

# 14 Unsatchemgeo: Modeling Water Flow and Multicomponent Solute Transport in a GIS Context

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## ABSTRACT

The one-dimensional version of the Unsatchem model was interfaced to a geographic information system (GIS). Unsatchem is a finite-element model of water flow in the vadose zone coupled with multicomponent solute transport, production and transport of CO<sub>2</sub>, and heat in addition to a major ion model of chemical speciation and kinetics. The new version, Unsatchemgeo, runs in a geographic context in association with the GIS, such that data required by the model are obtained directly from database tables and computed results are written to other database tables. This direct method for input and output of data is faster by a factor of 4.7 than an earlier approach utilizing the native macro language of the GIS. Support programs were written for initial generation of the INFO database and input of data in text form. To investigate the advantages and limitations of the coupled approach, Unsatchemgeo simulated water movement in a tile-drained agricultural field. Observed cumulative drainage flow from the tile drain system is greater than calculated drainage through the lower boundary of the model, by a factor in the range 1.2 to 2.1, for all times and at all locations. Also, the onset of increased tile drain flow occurs prior to the start of irrigations. These results and observations indicate the existence of water sources for drainage other than water supplied during irrigation of this field,

The Unsatchem model, a finite-element code for solution of coupled flow problems, treats water flow, multicomponent chemical transport, heat transport, CO<sub>2</sub> transport, and plant root water uptake in the vadose zone (Suarez & Šimunek, 1992; Šimunek & Suarez, 1994). This chapter reports the coupling of the one-dimensional version of Unsatchem to the ARC/INFO<sup>1</sup> GIS system. Coupling involved a rewrite of portions of the original Unsatchem program to facilitate operation in a geographic context and the addition of routines for interfacing Unsatchem to ARC/INFO. The chapter is concerned with issues relevant to data manipulation when coupling a complex model such as Unsatchem to a geo-

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<sup>1</sup> The use of brand names in this report is for identification purposes only and does not constitute endorsement by the U.S. Dept. of Agriculture.

graphic database. The emphasis of the chapter is on methodology. But, there also is a representative calculation of water flow in an irrigated, agricultural area. Results of this calculation are compared with measured tile drain flows.

## GIS

Geographic Information Systems (GIS) provide methods of storing, retrieving, and displaying geographically-based data. GIS is commonly used in scientific applications for spatial analysis that is analysis requiring both locational and attribute data (Goodchild, 1988). Use of GIS in hydrology has been expanded to include water flow modeling in both groundwater (El-Kadi et al., 1994; Roaza et al., 1993; Baker & Panciera, 1990) and in the vadose zone (Vaughan & Corwin, 1994). Coupling of the various flow models to a GIS creates a functional environment for display and spatial analysis of both input data and computed results.

One example of a groundwater flow model that was coupled to a GIS is MOC, a two-dimensional flow and transport model (El-Kadi et al., 1994). MOC is loosely-coupled to the GIS, meaning that the numerical model is running as a standalone program with data transfer accomplished by means of text files. The GIS contained data for specific locations where measurements were made. Interpolation of this spatial data provided property data for meshpoints in the numerical model. This was accomplished by combining a program written in a GIS programming language with an external gridding routine (El-Kadi et al., 1994).

A similar approach was developed for TETransgeo that calculates one-dimensional vertical redistribution of water and a single solute (Vaughan & Corwin, 1994). TETransgeo is a loose coupling of the original TETrans program (Corwin et al., 1991) to ARC/INFO involving the creation of internal data structures for storage of all the GIS-based data required for the model. The TETransgeo program is a standalone application with standard text file input and output. Thus, both TETransgeo and MOC are independent of any particular GIS system. When TETransgeo is run from ARC/INFO, the text file containing the input data for TETransgeo is written using a program developed in the AML programming language (Arc Macro Language) which is part of ARC/INFO. The text file is generated from data stored in the INFO database. Likewise, the AML program reads results generated by the model back into the INFO database. This design is good from the standpoint of flexibility, both MOC and TETransgeo could be coupled with any GIS, but there is a cost in terms of reduced efficiency of processing, at least, in the case of TETransgeo.

Coupling a GIS to a vadose-zone, water flow and transport model involves finding a model that performs a realistic calculation, but does not overwhelm the computational capability of a standard workstation (calculations discussed in this chapter were conducted on a Sun SPARC 2). Some possibilities for transport models are: (i) three-dimensional model run on a three-dimensional grid; (ii) two-dimensional model oriented to take advantage of symmetry in the flow field; or (iii) one-dimensional model calculated for vertical flow. The disadvantage of a three-dimensional model is complexity and lack of knowledge of boundary conditions especially on the sides of a model for a geographic area. Vertical transport

modeling of unsaturated flow in the root zone generally requires a grid-spacing of about 0.01 m. If the horizontal grid-spacing was approximately the same as the vertical spacing then modeling an area large enough that GIS methods were appropriate would be too large a problem. Adaptive mesh refinement would mitigate this problem but, for the near future, detailed three-dimensional modeling of water flow and chemical transport in the root zone on a scale appropriate to GIS is not a viable option. Calculations on the scale of field plots (<100 m<sup>2</sup>) may be a possibility.

A two-dimensional model is a more workable alternative in terms of problem size, but the usefulness of two-dimensional models is limited to situations where symmetry permits two-dimensional modeling of the flow field. Regions commonly treated by GIS are irregular and certainly soil units generally lack symmetry. While two-dimensional modeling may be applicable to areas where there is strong evidence for a planar flow field, such modeling will not be generally applicable in a GIS context.

The one-dimensional model appears to be the best choice for GIS applications, at least for the near future. One-dimensional water flow and solute transport calculations could be conducted in various ways: (i) at geographical locations on a grid; (ii) at individual point locations unconnected to a grid; or (iii) as calculations representing a small area characterized by a uniform set of material properties, boundary conditions and initial conditions. Method 1 requires data on material properties, boundary and initial conditions, and sources or sinks at each point on the grid. Taking actual field data at a large set of gridded points is logistically difficult and time-consuming, but kriging and cokriging algorithms could interpolate isolated measurements onto a grid. Method 2 simply runs the calculation at isolated points where actual measurements of soil properties and initial conditions were made. Method 3 would be best when applied to larger areas. An area could be divided into units where each datum relevant to the calculation is represented as a separate layer in the GIS. In each layer, polygons could be defined representing approximate invariability in the layer datum. The spatial overlay features of the GIS would then further subdivide the area into polygons defined as areas where material properties, boundary conditions and initial conditions were all spatially invariable.

### Unsatchem-One-Dimensional

Water flow in the one-dimensional version of Unsatchem is described by the Richards equation,

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[ K \left( \frac{\partial h}{\partial z} = 1 \right) \right] - S \quad [1]$$

where  $\theta$  is the volumetric water content (L<sup>3</sup>L<sup>-3</sup>),  $K$  is the hydraulic conductivity (LT<sup>-1</sup>),  $h$  is the hydraulic head (L),  $S$  is a source-sink term (L<sup>3</sup>L<sup>-3</sup>T<sup>-1</sup>),  $t$  is time (T), and  $z$  is the vertical coordinate increasing upwards. Unsatchem uses the water retention function proposed by van Genuchten (1980). The main assump-

tion in applying Eq. [1] to water flow in the vadose zone is no influence of the air phase on water flow.

Boundary conditions used in the demonstration calculation presented in this chapter are:

$$-K \frac{\partial h}{\partial z} - \mathbf{K} = q_0(t) \quad [2]$$

where  $q_0(t)$  is the prescribed water flux at the soil surface ( $z = L$ ). At the bottom of the soil column, there is a free drainage boundary condition (unit vertical hydraulic gradient),

$$\frac{\partial h}{\partial z} = 0 \quad z = 0 \quad [3]$$

The actual flux at the soil surface is calculated by the program and depends on atmospheric and soil conditions (Suarez & Simunek, 1992). The Unsatchem program has several other modules for calculation of multicomponent solute transport, heat transport, and so on, but the only module used in the demonstration calculation reported here is the water flow module.

## MATERIALS AND METHODS

### Coupling Unsatchem to a GIS

The main advantage of storing and manipulating geographically-based data in a GIS system as opposed to storing data in text files is access to the operations that can be performed by the system. These include preparation of maps, selection of records, sorting, calculations, and plotting. These GIS operations provide a much more flexible way of pre- and post-processing the data for a flow calculation. For Unsatchem, so much data is being processed that some kind of database storage would be useful even if the program were not run in a geographic context.

A GIS stores both geographic and attribute data. The attribute data consist of all the non-spatial information related to a geographic feature. Attribute data are stored and manipulated in the INFO portion of the ARC/INFO package. Examples of attribute data required by Unsatchem are daily actual evapotranspiration, parameters needed for determination of hydraulic conductivity, concentrations of dissolved chemical species, and many others. All these data are organized into INFO tables, each table having a certain theme. For example, a theme could be crop characteristics. The INFO table for crop characteristics is named RCROP and stores a crop identification number (CROPID), a crop name (CROPNM), a minimum rooting depth (XRMIN), and several other crop-specific items. Another example is the CROPSCHEDxx table which stores a schedule of planting dates and crop growth data for individual fields (Fig. 14-1). The xx portion of the table name is an identification number for a field. Tables that have such a number

COL	ITEM NAME	WIDTH	O.W.	TYPE	N.DEC
1	FSECID	4	5	B	
5	CROPID	4	5	B	
9	TRMIN	8	15	F	3
17	TRMED	8	15	F	3
25	TRMAX	8	15	F	3
33	XRMED	8	15	F	3
41	XRMAX	8	15	F	3

Fig. 14-1. INFO table definition for a crop schedule table. The width is in bytes, O.W. means output width in characters and types are binary integer and float. N. DEC refers to the number of decimal places. Details on the five variables are available (Simunek & Suarez, 1992).

appended to their names, contain data that are specific to that field. Tables containing data that are not field-specific have exclusively alphabetic names.

All INFO tables that are part of the database contain at least one item that is an integer identification number. These numbers are essential for maintaining the uniqueness of individual records in the table. The crop schedule table has two such numbers, the FSECID (field-sector identification number) and the CROPID (crop identification number). The field-sector identification number is a composite of a field identification number and sector number for a sector within the field. Sectors are necessary because fields are sometimes split up with different crops growing in separate areas. Other items in the CROPSCHEDxx table store significant dates such as the date for the start of root growth (TRMIN), the date of known rooting depth (TRMED), and the harvest date (TRMAX). Finally, this table stores the minimum rooting depth (XRMIN) and the known rooting depth (XRMED). Thus, the crop schedule provides data for the sequence of crops that were grown in a particular sector of a field during the period of a calculation.

Identification codes such as the field-sector number (FSECID) provide the means by which tables are related to each other. The operation, which uses a specific value of an identification code in one table to select a specific record from another table, is called a *relate*. Establishing relates between tables makes data from different tables accessible simultaneously. Thus, completely new, virtual tables can be created by combining items from various existing tables. For example, a relate between a table containing the geographic locations of points and the crop schedule table shown in Fig. 14-1 would facilitate the display of known rooting depths at individual locations. The relate would go from the FSECID number present in the location table to the FSECID number in the crop schedule (Fig. 14-2). The known rooting depth is stored in the crop schedule; thus, the single relate between the two tables is sufficient to display these data.

A stacked relate is one that involves more than just two tables. An application of a stacked relate is the generation of a crop map for some specified date. A crop map requires geographic information in the form of polygon data in order to draw the outlines of each sector. Such data are accessed by ARC/INFO, when a command to draw the map is issued. A special INFO table exists, called a polygon attribute table, which contains unique identification numbers for each poly-

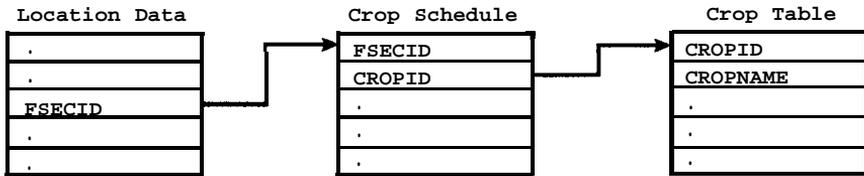


Fig. 14-2. Diagram illustrating the operation of relates between tables in the database. The matching of identification numbers in different tables allows individual items from several different tables to appear together in a newly-constructed table which may exist temporarily for the purpose of data representation in a map, graph or printed table. The table represented on the left is either a point attribute table or a polygon attribute table depending on how it's referred to in the text.

gon that is drawn. For the field-sector polygons, these numbers are the FSECID numbers. Figure 14-2 shows how the FSECID in a polygon attribute table (location data) can be used to access the crop name in a crop table through a stacked relate. Ultimately, this access makes it possible to draw the map and print the name of the crop growing in each sector based on the specified date. The first relate accesses the crop schedule from the polygon attribute table. Then, a specific record is selected from the schedule by invoking the criterion that the supplied date must lie between TRMIN and TRMAX. Once the record is selected, a unique CROPID is associated with the sector. The CROPID can then identify the crop name and other information about the crop including the number of the color that was assigned to that crop for purposes of map representation.

The preceding discussion is provided as an illustration of how a geographic database would be used to create maps within a GIS context. Maps of input data or the results computed by Unsatchemgeo may be prepared by similar techniques.

### Organization of the Unsatchemgeo Database

Creating a geographic context in which to run Unsatchem required rewriting several modules in the program, notably, all of the input and output routines. Also, the main program was modified to loop through all point locations within a field and to loop through all fields in a region. Both input and output data for the new program, Unsatchemgeo, are stored in a database rather than text files. This is more appropriate considering the large amount of data needed to characterize a geographic area.

The Unsatchemgeo database contains data at varying levels of specificity. Data, such as initial water content, are required at various depths for the water flow portion of the model. These data are highly-specific, having a separate value for each node in the finite-element calculation. There is a vertical array of nodes at each point location in the area. By contrast, only a single value is required for the maximum number of iterations allowed in the water flow model. This number will always be the same regardless of location; thus, there is a strong incentive not to include this number in tables that have records for each location, in order to avoid unnecessary duplication. This type of problem is addressed by organization of a database that is hierarchical, with tables near the top of the hier-

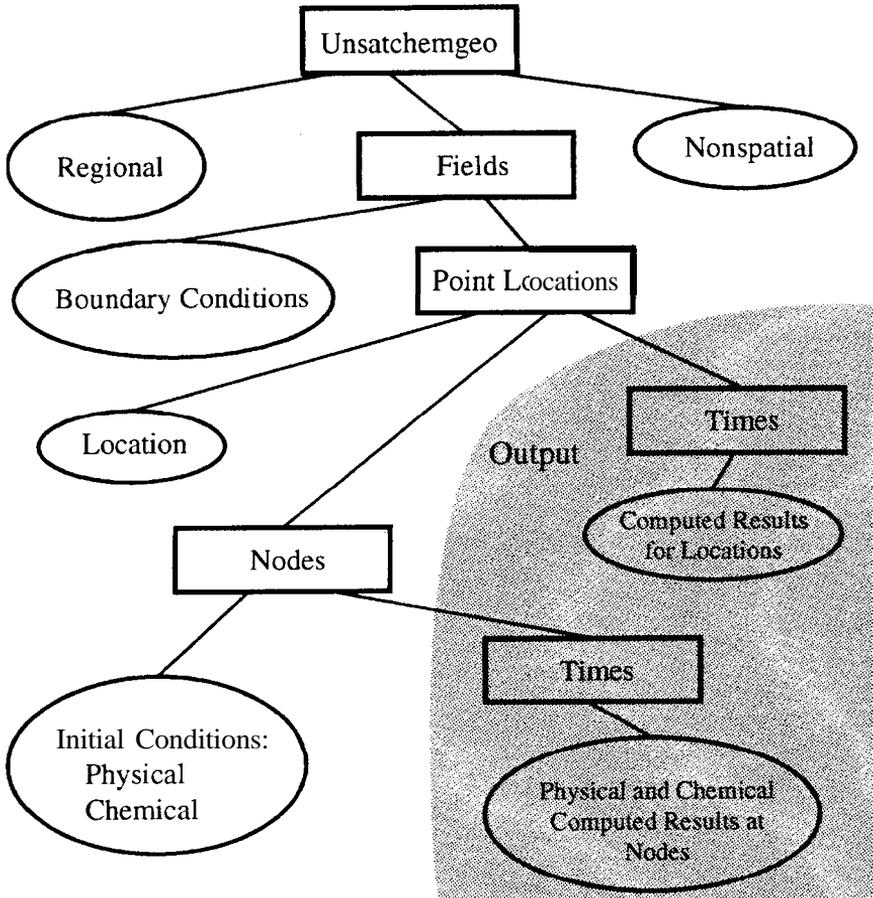


Fig. 14-3. Organization of data into database tables required for operation of Unsatchemgeo. The labels on the rectangular boxes in the unshaded area indicate the level of specificity of the input data. Boundary conditions, for example, are established for individual fields so they are field-specific. Each oval represents one or more database tables. The lowest level of specificity for output data is node-time, that is, a physical or chemical condition at a given node and some specified time.

archy containing fewer and more generalized data, while tables at progressively lower levels contain more specific data (Fig. 14-3). Links between the various tables are established by relates that are shown by connecting lines in the diagram.

The five rectangles indicate the varying levels of specificity (Fig. 14-3). At the top level, the *nonspatial* table contains only one record storing single values for various parameters relating to the calculation. An example would be maximum number of iterations. Other tables at this level include regional data, for example, soil properties such as saturated hydraulic conductivity. Tables at the *fields* level include storage of boundary conditions because, in the test case, these data are assumed uniform within a field. An example of data at the level of point

locations is the number of nodes to be used in the finite-element column at that location. Most input data are at the lowest level in the hierarchy and are specific to observation nodes. Normally, a subset of the nodes utilized in the finite-element grid are observation nodes. Initial conditions, such as measured soil water content, are stored in tables of observation nodes. Unsatchem does a linear interpolation to compute initial conditions at nodes located between the observation nodes (Suarez & Simunek, 1992).

When the Unsatchemgeo program is started, all INFO tables storing results of the calculation are purged of all records. Results are written either as time-stamped records for every time step, or, at designated times when a complete dump of all the current nodal values occurs. Thus, the location-specific and node-specific results are categorized separately (Fig. 14-3).

In view of the slow speed of Arc Macro Language (AML) programs and the large amount of data handled by Unsatchem, the approach to coupling the transport model to the GIS was fundamentally altered from the design for TETransgeo (Vaughan & Corwin, 1994). The Unsatchemgeo program is tightly coupled to the GIS meaning that data required by the program are obtained by reading directly from the INFO tables. This design change reduced the flexibility of Unsatchemgeo, but the presumed gain in efficiency was crucial because the Unsatchem model is computationally-intensive and a further speed reduction, due to slow AML processing of text files, would be unacceptable. Direct linkage to the INFO database bypassed the steps of reading and writing to external text files from AML or INFO programs. The relative speed of the AML processing approach and the direct method could not be assessed by comparing Unsatchemgeo and TETransgeo because the input and output operations were not easily separable from the rest of the code in either program. Instead, two test programs were written specifically to evaluate the two methods. These programs did nothing other than input and output operations. For an INFO table of 10 000 records, the AML method required 46.3 min for processing compared with 9.9 min for the direct method. Thus, a speedup factor of 4.7 was achieved. But, this number should not simply be generalized, the actual speedup for a program such as Unsatchemgeo depends on the type of calculation and other factors including output specifications. Another advantage of the direct method is robustness. If the Unsatchemgeo calculation should fail for any particular location, continuation at the next location is possible and results for all prior locations remain intact because they are now part of the INFO database.

### **Computer Programs Supporting Unsatchemgeo**

Unsatchemgeo reads data directly from INFO tables so some method for generating those INFO tables is required. This operation was divided into two parts. The first is creation of all the INFO tables from a text file containing table definitions (mkInfo program). The second is reading data from a text file into the INFO tables (rdInfo). These two programs are designed to be completely flexible, they will work with any program that requires INFO tables for input and output. In the rdInfo program, a distinction is made between scalar and vector data. Vector data, in this context, means data where multiple values for a single item

are provided. Unsatchemgeo and these two support programs have not been released for general distribution, as of this writing. But, a forthcoming U.S. Salinity Laboratory report will provide details regarding the operation of Unsatchemgeo and the two support programs, in addition to information on availability.

### **Test Application to the Broadview Water District Data Set**

A hierarchical system of INFO tables was created to store data for a study area consisting of 37 fields in the Broadview Water District of the San Joaquin Valley. The organizational approach divided up the water district into management units that are 64.7-ha fields. For some other area, the management units could be defined in a different way. A 100 by 100 m grid was overlaid on each field resulting in a set of 64 grid intersections. A subset of eight sampling points was statistically chosen from this set of intersections to retain the gross field variability (Lesch et al., 1992). Soil samples were taken at these locations at 0.3-m depth increments to a total depth of 1.2 m using an auger. Water content of these samples, collected in May of 1991, was determined by gravimetric methods. The gravimetric measurements of water content were converted to volumetric water content through the relationship with bulk density; however, bulk density measurements were not available for the samples collected in 1991. Therefore, a second set of soil samples was taken in May, 1993. In this sampling, two or three of the original sampling sites per field were revisited and sampled for bulk density at a depth of 0.3 m. Volumetric water content was calculated for the revisited sites from the bulk density data and the original gravimetric water content. Determination of volumetric water content at the remaining sites required spatial interpolation of the bulk density data. This was accomplished by ordinary punctual kriging of the entire bulk density data set. Initial conditions for the water flow calculation consisted of this set of volumetric water content data.

The top boundary conditions for the calculation were determined based on irrigation deliveries to individual fields. There is no information on precisely where irrigation water was applied within a field, but the timing and amounts of irrigation deliveries were carefully monitored. Irrigation events generally last 4 to 10 d and there are normally four to six irrigations during the summer growing season. The most common irrigation method in the Broadview Water District is flooding of furrows, but sprinklers also are used. In the calculation, evaporation of irrigation water was assumed to be zero. The prescribed infiltration rate was calculated for each irrigation event by dividing the total amount of water applied by the elapsed time during the irrigations. Thus, the boundary condition is assumed to be constant, uniform flux over an entire field during an irrigation. Unsatchemgeo recomputes the actual boundary condition at each time step. The user of the program can choose whether water will be allowed to pond at the surface, thereby creating a constant head boundary condition.

One field was chosen for a demonstration calculation. Soil in this field was mapped as Lillis clay by the Soil Conservation Service. This soil has between 50 and 60% clay content. Water retention and hydraulic conductivity data are not currently available for this soil and were estimated from a short database of soil properties related to soil texture (Carsel & Parrish, 1988). The van Genuchten

parameters ( $a$  and  $n$ ), the residual saturation,  $\theta_r$ , and the saturated hydraulic conductivity ( $K_s$ ) were assumed to be those listed for a sandy clay ( $a = 0.027$ ,  $n = 1.23$ ,  $\theta_r = 0.10$ ,  $K_s = 0.0288 \text{ m d}^{-1}$ ). The measured saturated water content was  $\theta_s = 0.45$ .

Unsatchemgeo determines potential root water uptake as the product of the potential transpiration rate and a normalized function that expresses the variation of root water uptake with depth (Suarez & Simunek, 1992). The function is further modified by the effects of water stress and osmotic stress (Feddes et al., 1978) to provide an actual transpiration rate obtained by integrating the product of all four of these functions from the surface to the current depth of the root zone. In the calculation discussed here, chemistry was not included, thus the osmotic stress could not be calculated. The rooting depth is determined from the Verhulst-Pearl logistic growth function or a function incorporating the growth degree day concept with the Verhulst-Pearl function (Simunek & Suarez, 1993).

Modeling of water flow was carried out for a field in which cotton (*Gossypium hirsutum* L.) grew during the period of the simulation. Root growth for cotton is assumed to follow the Verhulst-Pearl logistic root growth function with a maximum rooting depth of 2 m. The initial rooting depth is assumed to be 0.01 m. The time period of the simulation was 175 d starting on Day 128 of 1991. Daily actual evapotranspiration was calculated from,  $ET = ET_0 \times K_c$ , where  $ET_0$  is the reference crop evapotranspiration for grass (Jensen et al., 1990).  $K_c$  is the crop coefficient that varies over the growth period following a piecewise linear function. This function consists of an initial stage of slow growth, a period of rapid growth, a period of maturity when the coefficient is nearly constant, and a late stage of declining  $K_c$ . Values of  $K_c$  for cotton growing in the San Joaquin Valley were provided by the California Irrigation Management Information System. The soil depth range modeled in the calculation was 1.22 m. The boundary condition at the bottom of the simulated soil column was free drainage (Eq. [3]).

## RESULTS AND DISCUSSION

The new Unsatchemgeo program was applied to computation of vertical water flow in one field of the Broadview Water District. During the simulation period, the field was irrigated four times resulting in 0.43 m total depth of applied irrigation water. Within this field, the only spatially-variable quantity that is significant for the water flow calculation is initial water content. The solid lines on Fig. 14-4 are plots of the calculated cumulative amount of water drained from the soil column at each of the eight locations in the field. The first irrigation, from Day 177 to 186, caused an increase in drain flow starting about Day 185, but comparing this to the measured flow, which increases beginning about Day 160, suggests that the tile drainage system is taking water by lateral flow from other sources. Further evidence of the contribution of sources other than irrigation is the observed cumulative drainage that is greater than computed values for any of the locations by a factor of 1.2 to 2.1 (Fig. 14-4). Although lateral flow seems likely, there also is the possibility that some accidental spillage of water occurred in the area of the sump.

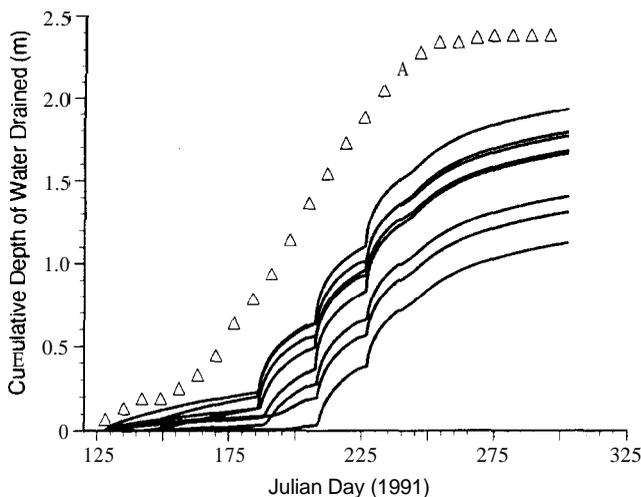


Fig. 144. Calculated cumulative drainage from 1.2 m soil columns (solid lines). Triangles represent cumulative tile drain flows based on weekly measurements. The observed cumulative drain flow exceeds the calculated flow by a factor between 1.2 and 2.1.

Initial mean volumetric water content at a location was calculated as the mean for the four observation nodes. The initial mean water content ranged from 0.361 to 0.424. But, there is no variability in computed water content among the various locations on Day 303, at the end of the computation, when the water content was 0.377. The lack of variability in water content at the end of the calculation is not surprising because the material properties and the boundary conditions are identical for all eight locations.

## CONCLUSION

The Unsatchem model was coupled to the ARC/INFO GIS. The one-dimensional version of the Unsatchem model was judged to be most appropriate for use in a GIS context. The I/O requirements of the Unsatchem model are too great for efficient operation of Arc Macro Language as an interfacing tool. Instead, lower-level routines written in a mixture of C and Fortran provided reasonably rapid processing. A demonstration calculation of water flow was run for eight locations within a single field in the Broadview Water District in California's San Joaquin Valley. Calculated cumulative drainage varied substantially due to differences in initial water content, although the calculated final water contents are identical at all locations. The observed drain flows start prior to the first irrigation raising the possibility of drainage from sources other than irrigation of the field.

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