highly probable source of local groundwater contamination located to the east of the main plume. This con-

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4 *Soil sampling* refers to the collection of soil samples for the primary purpose of investigating for the existence of contaminants.

5 The **vadose zone** is the portion of the soil column that normally contains air as well as water.

6 *Soil borings* are borings made primarily to obtain information regarding the conditions and properties of the soil, especially the degree of their contamination.
clusion is based on documented TCE use, poor disposal practices, and the
reports of witnesses indicating the presence of an abandoned well on-site and the
possibility of disposal there. More monitor wells are needed in the area to define
Burr-Brown’s contribution and differentiate it from possible contributions from
its neighbor to the south, West-Cap Arizona.

10. **West-Cap Arizona** is a possible source of local groundwater contamination
directed to the east of the main plume. This conclusion is based on documented
TCE use and the high probability of long term inadequate disposal practices. A
monitor well, SF-3, located down-gradient of part of the facility, may not be
situated properly to monitor contamination from all portions of the plant. More
on-site investigation and additional monitor wells are needed to more completely
assess West-Cap’s pollution potential.

11. The **Arizona Air National Guard** facility located at the northern edge of the air-
port is a probable source of local groundwater pollution east of the main plume.
This conclusion is based on circumstantial evidence, largely the Guard’s location
relative to the known extent of contamination, the documentation of at least some
TCE use, and the presence of possible pollution sources at the oil–water separa-
tors. It is not yet clear how activities at the Guard facility specifically relate to
observed contamination. An ongoing *Installation Restoration Program* study
of hazardous waste generated at the facility should allow better understanding of
this relationship.

12. The **abandoned fire-drill areas** located near runway 3 were in use from 1964
until sometime in the 1970’s. While these areas received primarily JP4 jet fuel,
they also received waste materials, possibly including TCE, from the Arizona
Air National Guard. Intermediate-depth soil sampling performed by EPA at these
sites failed to confirm vadose zone contamination emanating from them. The fire-
-drill areas currently in use are located in the southeastern portion of the airport
north of runway 29. **Shallow soil sampling** here revealed high concentrations
of a range of contaminants, including TCE. **Deep soil borings** contained traces
of TCE and higher levels of toluene and benzene, indicating that downward mi-
gration of contaminants from this source has taken place. The fire-drill areas
currently in use are a potential source of groundwater contamination. No local
wells exist to determine the extent of this contamination, however.

13. The possibility that surreptitious dumping of TCE or chromium at as yet undis-
covered locations near the airport contributed to groundwater pollution was not
addressed in this investigation. The location and amounts of contaminants in the
local groundwater system appear to be explainable on the basis of the activities
previously discussed.

To summarize, there appear to have been two important sources of groundwater pol-
lution which contributed to the main contaminant plume near the Tucson International
Airport. Air Force Plant #44 appears to have been the more significant of these, while
the activities of the Grand Central Aircraft Company appear to have been less impor-

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7 A *monitor well* is one that has been constructed primarily to sample groundwater for contamination
and to measure groundwater elevations. It is normally sampled on a regular basis, such as every three
months.
tant. The Burr-Brown Corporation, West-Cap Arizona, and the Arizona Air National Guard are probably responsible for two smaller contaminant plumes located east of the main plume. Other potential sources were considered to be less significant, if indeed they were sources as all, or could not be fully evaluated on the basis of available data.

1.2 AREAL EXTENT OF A MODEL

Let us now consider the first of the model construction steps outlined above, determination of the areal extent of a model. The areal extent of a model must be such as to

1. **Incorporate all locations where model heads are expected to change in response to stresses** imposed on the model. For example, when pumping at one or more wells to create a *cone of depression*, the model should be large enough to include all areas where a decline in water level can be expected to be significant. By *significant* we mean declines that are likely to impact the overall groundwater flow and transport in the area of interest. Since such water-level changes normally are determined via the model output, such an area nearly always can only be approximated;

2. **Incorporate the area of interest to the client.** As an example, the client may be interested in seeing the simulated water levels or flow directions over an area larger than the area where water-level changes are to be expected. In order to have this flow information available for output, the applicable area should be encompassed within the perimeter of the model;

3. Result in a model that is **consistent with available computational capabilities.** In other words, if a personal computer is the largest computer platform available, the model size should be no greater than that for which an acceptable turnaround time can be realized on the personal computer platform. It is inappropriate for a groundwater professional engaged in modeling to remain idle for extended periods of time waiting for modeling results because of computational limitations.

4. To the degree possible, coincide with an **area defined by distinct and easily evaluated hydrological boundary conditions.**

**Tucson Example**

Via this field example we demonstrate, step by step, throughout the remainder of the book, how to utilize the GMA to model groundwater flow and transport. As noted in Part 3, the GMA is composed of the Argus ONE GIM system and the *PTC* groundwater flow and transport model. The GUI that interfaces these two programs is a plug-in extension (*PIE*). The *PTC* GUI-PIE installs its menu commands in Argus's

---

8 A *cone of depression* is the area around a well whereat the water levels drop in response to pumping at the well.
PIEs menu. Thereafter it acts as a control panel for the creation of new PTC projects, the editing of control parameters of existing PTC projects, the execution of PTC, and postprocessing of the PTC output.

Since this is the first time we have faced the prospect of actually accessing the GMA environment, it seems appropriate to provide an abbreviated overview of the software that is used. More detail on each step may be found in subsequent sections of this book.

The steps involved in the creation, execution, and evaluation of a groundwater-flow model are the following:

1. After starting Argus ONE, the Argus ONE window appears and the user begins model development by selecting New PTC Project... from the PIEs menu.
2. A dialog box presenting the choices such as mesh type and number of geological (formations) layers then appears. The choice that is made causes the PIE to structure the kinds of geospatial coverages (information and data layers) required for a PTC simulation and automatically makes them available to the user for data entry and manipulation.
3. Next, the user may enter simulation-control parameters (those that are not spatially dependent, such as time-step size) into an interactive, tabbed-dialog box that appears on the computer screen. Upon completing data entry or editing of these values, the user closes the dialog and returns to the Argus ONE window.
4. The user should then modify the default information in any geospatial information layer by manually drawing closed or open contours or points to represent the desired spatial distributions of hydrogeologic and hydrologic parameters, fluid sources and sinks, and boundary conditions. One must also specify a desired finite-element mesh density. As an alternative to drawing, any of these spatial distributions may be imported directly from other applications that can generate either simple text files, DXF (Autocad format) files, or Shape (ArcView format) files.
5. The user now requests that Argus ONE create the finite-element mesh. Before proceeding to run PTC, the user may modify any of the spatial or nonspatial information already input.
6. The user then selects the PTC Mesh layer, and from the PIEs menu proceeds to “export” the geospatial and nonspatial information by selecting the Run PTC option. At this point Argus ONE writes out the standard input-data files for PTC to the directory selected, and runs the PTC simulation. When the simulation is complete, the user may choose to plot any of the simulation results within Argus ONE in a postprocessing step provided by the PTC PIE.

The power of the GMA approach in hydrogeologic hypothesis testing and practical modeling should be apparent at this point to any experienced modeler. In particular, it is straightforward to return at any point in the model formulation to any type of spatial information already input to the PTC–Argus ONE environment. It is
also easy to make major modifications to this information or to the finite-element mesh, to export once again from Argus ONE, to run PTC, and finally, to graphically evaluate the results of new simulations. Each cycle of changing information, running PTC, and inspecting the results can take as little as a few minutes.

Let us now return to the practical aspects of setting up a model. To access the interface, activate Argus ONE. An existing project can now be selected by clicking on File and then Open. From the resulting dialog box, one can then select an existing .mmb file produced during an earlier investigation (Figure 1.3).

Alternatively, if a new project is to be considered, one can click on the PIEs menu and select New PTC Project. . . . Plug-in extensions (PIEs), as noted earlier, are functions or groups of functions that add capabilities to the basic structure of Argus ONE. The PTC PIE contains the following functions:

1. A function to create an Argus ONE project for PTC. This function is executed by selecting PIEs | New PTC Project . . .
2. A function to edit the project information, executed by selecting PIEs | Edit Project Info. . . .
3. A function to run PTC, executed by selecting PIEs | Run PTC.

FIGURE 1.3. The first step in setting up the PTC model using Argus ONE is to establish that the model to be used is PTC. This is accomplished by selecting New PTC Project . . . from the PIEs menu.