HYDROLOGICAL APPLICATIONS OF GIS

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REGIONAL-SCALE ASSESSMENT OF NON-POINT SOURCE GROUNDWATER CONTAMINATION

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ABSTRACT

Predictive assessments of non-point source (NPS) pollution can have great utility for environmentally focused land use decisions related to both the remediation of existing groundwater contamination and the regulation of current (and future) agrochemical use. At the regional scales associated with NPS agrochemical applications there are staggering data management problems in assessing potential groundwater vulnerability. Geographical information system (GIS) technology is a timely tool that greatly facilitates the organized characterization of regional-scale variability. In this paper we review the recently reported (Loague *et al.*, 1998a,b) simulations of NPS groundwater vulnerability, resulting from historical applications of the agrochemical DBCP (1,2-dibromo-3-chloropropane), for east-central Fresno County (California). The Fresno case study helps to illustrate the data requirements associated with process-based three-dimensional simulations of coupled fluid flow and solute transport in the unsaturated/saturated subsurface at a regional scale. The strengths and weaknesses of using GIS in regional-scale vulnerability assessments, such as the Fresno case study, and the critical problem of estimating the uncertainties in these assessments (owing to both data and model errors) are discussed. A regional GIS-driven integrated assessment approach is proposed, which is based upon cost–benefit analysis, and incorporates both physical and economic factors that can be used in a regulatory decision process.

KEY WORDS non-point source pollution; groundwater contamination; regulation of agrochemicals; Fresno County, California; GIS; DBCP

INTRODUCTION

Non-point source groundwater vulnerability

It is now well know that groundwater contamination is one of the US's most important environmental quality concerns. The assessment and remediation of non-point source (NPS) groundwater contamination, from the past, present and future use of agrochemicals, can easily pose problems that have significantly greater economic effects than those that have long been recognized for point sources (Loague *et al.*, 1996). In many instances, agrochemicals applied at or near the surface, with little perceived threat of contaminating the groundwater below, have leached to considerable depths. One of the greatest challenges today is to quantitatively assess the vulnerability of precious groundwater resources at regional scales, as they are affected by the long-term applications of agrochemicals that cover thousands of hectares (Kellogg *et al.*, 1992; National Research Council, 1993; Corwin and Loague, 1996; Corwin *et al.*, 1997).

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Modern agriculture is at the root of the NPS groundwater contamination problem, i.e. large-scale agriculture depends upon agrochemicals. The goal of sustainable agriculture is to meet the needs of the present without compromising the ability to meet the needs of the future. Ideally, it strives to optimize food production while maintaining economic stability, minimizing the use of finite natural resources and minimizing environmental effects. This presents a formidable dilemma because agriculture remains as the single greatest contributor of NPS pollutants to soil and water resources (Humenik *et al.*, 1987). Point source and NPS pollutants differ in the scale of the areal extent of their source. Point source pollutants are those isolated to a single point location, such as a hazardous waste spill or a dump site. In contrast, NPS pollutants are spread across broad areas encompassing hundreds, thousands or even millions of hectares of soil and millions of litres of water. Obviously, land use decisions related to NPS groundwater contamination are very different from those for point sources. For example, it is just not possible to dig up California's San Joaquin Valley and place the contaminated soils in a secure landfill as might be the remedy for soils tainted by a leaking storage tank.

Khan *et al.* (1986) were among the pioneers in the development of regional-scale rating maps for pesticide leaching. In general, most of the NPS vulnerability assessments undertaken up until now have not considered the dynamics of a stressed saturated subsurface (i.e. groundwater pumping) at the regional scale. More importantly, leaching indices of the type used by Khan *et al.* (1986), which screen/rank chemical vulnerability, do not provide an estimate of the chemical concentrations loaded to the water table, which are essential in the decision management arena. The use of process-based numerical simulation models for the assessment of groundwater vulnerability at regional scales, albeit data and computationally intensive, is perhaps the most effective means of addressing problems that in all likelihood will not be investigated thoroughly through field study because of the lag times associated with the unsaturated zone, which can easily span several decades. For example, simulation is perhaps the easiest way to assess the lingering effect of legacies, i.e. agrochemicals long since out of use whose fate and transport are still of great concern. For the agrochemicals currently in use, and those that may be developed for use in the future, simulation allows one to look well into the future and consider alternative management strategies. The simulation effort reviewed in this paper was conducted (Loague *et al.*, 1998a,b) to estimate the regional-scale fate and transport history of DBCP (1,2-dibromo-3-chloropropane) in east-central Fresno County (California). The Fresno DBCP case study is a process-based NPS vulnerability assessment, coupling the unsaturated near-surface to the saturated subsurface, i.e. going well beyond the typical screening model approach.

Geographical information systems (GIS)

A geographical information system (GIS) is an integrating information technology that can include aspects of surface culture, demographics, economics, geography, surveying, mapping, cartography, photogrammetry, remote sensing, landscape architecture and computer science. GIS technology links the characteristics of a place, a resource and/or a feature with its spatial location. The principles and nuances of GIS techniques are reviewed by Burrough (1986). Goodchild (1993) defines a GIS as a 'general-purpose technology for handling geographic data in digital form with the following capabilities: (i) the ability to preprocess data from large stores into a form suitable for analysis (reformatting, change of projection, resampling, and generalization), (ii) direct support for analysis and modeling, and (iii) postprocessing of results (reformatting, tabulation, report generation, and mapping)'. In the context of NPS vulnerability assessments, a GIS is a tool used to characterize the full information content of the spatially variable data required by solute transport models. The advantages of GIS in its application to general spatial problems, as identified by Walsh (1988), include 'the ease of data retrieval; ability to discover and display information gained by testing interactions between phenomena; ability to synthesize large amounts of data for spatial examination; ability to make scale and projection changes, remove distortions, and perform coordinate rotation and translation; and the capability to discover and display spatial relationships through the application of empirical and statistical models'.

The use of GIS in environmental modelling has proliferated over the past two decades. However, to date, no generalized GIS system has the data representation flexibility for space and time together with the algorithmic capability needed to construct process-based models internally; consequently, environmental models and GIS must be coupled. Three of the most common strategies for linking a GIS to an environmental model (illustrated in Figure 1) are: (i) loose coupling; (ii) tight coupling; and (iii) an embedded system approach. A loose coupling involves data transfer from one to another by storage of data in one system and subsequent reading of the data by the other. The important characteristic of loose coupling is the separate functionality of the programs that implement the GIS and those that implement the models. Characteristically, a tight coupling provides a common user interface for both the GIS and the model i.e. the information sharing between the respective components is transparent. A tightly coupled model and the GIS must share the same database. As the degree of coupling between the GIS and the model increases, to the point where the model's functions are essentially part of the built-in functionality of the GIS, the model becomes embedded. In embedded systems, the coupling of software components occurs within a single application with shared memory rather than sharing the database and a common interface. The majority of the GIS linked environmental modelling applications that have been described in the literature are based upon loose coupling. The regional-scale, process-based NPS groundwater vulnerability assessment reviewed here is an example of a loosely coupled system.

AN ASSESSMENT OF REGIONAL-SCALE NON-POINT SOURCE GROUNDWATER VULNERABILITY: THE FRESNO CASE STUDY

Between the late 1950s and the time of its statewide cancellation in August 1977, there was widespread use of DBCP (1,2-dibromo-3-chloropropane) throughout the San Joaquin Valley (SJV). Almost 20 years after the cancellation, DBCP-contaminated groundwater persists as a problem in California: note, the maximum contaminant level (MCL) set for DBCP in the US for groundwater is 0·2 μg/l, the current detection limit for DBCP is approximately 0·001 μg/l.

Recently, environmental quality-driven lawsuits, for several hundred millions of dollars each (see Curtis and Profeta, 1993), have been brought against the manufacturers of DBCP related to the groundwater contamination problems in the SJV. A central issue in these cases has been whether the manufacturers of DBCP should have been expected to know that the chemical could potentially leach to groundwater and, thereby, be financially responsible for the remediation costs. The original objective of the case study (Loague *et al.*, 1998a,b) reviewed in this paper was to address, from a simulation perspective, if 'label recommended'

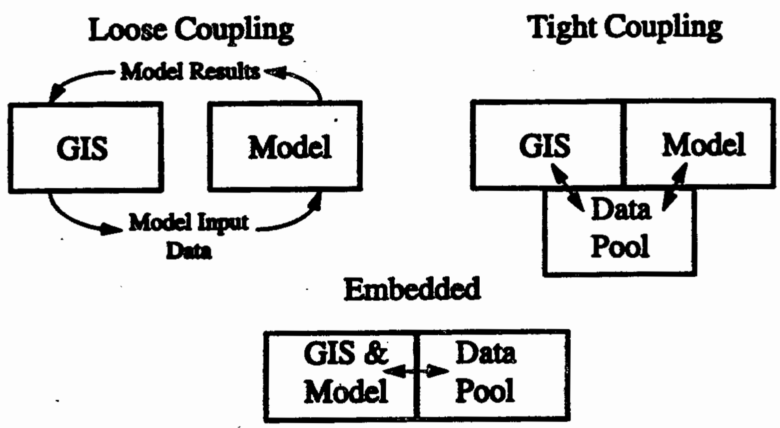

Figure 1. Three of the most common types of coupling of a GIS to an environmental model; loose, tight and embedded (after Corwin *et al.*, 1997)

NPS applications are likely to be the principal source of the DBCP groundwater contamination in Fresno County. The Fresno case study, as presented here, is a brief summary of a two-part paper by Loague and co-workers; readers interested in the details of the modelling effort are directed to Loague *et al.* (1998a,b).

The Fresno case study boundary value problem

The San Joaquin Valley, at the southern end of California's Central Valley, extends in a south-easterly direction for approximately 400 km from just south of Sacramento. East-central Fresno County (Figure 2), situated between the San Joaquin River to the north and the Kings River to the south, is the largest agricultural county in the valley. The Fresno area is a structural depression filled with thousands of metres of sedimentary material. The estimated spatial distribution of soils in the study area is shown in Figure 3. The spatial distribution of DBCP use in the study area, between 1960 and 1977, was estimated using land cover maps for different years (e.g. Figure 4). The location of an agricultural crop on a land use map was used as an indication of the DBCP application rate for that site at that time. The DBCP application rates used for the different crops considered for the study area are given in Loague *et al.* (1998a). The water table maps constructed for the study area (e.g. Figure 5) were based upon annual estimates of the water table depth made by the Fresno Irrigation District. The areas within the study area not covered by the District's estimates were estimated for this study using nearest-neighbour extrapolation. The three-dimensional characterization of the regional geology for the Fresno study area was represented, as shown in Figure 6, by three different formations: (i) younger sediments; (ii) older sediments; and (iii) bedrock. The estimates of the formation geology and pump test information were used to characterize the distribution of saturated hydraulic conductivity (Loague *et al.*, 1998b). The pumping histories from 408 wells within the study area were included in the simulations.

The numerical model used for the one-dimensional simulations (Loague *et al.*, 1998a) of dissolved phase DBCP concentration profiles in the unsaturated zone was PRZM-2 (Mullins *et al.*, 1993). The potential fate and transport of DBCP between the surface and the water table for multiple NPS applications, related to different and changing land use between 1960 and 1977, was quantitatively estimated for 1172 elements for a 35-year period. The aggregate of the DBCP concentrations loaded to the water table for each grid element make up the annual loading files for the three-dimensional saturated transient transport simulations. The numerical models used for the three-dimensional simulations (Loague *et al.*, 1998b) of saturated subsurface

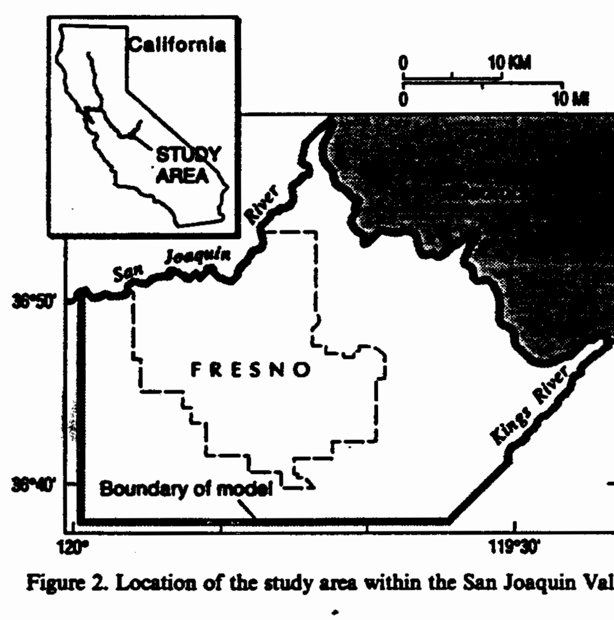

Figure 2. Location of the study area within the San Joaquin Valley

fluid flow and DBCP transport are MODFLOW (McDonald and Harbaugh, 1988) and MT3D (Zheng, 1992), respectively. Recharge to the water table for the saturated simulations was estimated as the residual (precipitation plus irrigation minus evapotranspiration) in the PRZM-2 water balance simulations. The area focused upon for the saturated simulations was represented by a three-dimensional finite-difference grid made up of 76440 elements, i.e. 2184 1 km^2 surface elements with 35 layers. The total volume of the boundary value problem is approximately 3604 km^3.

The steps used by Loague *et al.* (1998a,b) to simulate the effect of multiple DBCP applications under changing landuse and groundwater pumping/recharge in the Fresno study area are summarized below.

1. Approximate the climatic history (1950–1994) using rainfall, temperature and pan evaporation data from the Fresno area.
2. Approximate the distribution of the major soil orders, based upon soil taxonomy and the mapped soil series.
3. Approximate the land cover history (1958-1994), based upon aerial photographs.
4. Approximate the average irrigation history (1960–1994).
5. Approximate the water table depth history (1960–1994).
6. Simulate (with PRZM-2) the transient vertical unsaturated fluid flow and DBCP transport for 1172 separate 1 km^2 elements (1960–1994).
7. Abstract the DBCP concentration at the water table for each element (1960–1994), based upon the simulated last day of the year concentration profiles.
8. Approximate the geology, based upon well logs.
9. Approximate the distribution of saturated hydraulic conductivity.
10. Approximate the recharge history (1960–1994).
11. Approximate the pumping history (1960–1994).
12. Simulate (with MODFLOW) three-dimensional groundwater flow for 35 separate years (1960–1994) i.e. one steady-state simulation for each year.
13. Simulate (with MT3D) three-dimensional saturated transient DBCP transport for 35 years (1960–1994).

The Fresno case study results

The aggregate of DBCP loaded at the water table for the entire simulation period is shown in Figure 7; Loague *et al.* (1998a) show snapshots of the water table loading for several individual years. The near-surface simulation results for the 35-year period lead to the following general comments related to the concentrations of DBCP loaded to the water table (Loague *et al.*, 1998a).

1. The areas most likely to facilitate DBCP leaching through the entire unsaturated soil profile are targeted.
2. The first appearance of DBCP above the detectable limit at the water table is simulated as most likely occurring between 1961 and 1965.
3. The estimated concentrations reaching the saturated subsurface exceed the MCL at several locations at different times. The first appearance above the MCL was between 1965 and 1970; by 1990, the concentrations are below the MCL.
4. Relative to the size of the study area, the extent and duration of the estimated contamination is small.
5. Concentrations are a function of the application rates and frequency; the highest estimates are associated with citrus and vineyards, the lowest estimates are associated with cotton.

6. Concentrations are a function of the unsaturated profile thickness. The longer the residence time the chemical has in the unsaturated zone the more opportunity there is for decay and vapour diffusion.
7. Concentrations are a function of soil hydraulic properties. The higher estimates are associated with the Alfisols and Entisols, the lower estimates are associated with the Inceptisols, Mollisols and Vertisols.
8. Concentrations are a function of near-surface sorption. The higher estimates are associated with the Entisols and Vertisols, the lower estimates are associated with Mollisols.

Figure 8 illustrates the simulated water table elevations for the study area for a single year and the simulated concentrations for the DBCP plume for three individual years; Loague *et al.* (1998b) show observed versus predicted water table elevations and DBCP concentrations for several individual years. The simulation results for the saturated subsurface for the 35-year period lead to the following general comments related to the fate and transport of DBCP in the study area (Loague *et al.*, 1998b).

1. The MODFLOW and MT3D simulations appear, in a qualitative sense, to be quite reasonable without the aid of calibration.
2. The direction of groundwater flow and the movement of the plume is from the east to west.
3. The plume evolves (grows and retracts) with time owing to the loading rates at the water table.
4. The plume does not migrate into the older sediments during the simulation period.
5. The simulated concentrations, for the base case, are below the MCL.
6. The shape and movement of the plume correlates well with the estimated application history.

DISCUSSION

The Fresno case study and GIS

The coupled modelling approach employed for the Fresno case study facilitated the simulation of an extremely complicated problem in an efficient manner. GIS facilitated the preparation of the individual data overlays (e.g. soils, land cover, water table depth, geology). In addition, GIS greatly enhanced the presentation of the simulation effort reported here and by Loague *et al.* (1998a,b). For example, Figures 3–6 begin to show the variability of the tremendous amount of information needed to excite the models, while Figure 7 shows the variability in the near-surface leaching results.

The PRZM-2 simulations were designed to characterize the non-intuitive interplay between climate, soil type, land use and chemical properties as related to the long-term leaching of DBCP in the Fresno study area. The results from the near-surface portion of the Fresno case study (Loague *et al.*, 1998a) illustrate, for the best estimates of historical chemical use patterns, soil properties and water table depths, that DBCP can be expected to leach to groundwater in Fresno County as a result of regional-scale, agricultural-related applications. The simulated leaching history for DBCP in Fresno County suggests that the pesticide has migrated from the surface to the water table in detectable concentrations and at some locations these concentrations exceed the MCL. The results suggest that future DBCP loading at the water table, resulting from past applications, will be below the detectable limit.

The MODFLOW and MT3D simulations were designed to characterize the non-intuitive interplay between DBCP loading at the water table, recharge, pumping and regional groundwater flow as related to the long-term fate and transport of DBCP in the Fresno study area. The results from the saturated subsurface portion of the Fresno case study (Loague *et al.*, 1998b) illustrate the three-dimensional evolution of the DBCP plume in the Fresno study area over a 35-year period based upon our best estimates of hydrogeological parameters, water table depths and pumping rates. The simulated DBCP concentrations are limited to the relatively shallow younger sediments and are generally well below the MCL. The simulations suggest that NPS applications of DBCP are not responsible for the observed 'hot spots' in the study area (see

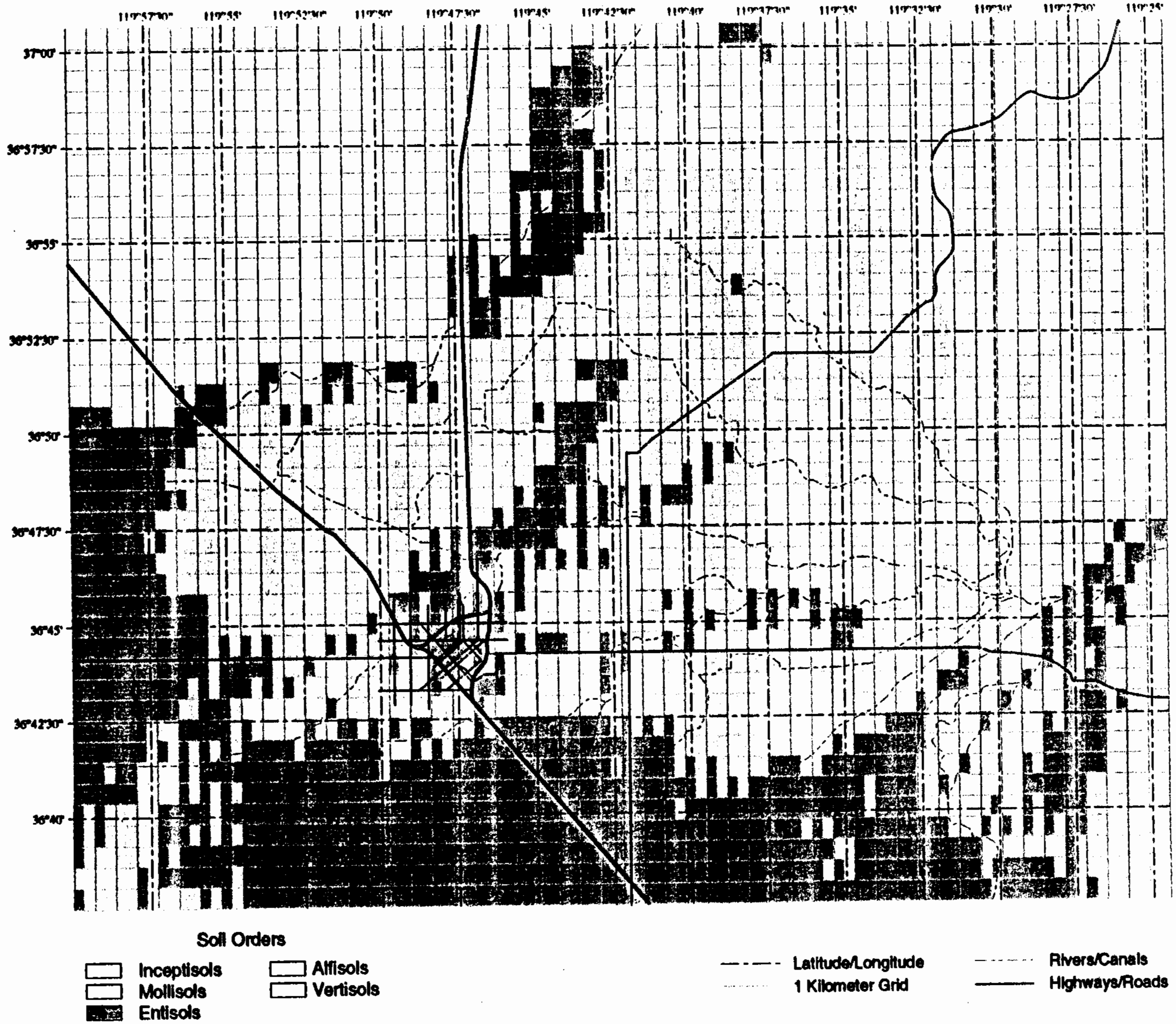

Figure 3. The distribution of soil orders within the study area. The study area corresponds, approximately, to east-central Fresno County; the location of the city of Fresno is earmarked by the road intersections in the lower left quarter of the map

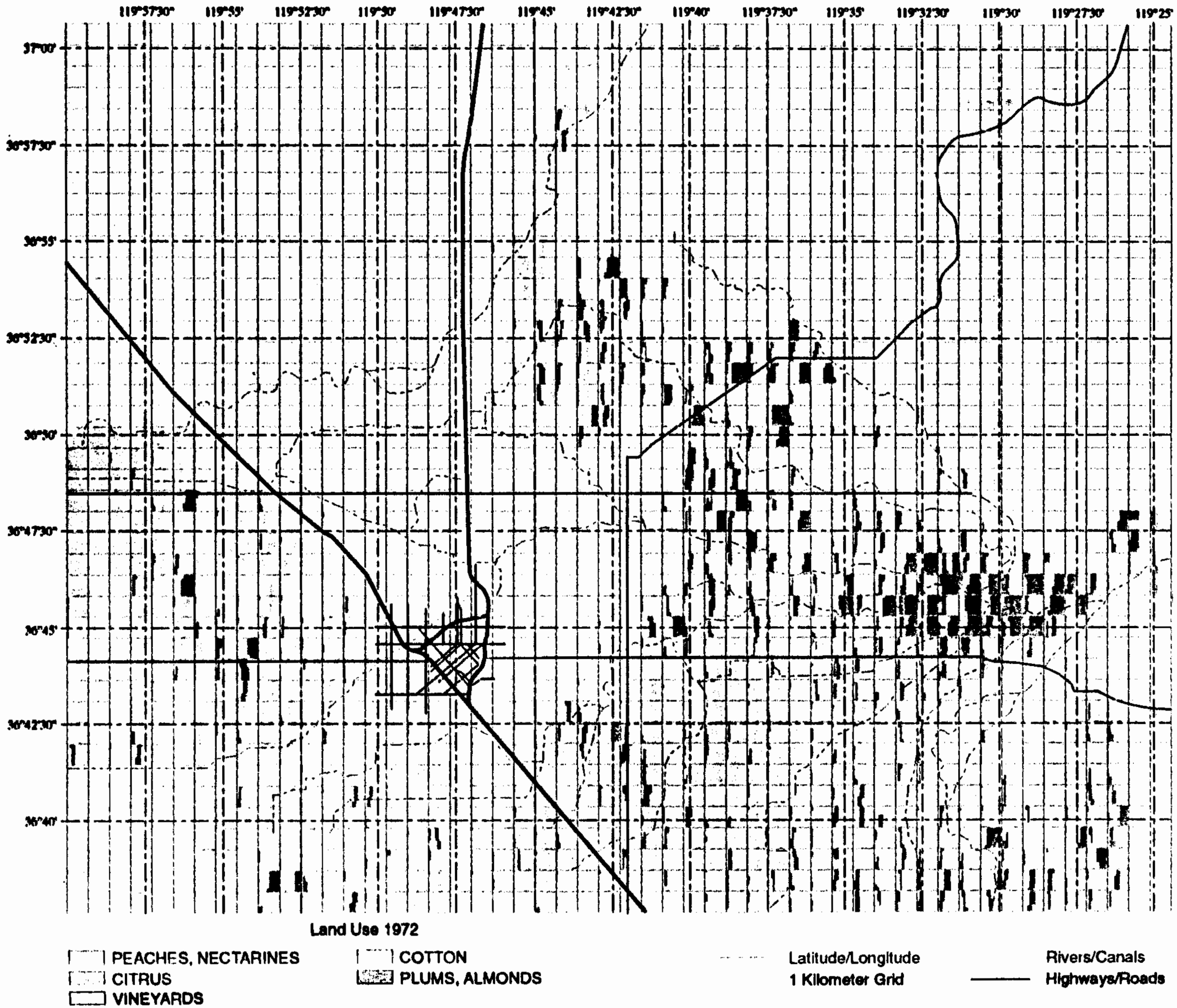

Figure 4. Land cover representation (1972) for the study area

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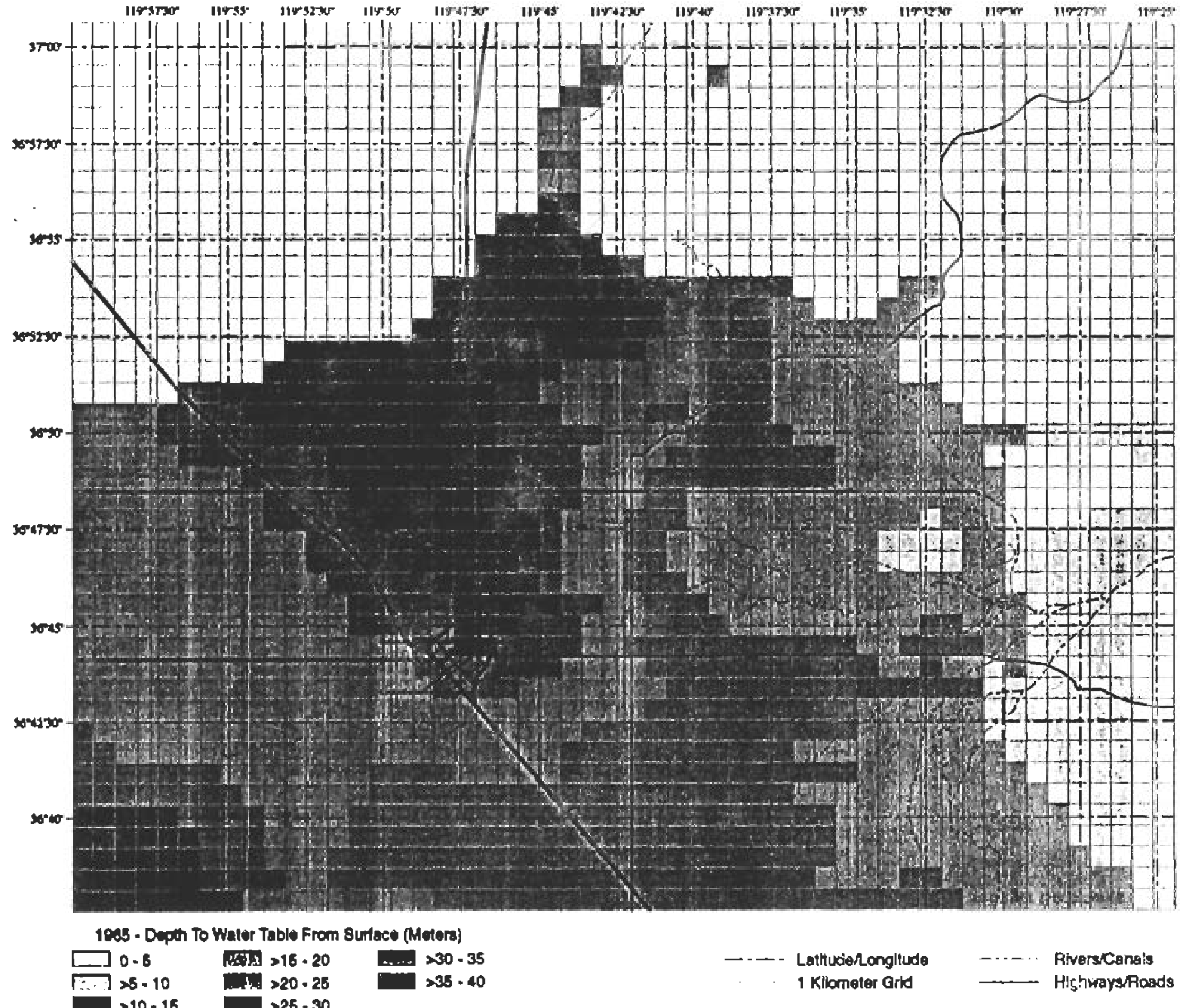

Figure 5. Estimated depth to the water table (from the land surface) for the study area in 1965

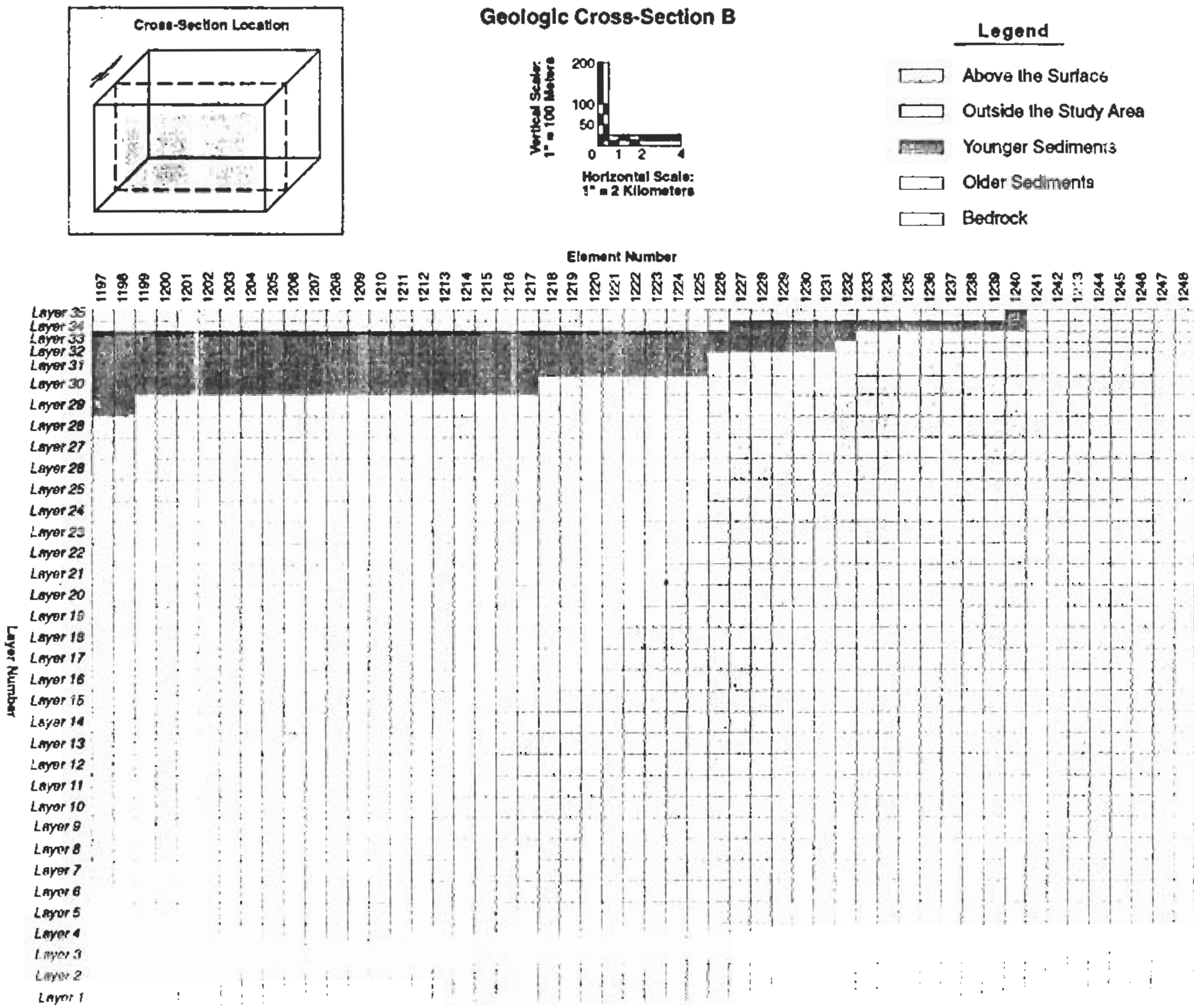

Figure 6. Estimated east west cross-section of the study area geology. The upper portion of the sedimentary sequence is dominated by late Cenozoic stream deposits which contain the water-bearing zones of interest in the simulation effort (see Loague *et al.*, 1998b)

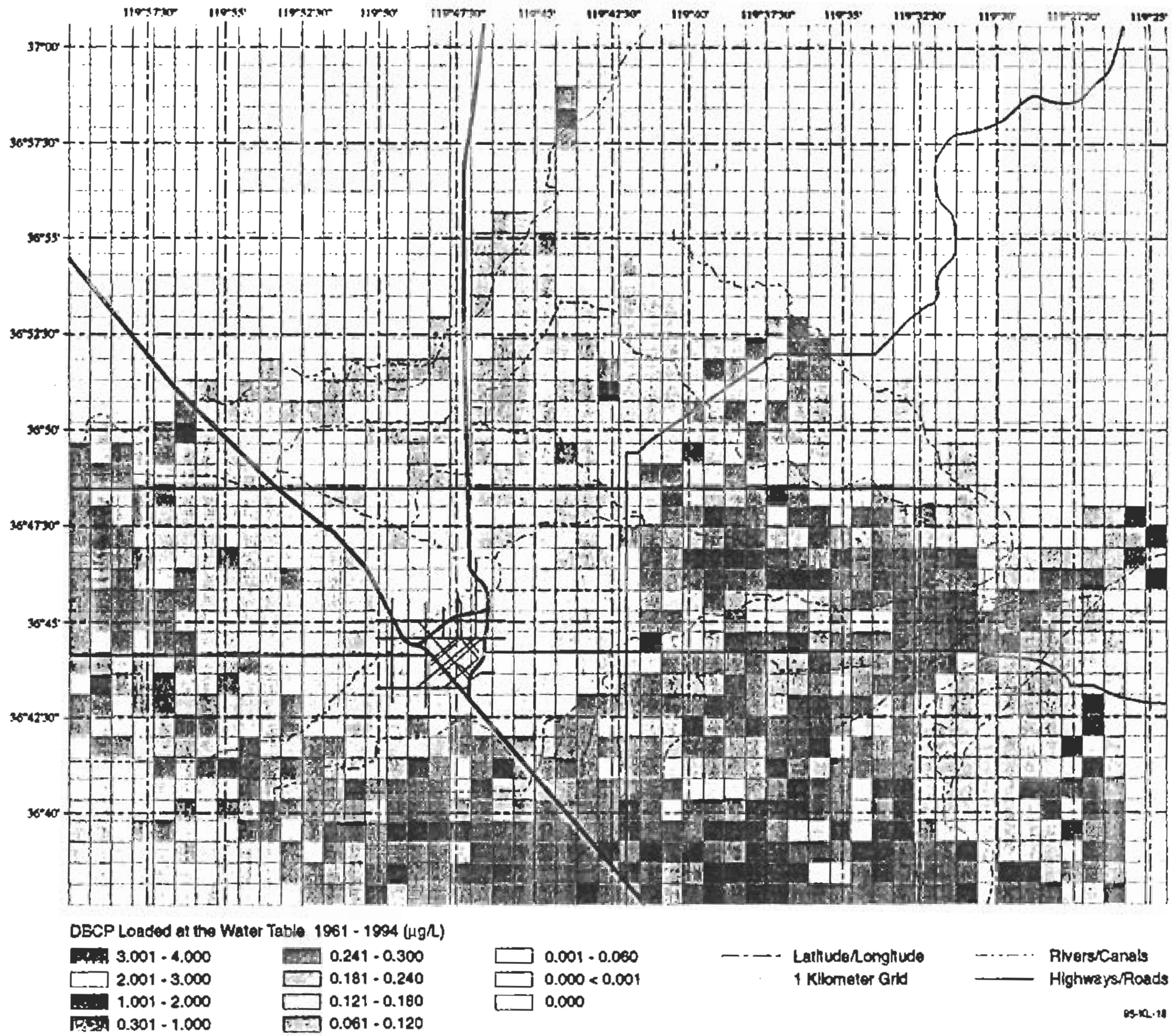

Figure 7. Total simulated DBCP loading at the water table between 1960 and 1994 for the study area

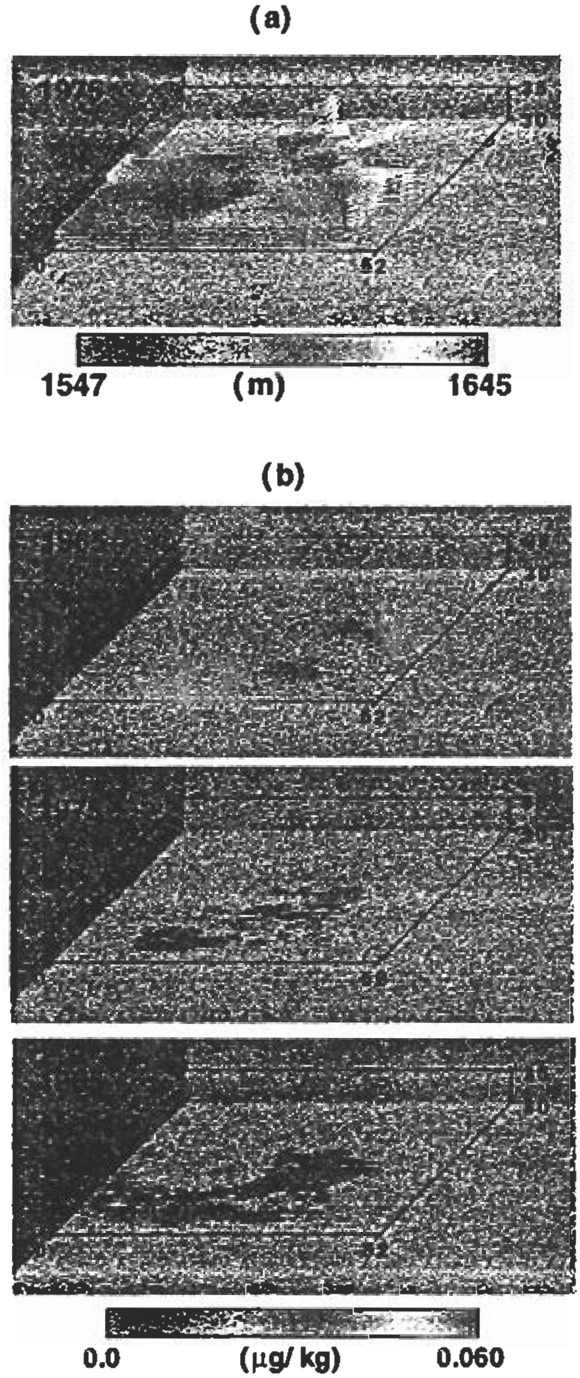

Figure 8. (a) Simulated water table elevations for the study area for 1975. (b) Simulated DBCP concentrations for the study area for 1965, 1975 and 1985

Loague *et al.*, 1998b); it is quite possible that these isolated high concentrations are a result of point source loading (e.g. spills at field mixing sites, down-well dumping and/or burial).

Uncertainties in regional-scale assessments

Why model? In general, there are two idealized uses for simulation in hydrology. The first is the prediction (or forecasting) of future events based upon a calibrated and validated model. The second use is the development of concepts for the design of future experiments to improve the understanding of processes. The Fresno case study reviewed in this paper was intended for both prediction and concept development.

There are three sources of error inherent to modelling in hydrology: (i) model error; (ii) input error; and (iii) parameter error. Model error results in the inability of a model to simulate the given process, even with the correct input and parameter estimates. Input error is the result of errors in the source terms (e.g. soil water recharge and chemical application rates). Input error can arise from measurement, juxtaposition and/or synchronization errors. Parameter error has two possible connotations. For models requiring calibration, parameter error is usually the result of model parameters that are highly interdependent and non-unique. For models with physically based parameters, parameter error results from an inability to represent aerial distributions on the basis of a limited number of point measurements. The aggregation of model error, input error and parameter error is the total (or simulation) error. For multiple-process and comprehensive models, simulation error is complicated further by the propagation of error between model components.

In general, the methods for characterizing uncertainty can be grouped into three categories (Loague and Corwin, 1996): (i) first-order analysis; (ii) sensitivity analysis; and (iii) Monte Carlo analysis. First-order analysis is a simple technique for quantifying the propagation of uncertainty from input parameter to the model output. The first-order approximation of functionally related variables is obtained by truncating a Taylor series expansion (about the mean) for the function after the first two terms. Sensitivity analysis is used to measure the effect that changing one factor has on another. The sensitivity of a model's output to a given input parameter is the partial derivative of the dependent variable with respect to the parameter. Monte Carlo analysis is a stochastic technique for characterizing the uncertainty in complex hydrological response model simulations. The Monte Carlo method considers each model input parameter to be a random variable with a probability density function (PDF). Monte Carlo simulations are based upon a large number of realizations, from every input parameter distribution, created through sampling the different PDFs with a random number generator. A separate hydrological response simulation is made for each parameter realization. The number of possible simulations, based upon all the combinations of parameter realizations, is infinite; therefore, a finite number of cases (usually several hundred) are usually investigated. Estimates of the average simulated hydrological response, and the associated uncertainty, are made from the combined outputs of the simulations (i.e. the total ensemble of the different realizations). Loague and Corwin (1996) provide examples of first-order uncertainty analysis, sensitivity analysis and Monte Carlo simulation.

Assessments of NPS groundwater vulnerability rest upon soil, climatic and chemical data that are extremely sparse at regional scales and, therefore, contain considerable uncertainty. The implications of the uncertainties associated with data and model errors, as well as data worth consideration, are discussed in the review by Loague *et al.* (1996) for regional-scale groundwater vulnerability assessments in Hawaii. The ongoing phase in the coupled simulation effort discussed in this paper is the quantitative characterization of the uncertainties (i.e. model and data errors) for the regional-scale NPS assessment of groundwater vulnerability for east-central Fresno County.

Risk assessment for regional-scale vulnerability

Management decisions that result from environmental policy assessments of NPS pollution require an approach that integrates physical and social sciences in a decision framework. Conceptual economic models for estimating the effects of agricultural production and environmental residuals have been developed, in a point source framework, in parallel with, but not rigorously coupled to, physics- and chemistry-based process models of near-surface solute transport. These economic models are based on an individual farm unit's production. The farm unit models are used to evaluate agricultural and/or environmental policy issues both on an individual basis and on a regional scale. While these models are of value, we do not consider them to be relevant for regional-scale policy analysis because of the uncertainties inherent in spatial environmental data.

At a regional scale, the utility of scientific data lies in the ability to screen areas of greater (lesser) potential for groundwater contamination. Instead of collecting soils information at a sufficient number of sites to be able to apply geostatistics efficiently for identification of spatial structure, for use in GIS-based regional-scale environmental risk assessment, Loague *et al.* (1996) propose a regional integrated assessment (RIA) approach. The RIA method, based on cost–benefit analysis, incorporates both physical (spatial point processes) and economic (states of nature) variables in a regional screen that can be included as a protocol in a regulatory decision process. The screening process uses GIS as an analytical tool to identify areas that have a relatively high probability for loss based upon a variety of physical factors. For example, physical factors, such as mobility indices, may be used to represent dynamic hydrological processes. The model is then cast in a decision framework and follows a generic procedure. The results of an RIA would be presented as an environmental risk map. The following four steps make up an RIA evaluation (Loague *et al.*, 1996).

1. Areas that would require mitigation are identified.
2. For each area, a probabilistic hazard map (includes mean and variance) is estimated and compiled as a function of physical attributes.
3. The cost of the required mitigation in each area is estimated.
4. For each area identified as requiring mitigation, the expected mitigation cost (loss) avoided is estimated as the product of the probability of the hazard and the cost of mitigation.

CONCLUSIONS

GIS-based models of NPS pollutants in subsurface soil and water systems have proliferated over the past decade. The acknowledged trend in the coupling of GIS with environmental models will continue at an even greater pace because of the introduction of cheaper, desktop GIS software that is customizable to the application and to the growing demand for spatial environmental information. Without question, GIS is serving as a catalyst to bring solute transport modelling, data acquisition and spatial databases into a self-contained package to assess NPS pollutant problems. Yet, a cautionary footnote is needed, because the sophisticated visualizations created from GIS should never disguise the legitimacy of the rendered results nor should simulated results ever supplant field observation (Corwin *et al.*, 1998).

The case history simulations discussed in this paper provide a good starting point for understanding the regional-scale fate and transport of DBCP in east-central Fresno County, which could not have been obtained without the coupled process-based simulation effort and GIS. It is our opinion that for regional-scale groundwater vulnerability assessments to be of any significance relative to future regulation of agrochemical use the approaches to be developed must include: (i) concentration profile estimates in time and space; (ii) epidemiologically based contamination levels of concern relative to human health; and (iii) economic constraints. The next step in our own work is to incorporate economic constraints into stochastic–conceptual groundwater vulnerability assessments at regional scales.

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