

APPENDICES

APPENDIX 1

NUMERICAL SIMULATION OF GROUNDWATER FLOW

AT A SUPERFUND SITE:

CAPE COD STUDY

Cape Cod Study¹

Background

- site studied as part USGS program
- treated sewage through infiltration beds to aquifer since 1936 - 0.46 Mgal/d
- plume 11,000 ft long, 3000 ft wide and 75 ft thick
- chloride, detergents, boron, and 100 organic compounds (e.g., trichloroethene, tetrachloroethene dichlorobenzene)

Objectives in Modeling

- early stage - to understand processes and predict system response
- our use - to understand how models set up and applied

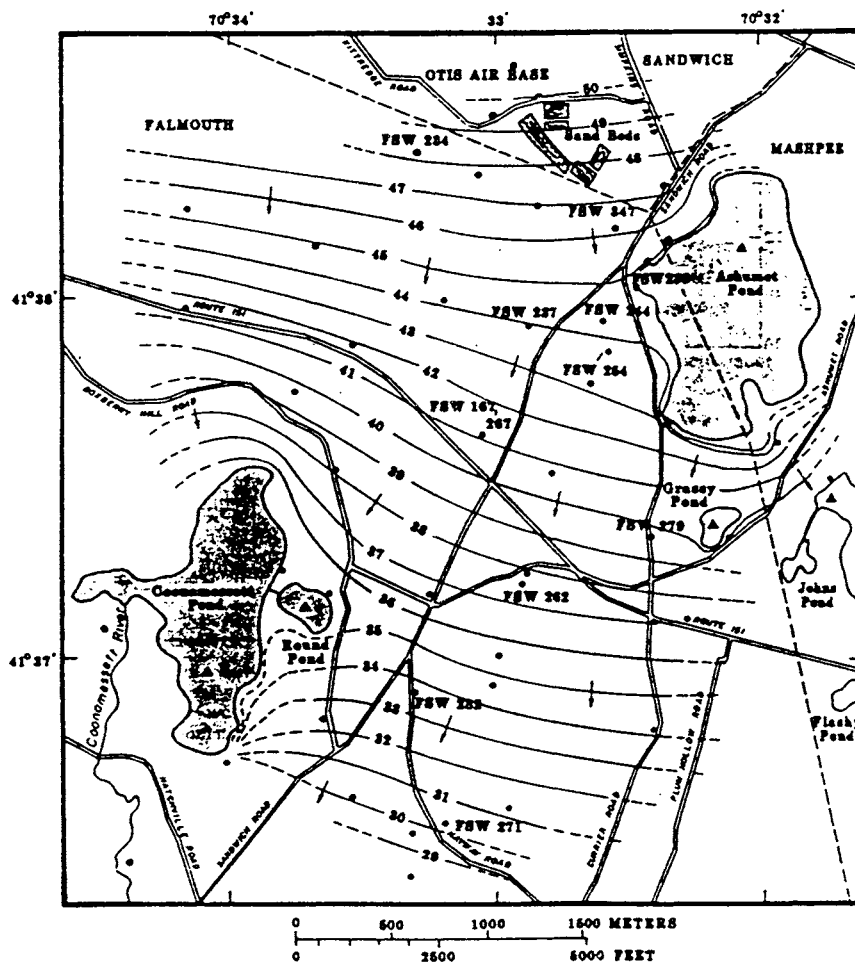
¹Adapted from USGS Open-File Rep. 84-475; 86-481

Geology

- glacial deposits overlying crystalline bedrock
- uppermost 90-140 ft stratified sand and gravel overlies silty sand and till

Hydrogeology

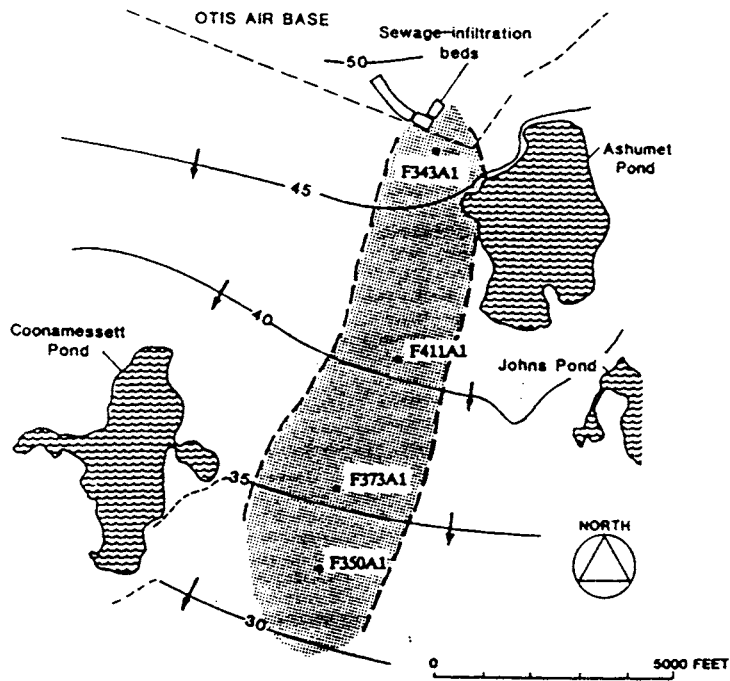
- hydraulic conductivity - 380 ft/d
- estimated, average groundwater velocity 1.5 ft/d



+ 35 --- WATER-TABLE CONTOUR, NOVEMBER, 1979---
 Shows altitude of water table. Contour interval 1 foot. Datum is sea level. Arrows show direction of ground-water movement. Contours dashed where inferred.

FSW 234
 ● WATER-LEVEL OBSERVATION WELL
 Number is well designation used in tables 2 and 4.
 ▲ POND AT WHICH WATER LEVEL WAS MEASURED

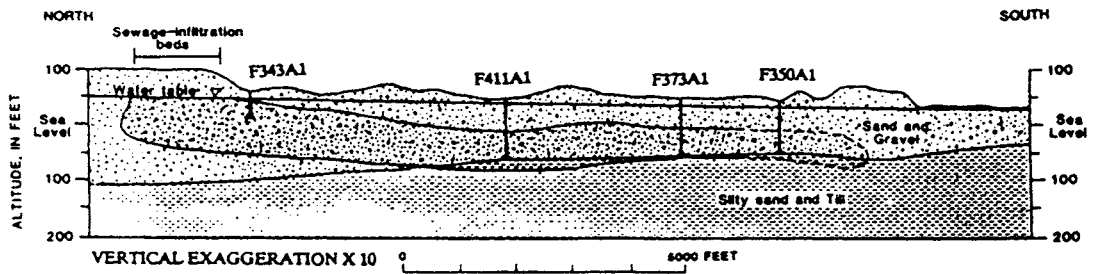
Plume Geometry



EXPLANATION

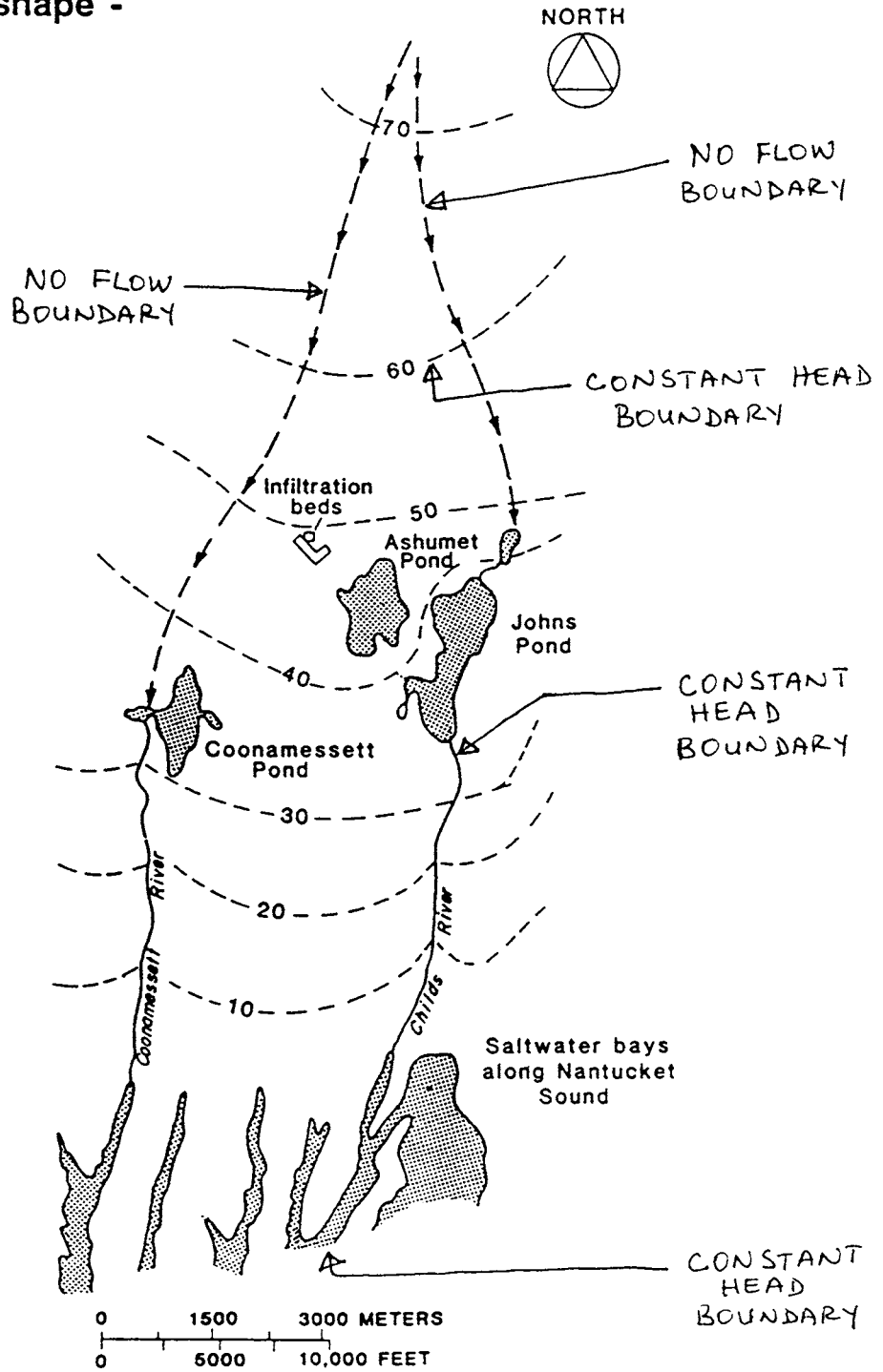


GENERAL AREA OF PLUME OF SEWAGE-CONTAMINATED GROUND WATER, AUGUST 1985—Area delineated by field observations of elevated specific conductance and foaming caused by detergents



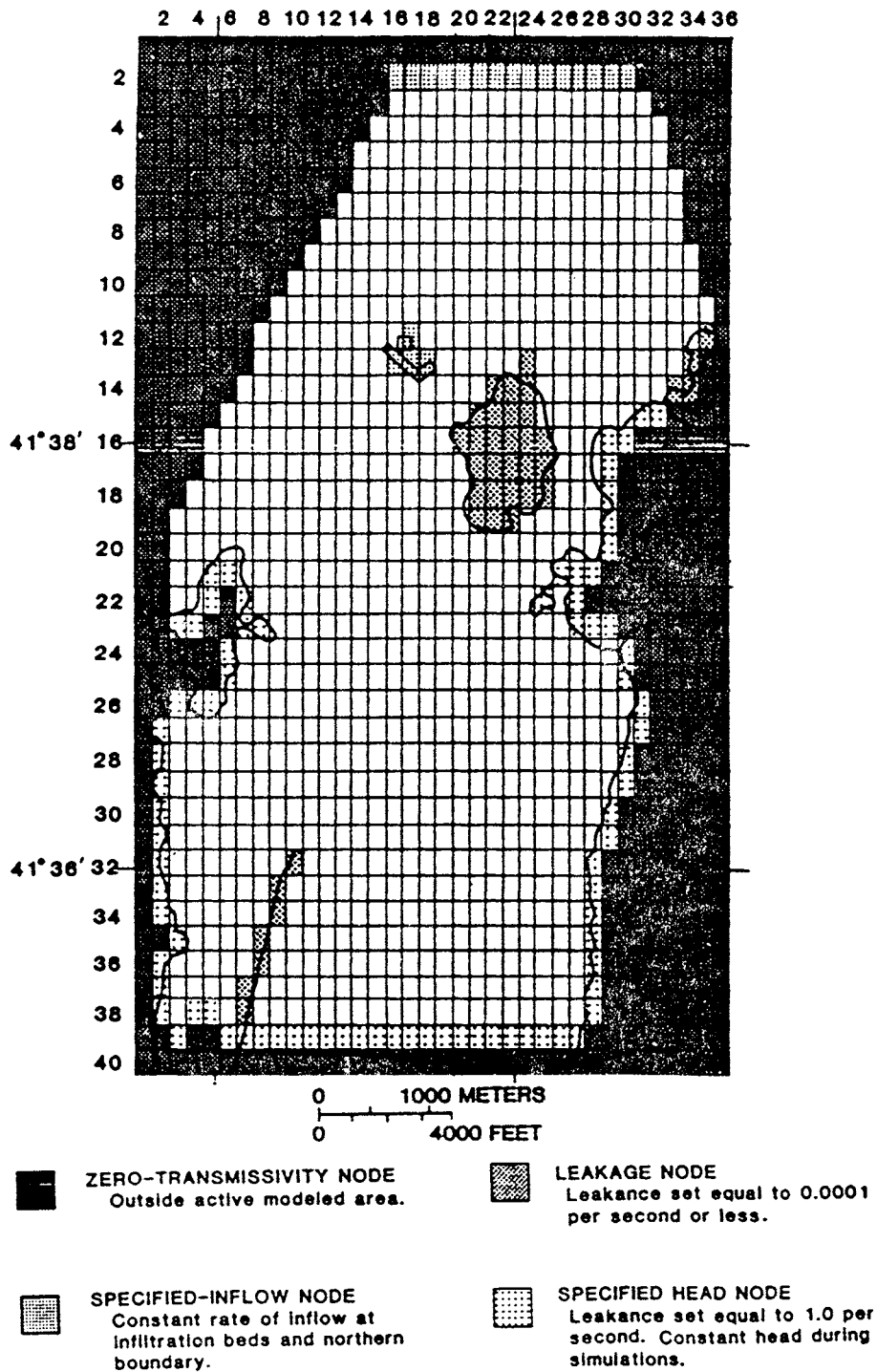
Critical Steps in Developing a Model

- processes involved?
- equations to describe these processes?
- region shape -

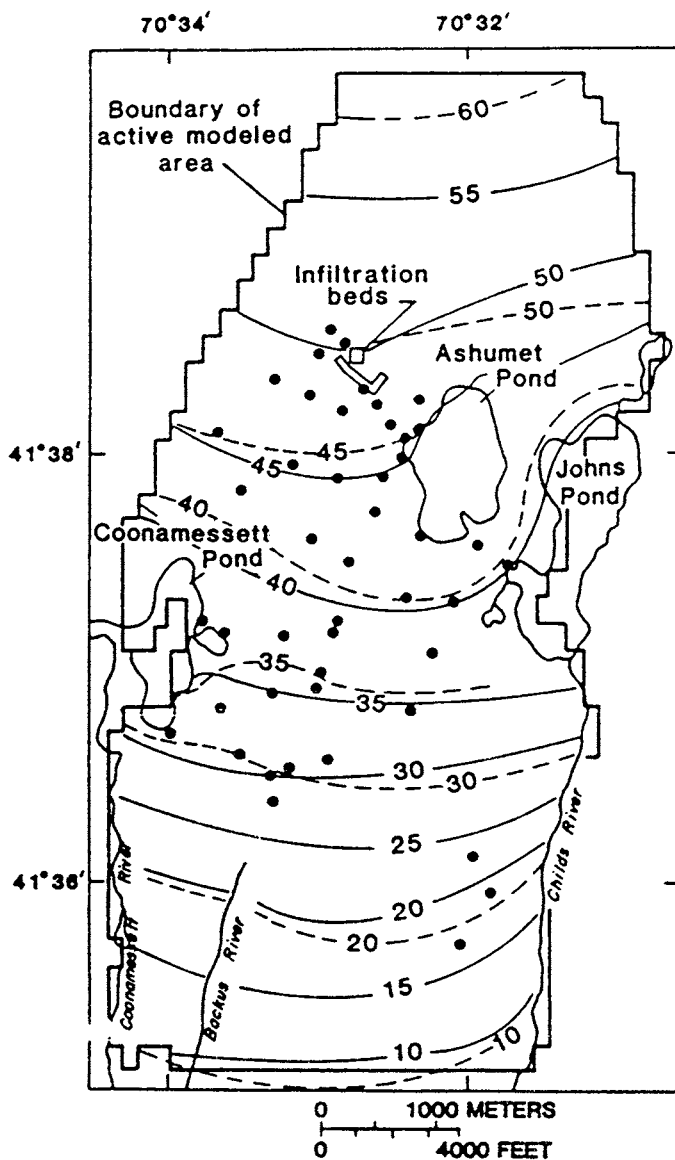


Flow Model

- discretization and boundary conditions
- parameter values - preliminary estimates from field data and guesses refined in calibration



Observed and Computed Water Table



EXPLANATION

- 40--- WATER-TABLE CONTOUR, NOVEMBER 1979--
Shows altitude of water table. Contour interval 5, 10 feet. Datum is sea level.
- 40— COMPUTED WATER-TABLE CONTOUR,
FLOW-MODEL CALIBRATION--
Shows altitude of simulated water table.
Contour interval 5 feet. Datum is sea level.
- WATER-LEVEL OBSERVATION WELL--
Site where computed and observed water
levels compared during calibration.

APPENDIX 2

HYDRAULIC TRAP FOR PREVENTING COLLECTOR WELL CONTAMINATION: FORWELL CASE STUDY

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A Hydraulic Trap for Preventing Collector Well Contamination: A Case Study

by Duke U. Ophori^a and Robert N. Farvolden^b

ABSTRACT

A hydraulic trap in the form of a purge well is proposed for the Forwell collector well K-71. The trap, which will protect well K-71 from contamination by contaminants migrating downgradient from the old Breslube waste disposal site, is based on a qualitative flow net obtained from a finite-element model of the Forwell Aquifer. The trap constitutes pumping at the position of observation well OW 9-80 at a continuous rate of at least $6.1 \times 10^{-3} \text{ m}^3/\text{s}$. The uniqueness of the trap lies in its simplicity and relatively low cost.

INTRODUCTION

The Forwell induced infiltration well field supplies about 6,818.4 m³/day of water to the cities of Kitchener-Waterloo, Ontario, something less than 10% of the total demand. On the basis of recommendations by the Grand River Induced Infiltration Committee (GRIIC) reports (1976 and 1977), several developmental processes have been undertaken to improve production by two "30.48-meter" horizontal collectors (K-70 and K-71) presently inducing infiltration from the Grand River. Also, canals have been dug around each collector to enhance infiltration and stabilize the cone of influence. The waste disposal site of the old Breslube petroleum refinery plant, which lies to the east of the well field, is a potential threat to the quality of water pumped from the collectors.

The waste disposal site is located at the highest topographic elevations in the area. The water level in the Forwell Aquifer is also highest around the disposal site, and slopes toward the collectors and the Grand River. Under these conditions, contaminants which escape into the aquifer from the disposal site could be expected to migrate toward the collectors and the Grand River under natural ground-water flow. Furthermore, the rate of contaminant migration might be enhanced by production from the collectors.

The topography of the Forwell site and the water-level configuration of the Forwell Aquifer are shown in a stratigraphic cross section of the site in a later section.

Drawdown cones of influence associated with induced infiltration well fields are commonly stabilized by infiltration from nearby rivers after long continued pumping. In the highly permeable river-connected Forwell Aquifer, stabilization was rapidly approached and in conjunction with a digital model of the aquifer has been advantageously employed in the design of the hydraulic trap in this study.

SITE DESCRIPTION

Location

The site is located about 4,828 m east of Kitchener, Ontario, Canada, approximately 2,414 m south of the Highway 7 bridge over the Grand River near Breslau and about 1,609 m southeast of the bridge (Figure 1). It is accessible by a laneway from regional road 17 at a point about 805 m south of the railway tracks in Breslau.

Geology

Chapman and Putnam (1966) described the Waterloo Hills physiographic region of which the Forwell site is part, and Karrow (1968, 1971, 1974) has done considerable detailed work in this area since then. Figure 2 shows the surficial glacial

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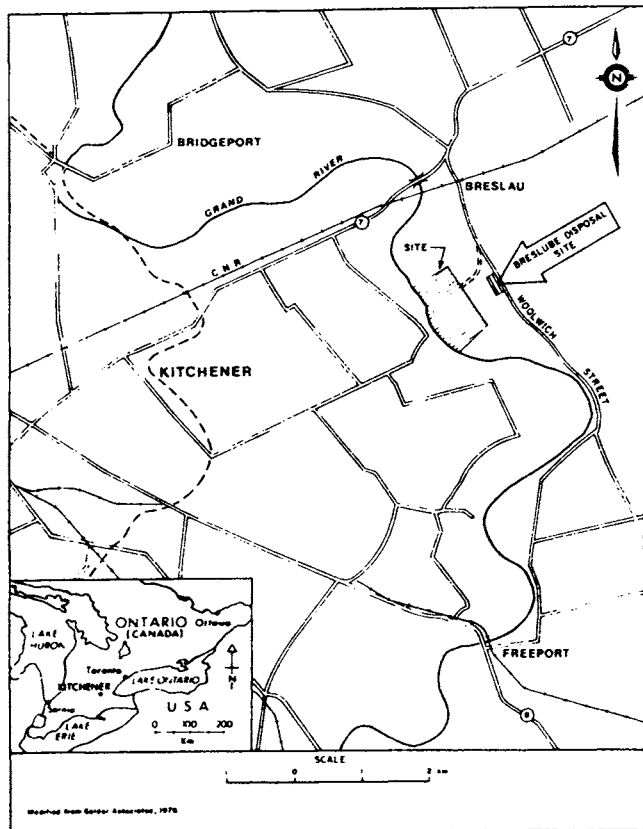


Fig. 1. Location map.

and postglacial deposits in the vicinity of the site. The surface is composed of sandy till ridges and hills of kames or kame moraines with outwash sand occupying the intervening hollows. The site itself lies in a major outwash channel in which the modern Grand River flows. The outwash deposits are predominantly uniform sand and gravel, occasionally silty. In the study area, the Grand River has an average gradient of 0.0013 (Karrow, 1968). The relatively low-gradient, broad-sweeping meanders and extensive floodplains indicate that the river is quite mature at the site. The glacial drift which varies in thickness from 9.1 to 24.4 m in the floodplains and up to 91.4 m in the uplands, consists of various interbedded till units, glacio-lacustrine deposits and outwash deposits (Karrow, 1961; 1968; 1971). Numerous and extensive coarse gravel and sand deposits occur along the Grand River spillway. At present, the Grand River appears to be depositing gravelly materials along many of its meanders (Baechler, 1974).

The study site is underlain by gently dipping Silurian sedimentary rocks. Thus, bedrock consists of the Salina and Guelph Formations, comprising mainly dolomite and limestone. In addition, the Salina Formation contains interbedded shales and some gypsum as secondary fillings in pores (Hewitt and Freeman, 1972). The relationship between the various deposits at the Forwell site is illustrated in Figure 2a. The position of this geologic cross section is shown in Figure 3.

Hydrogeology

General

The hydrogeology of the site is based mainly on a number of domestic water wells and test wells installed by International Water Supply Ltd. (IWS) between 1948 and the present, reports by Golder Associates Ltd. (GA) and Hydrology Consultants Ltd. (HC), and the GRIIC.

As a result of sand and gravel mining operations, the surface of the site is hummocky. Several deep pits contain ponded water at varying elevations which evidently infiltrates to deeper zones. South of the site, a creek draining the glacial till upland to the east of the site runs into the Grand River. The influent nature of the creek is caused by the hydraulic gradient resulting from the lower hydraulic head in the aquifer than that of the surficial water (GA, 1976). This influent stream which infiltrated 53,019.9 m³/day of water into the lower aquifer in the past (GA, 1976), is presently contained downstream along its course.

In general, four basic stratigraphic units have

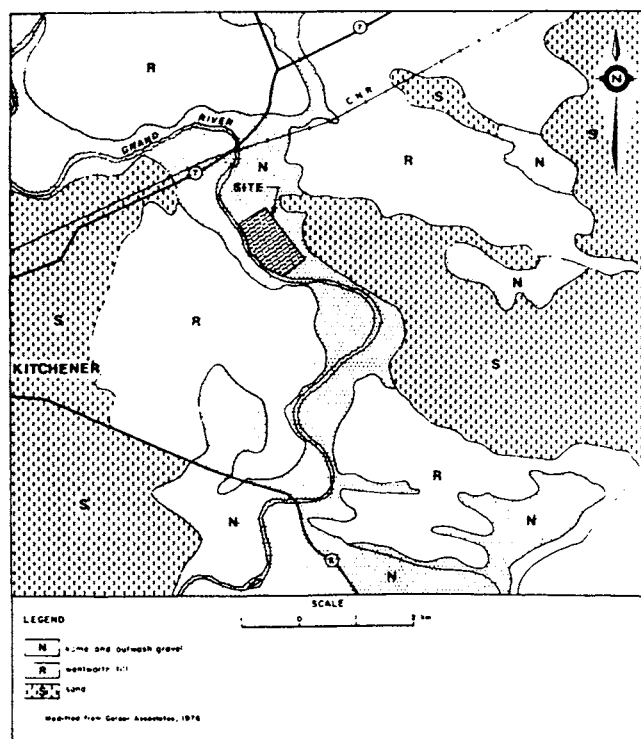


Fig. 2. Surficial geology

aquifer. The aquifer materials have been variously described by different workers. A general consensus is that the aquifer consists mainly of sand and gravel, everywhere silty and bouldery. Occasionally, the materials are clayey (IWS, 1979), cemented (IWS, 1966) or clean (IWS, 1966; GA, 1976; GRIIC, 1976). Data on available samples agree with this description. The silty sand and gravels are moderately permeable at about 10^{-6} m/s while cleaner sections have permeabilities of 10^{-4} m/s (GA, 1976).

The lower aquifer is the major water-bearing unit at the Forwell site and the one referred to as the Forwell Aquifer in this study. In the absence of pumping, ground-water movement in the aquifer is toward the Grand River. Aquifer conditions vary from confined artesian in the east to unconfined water table near the Grand River (IWS, 1980). This aquifer is hydraulically connected to the Grand River (GRIIC, 1976).

Bedrock

The map by Miller *et al.* (1979) shows the topography of the westward gently-sloping bedrock surface. The bedrock consists of dolomite and shale of the Silurian Salina Formation which, over most parts of this location, underlies the lower aquifer. The Salina Formation is known to contain very hard and sulphate-laden water. The direction of ground-water movement is likely similar to that in the lower aquifer (GA, 1976).

METHOD OF STUDY

The study was carried out in four stages. The first stage involved an extensive literature review of earlier reports on the Forwell site and its immediate confines. All available data relating to the site were assembled and examined. These data included results of previous test drilling and geophysical surveys along the Grand River carried out by IWS, borehole data from the exploratory drilling program by the GRIIC, and data from other studies. Chemical and water-level data since 1979 were also supplied by the Regional Municipality of Waterloo. Results of two pumping tests by previous investigators were evaluated. The first test was conducted by the GRIIC in 1975. A test well located near the present K-71 was pumped for 119 hours at a constant rate of 1.4×10^{-2} m³/s. A total of six observation wells situated at various distances from the test well and river were monitored. In the second pumping test of July 1976, the same test well was pumped for 460 hours at the rate of 1.7×10^{-2} m³/s and 11 observation wells were

monitored. The Thiem steady-state method of analysis defined an average transmissivity of 2.9×10^{-3} m²/s for the Forwell Aquifer. Gevaert (1979) reported a storativity value of 0.08, radius of influence of 213 m; distance from pumped well to effective recharge boundary of 106 m, percentage of water diverted from the river as 77 and an infiltration rate of 4.9×10^{-7} m/s at the site. Further details of the pumping test analyses may be obtained from GRIIC (1976) and Gevaert (1979). A careful study of the observation well hydrographs for both tests reveals that near-steady-state conditions were obtained at the site after two days of pumping.

As part of this study, additional data from more test holes and piezometers were necessary to define the cone of influence adequately, at the second stage. A total of six water-table piezometers were installed with a truck-mounted CME 55 drill rig, using both solid- and hollow-stem augers. These piezometers were restricted to the area around K-71 as it was hoped that definition of the cone of influence of pumping of K-71 would be sufficient to yield the desired results. All installations for the October 1981 pumping test are shown in Figure 3.

To provide a response in the aquifer that can be attributed to a specific pumping rate, well K-71 pumping at a rate of 2.8×10^{-2} m³/s was shut down and allowed to recover from October 14-17, 1981. The recovery data for two observation wells, like those of the earlier pumping tests, suggest that near-steady-state conditions are approached after about two days (Ophori, 1982). The recovery test was followed by a three-day pumping test during which well K-71 was pumped at a constant rate of 1.7×10^{-2} m³/s. This rate was considered high enough to produce the necessary response in the system as well as to facilitate comparison between earlier and present results in the area around K-71. Ten observation wells were monitored and measurements were taken before and after the pumping test in 15 other wells from October 17-20, 1981 (Figure 3). Typical observation well hydrographs (Figure 4) show that most of the drawdown occurred in the first ten hours; thereafter, drawdown was slow but continuous. At about 45 hours, drawdown became negligible with time but water levels were influenced by a rise in river stage approximately six hours later. It is obvious that near-steady-state conditions were approached after 48 hours of pumping.

In Figure 5, the water-table configuration after 48 hours of pumping in October 1981 is compared with that of August 1981. The August

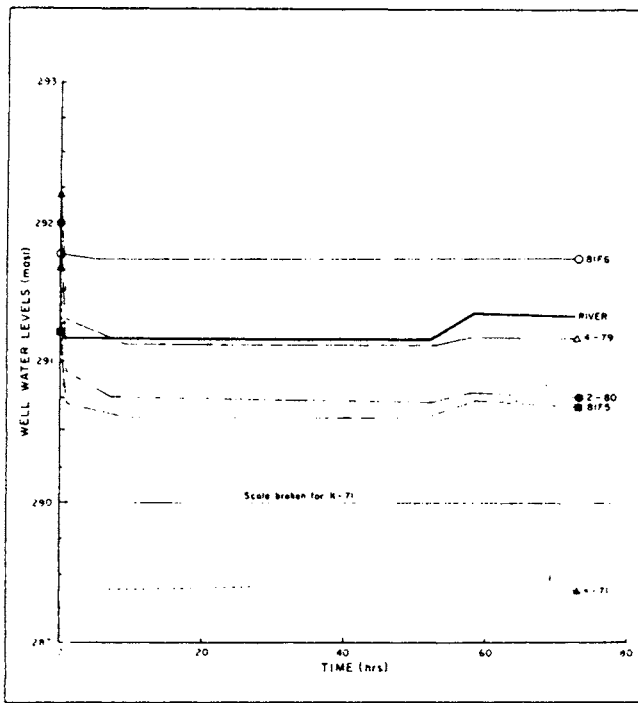


Fig. 4. Hydrographs of typical observation wells.

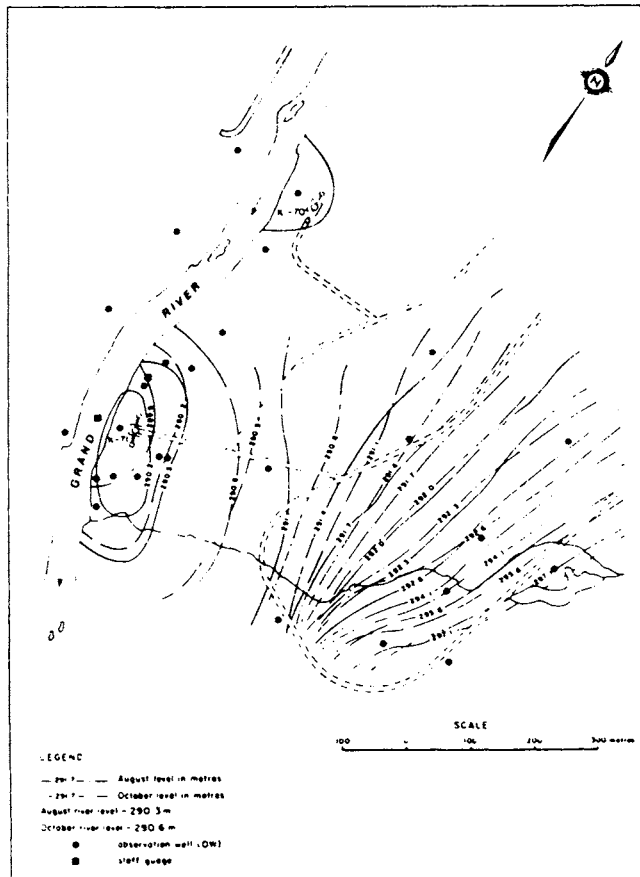


Fig. 5. Comparison of August and October 1981 steady-state water levels.

configuration was prepared from water-level data supplied by the Regional Municipality of Waterloo after one month of continuous pumping at the normal average production rate of $2.8 \times 10^{-2} \text{ m}^3/\text{s}$. Within the cone of influence, there is a 0.3 m rise in ground-water levels from August to October. A careful observation reveals that this 0.3 m difference is closely related to river-stage fluctuation from August to October 1981. This favorable comparison of water levels is a further evidence that near-equilibrium conditions prevailed at the end of the pumping test, and predictions based on this test would be valid with little or no error. An attempt to analyze the recovery data by the Theis recovery method as described by Kruseman and de Ridder (1970) yielded transmissivity values much higher than expected for the aquifer. Nonetheless, the recovery test gave a useful guide to expected drawdown and pumping period necessary to establish near-steady-state conditions. A knowledge of this limiting period was important in order to avoid errors in interruption that might be misleading in setting up the normal pumping schedule at this site. A reliable set of data for transient conditions was difficult due to complex boundary conditions. The Thiem steady-state method as outlined in Kruseman and de Ridder (1970) was used to evaluate the aquifer transmissivity. The method is valid for an aquifer system with a recharge boundary, provided piezometers considered are in a line parallel and not too close to the recharge boundary (Walton and Ackroyd, 1966). An average transmissivity value of $3.0 \times 10^{-3} \text{ m}^2/\text{s}$ was calculated by this method. A second transmissivity value of $3.7 \times 10^{-3} \text{ m}^2/\text{s}$ was estimated for the aquifer, using the method of Rorabaugh (1956). These transmissivity values fall within the range of transmissivities reported by GRIIC (1976) and Gevaert (1979). Detailed explanation of these methods and further analysis of the data is presented in Ophori (1982).

At the third stage, the hydrologic and hydraulic parameters obtained from the earlier stages of the study were incorporated in the development of a model to simulate the actual ground-water flow when near-steady-state conditions prevailed. Boundaries were inferred and adjusted to obtain realistic results.

Finally, at the fourth stage, the model was used to determine the effect of a hydraulic trap in the form of a purge well which would provide protection against contamination from the Breslube site.

MODEL DESCRIPTION AND CALIBRATION

The general partial differential equation that approximately governs the flow of water in a two-dimensional isotropic aquifer is

$$\frac{\partial}{\partial x} \left(T \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(T \frac{\partial h}{\partial y} \right) - S \frac{\partial h}{\partial t} - Q - \frac{K}{b} (h - h_a) = 0 \quad \dots \dots (1)$$

where

T is the transmissivity of the aquifer, $L^2 T^{-1}$;

h is the hydraulic head in the aquifer, L;

S is the storage coefficient of the aquifer, dimensionless;

Q is the flux of a source or sink, $L^3 T^{-1}$;

x and y are the space coordinates, L;

K is the vertical hydraulic conductivity of a confining layer, LT^{-1} ;

b is the thickness of a confining layer, L; and

h_a is the hydraulic head in the adjacent aquifer, L.

The mathematical model used to approximate (1) was that from the Pinder and Frind (1972) finite-element solution of the differential equation for transient flow in plan view. This solution used the Galerkin procedure to generate the approximating integral equations and evaluated them with iso-parametric quadrilateral elements by numerical integration. For a complete explanation of this method, the reader is referred to the paper by Pinder and Frind (1972). Although the method assumes a confined aquifer, it can be applied to an unconfined aquifer in which drawdown is small in comparison to the saturated thickness (Muskat, 1937; Kazmann, 1946; Lohman, 1972). Moreover, the Forwell Aquifer exhibits both confined and unconfined conditions (IWS, 1980).

In the present study, the domain was approximated by finite triangular elements which requires a modification of the original program of Pinder and Frind (1972). The grid had 110 nodes and 191 elements with a maximum bandwidth of 23. Small triangular elements were used near the pumping well, and the size increased with distance (Figure 6).

The image-well theory was incorporated into the model to simplify the complex boundary conditions imposed on the system by the Grand River and canal around K-71. Furthermore, it was hoped that the theory would reduce the computing cost of developing the model by eliminating the

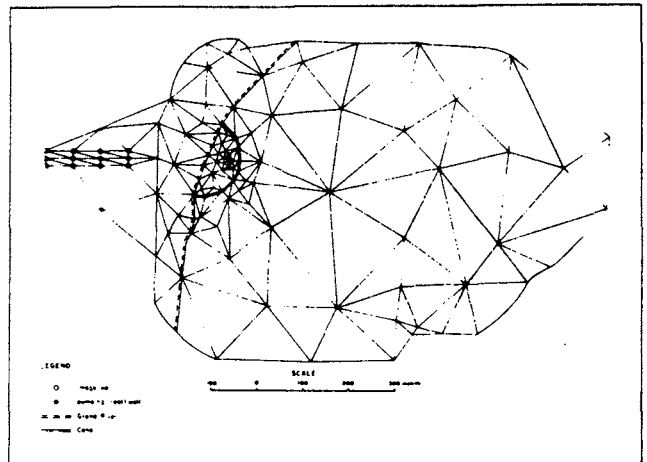


Fig. 6. Finite-element grid.

number of runs that would be required to obtain reliable flux into the system at the river and canal nodes. Figure 7 shows the observed drawdown cone at the end of the pumping test. But for the immediate vicinity of the pumping well, the cone is highly asymmetrical and resembles that expected for a single recharge boundary on the river side of the pumping well. Consequently, the entire

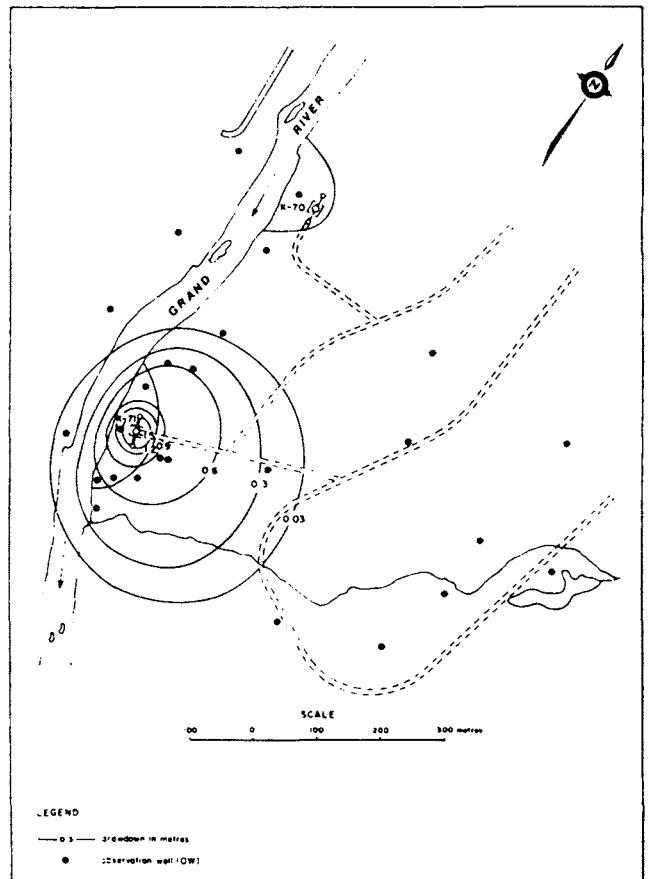


Fig. 7. Drawdown cone at the end of October 1981 pumping test.

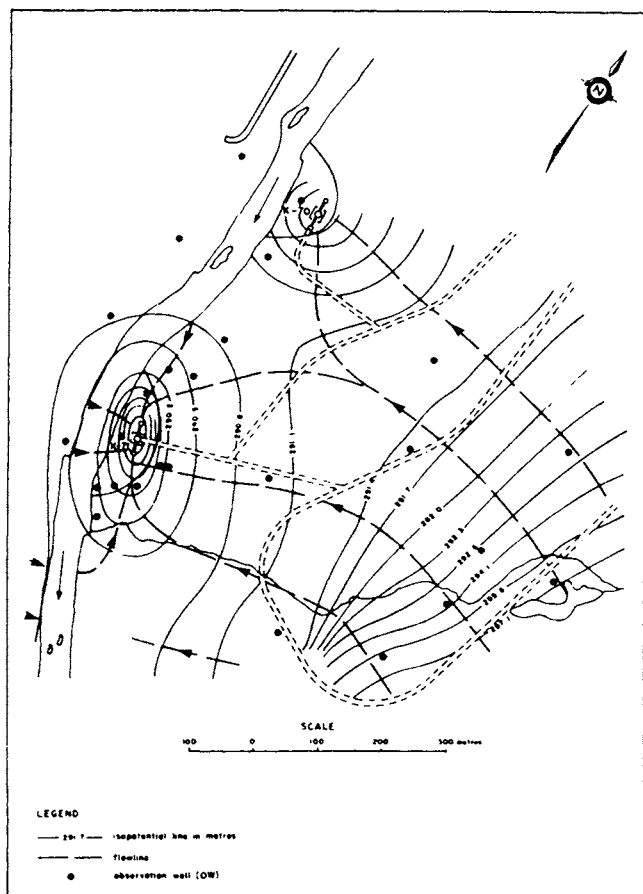


Fig. 8. Simulated steady-state flow net.

channel system was approximated by a single recharge boundary which was replaced by a line source and finally by image wells as suggested in Rorabaugh (1956). To simulate the long horizontal screen, the collector well (K-71) was modeled by three real wells equally spaced and each pumping at one-third the test pumping rate of K-71 ($1.7 \times 10^{-2} \text{ m}^3/\text{s}$). Three equivalent recharging "image wells" were placed at a distance "a" beyond the line source. This approach is a simplified form of those described by Ferris (1959), Walton and Walker (1961), Walton and Schaefer (1956), and Walton (1970).

To further simplify the problem, the system was started as hydrostatic and the water-level datum was chosen to be zero.

As data were insufficient to describe the areal extent of the aquifer rigorously, the north boundary of the model was fixed by the ground-water divide which separates the flow fields of K-70 and K-71. This divide was confirmed by field measurements of ground-water levels due to pumping of each of K-70 and K-71. The other boundaries were located far enough from the pumping center so that no-flux conditions could be assumed. The west boundary was adjusted to accommodate the

image wells at a distance "2a" from the real wells with which they produce the effect of the line source midway between them. The lower calculated transmissivity of $3.0 \times 10^{-3} \text{ m}^2/\text{s}$ seemed more reliable, and together with a storativity value of 0.08 adapted from Gevaert (1979), were used in the model.

The model was calibrated with the aid of the information above and a computer program which solves equation (1). An attempt was made to simulate the observed near-steady-state drawdown cone and hence head distribution in the aquifer. This procedure is based on the assumption that a particular head distribution is the result of a unique set of aquifer boundaries and properties.

Several runs were processed varying the positions of the image wells. In each case, the transient model described earlier was run till near-steady-state conditions prevailed—that is, after long-continued pumping. Best results were simulated with the image wells at a distance "2a" of 304 m from the real wells. The resulting near-steady-state flow net (Figure 8) compares favorably with the observed flow net (Figure 9) indicating that the model closely describes the hydrogeologic condi-

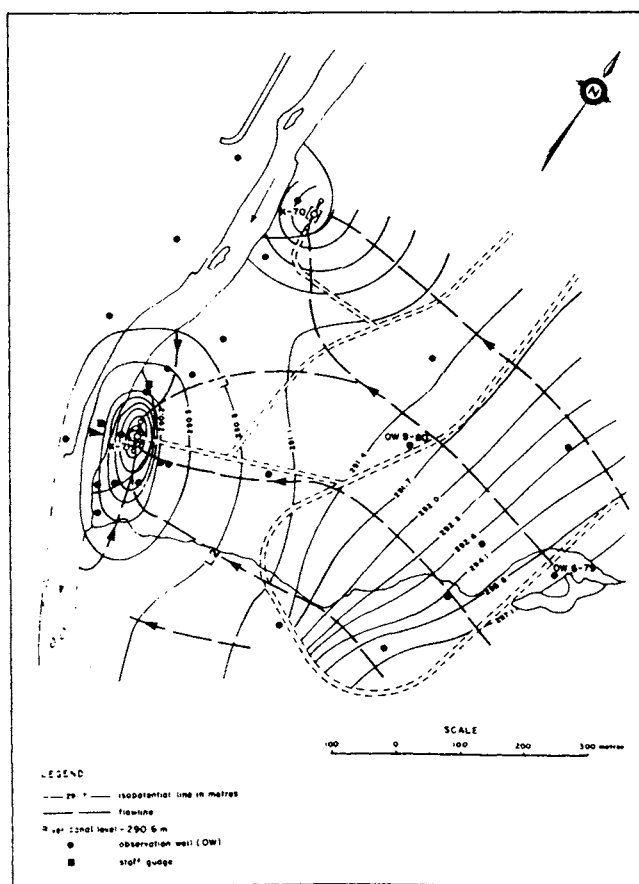


Fig. 9. Observed steady-state flow net.

tions at the Forwell site. The slight variation in the 290.5 m isopotential line may be caused by local variation in the aquifer parameters. An approximate distance of 152 m to effective recharge boundary is inferred by these results. This value is in agreement with those calculated earlier at the site (Gevaert, 1979; Ophori, 1982). As a similar interpretation seems feasible for K-70, it is concluded that for the pumping rates considered in this study, the Forwell Aquifer behaves as though it has boundaries beyond the cone of influence of pumping on one side and has a perfect recharge line source on the other side, 152 m west of K-71.

POLLUTION HAZARDS

The Breslube oil reclamation plant (Figure 1) which operated from the early 1960's until the late 1970's used lagoons to dispose of the oily acid sludge waste and waste water high in phenols derived from reclamation processes. Some test pits were excavated through contaminated silty sand fill, silt, and sand and gravel saturated up to 3.1 m with a black oily substance (International Water Consultants (IWC), 1980; GA, 1976).

The contamination from the lagoon has migrated into the upper aquifer, grossly contaminating an estimated 40,470 m², representing about 27,276 to 36,368 m³ of contaminated water (IWC, 1980). Water from this layer is typically odorous and grey when initially discharged and contains phenol concentrations from 7,000 to 22,000 ppb along with other parameters in the well characterization group (IWC, 1980). Heavy metals were either not detected or were present in low concentration, suggesting that they are held in the soil close to the lagoon.

Phenol concentrations of up to 11,000 ppb and 8,000 ppb have been measured in ponds and streams recharged by the lagoons and which then drain to the Grand River downstream from K-71 (Figure 9a). Analyses by the Regional Municipality of Waterloo over several years show that the level of phenols in observation wells fluctuates widely with highest values associated with low-flow conditions. High-phenol concentrations measured in the aquifer water below the intermediate confining layer at OW 6-79 (IWC, 1980) indicate that contaminants have passed through this layer in less than 20 years. The transit time is significantly less than would be expected if the overall permeability of the confining layer was as determined in the laboratory (IWC, 1980), suggesting that the layer has higher in-situ permeability including secondary permeability.

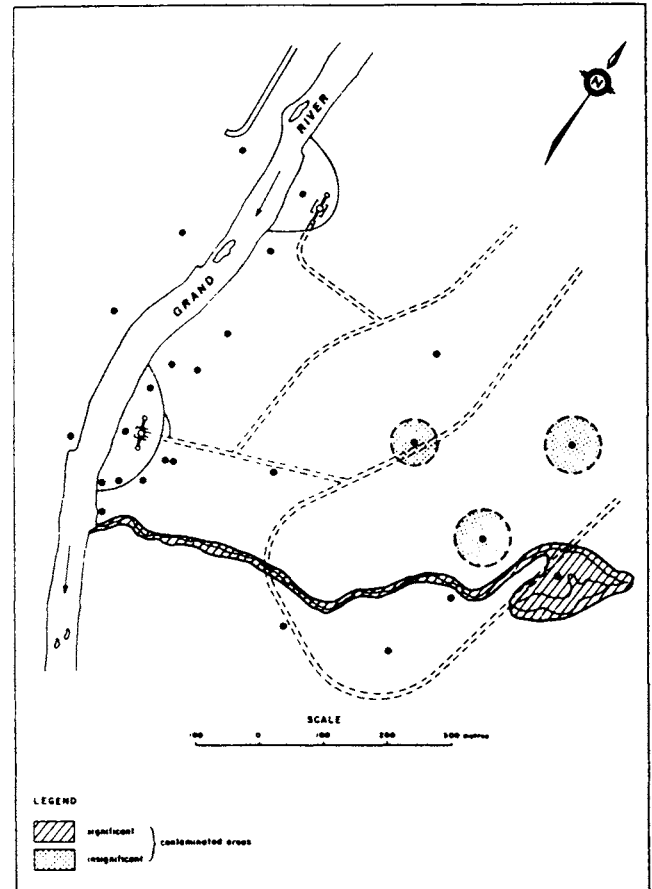


Fig. 9a. Distribution of contaminants.

Contamination is less in the lower aquifer, and consists of soluble compounds with a maximum concentration of 90 ppb. Three centers of relatively high-contaminant concentration have been located (IWC, 1980).

1. At OW 6-79 immediately west of the lagoon. It was estimated that it would take about 2.5 years to flow from the area of the lagoons to the collectors;

2. Between the lagoons and the collector wells and centered on OW 13-79 with estimated migration time to the collectors of 1.5 years; and

3. Near K-71 and the stream resulting from creek leakage especially where the intermediate confining layer is absent. There is already a low level of phenol present in the area of K-71, at least in the upper portion of the aquifer.

Following these results, three corrective measures for the lower and eight for the upper aquifers were suggested by IWC (1980). The suggested measures for the lower aquifer include: (a) the containment of the creek, which conveys contaminated water from the pond to the Grand River, in a corrugated metal pipe; (b) installation of a purge well or wells northwest of OW 9-80,

Table 1. Chemical Data of July, August, and September 1981 (ppm) (Supplied by Reg. Mun. of Waterloo)

LOCA-TION	DATE	HARD-NESS	ALKAL-INITY	IRON	CHLO-RIDE	PH	CONDC-TIVITY	SULP-HATE	PHENOLS (ppb)
1-67	July 20	224	213	31	57	8.4	539	48	<1
5-76	July 20	396	830	66	19	7.3	730	87	<1
8-76	July 20	324	610	78	4	7.4	550	39	<1
1-79	July 20	384	293	35	34	7.3	760	102	<1
3-79	July 20	404	712	138	26	7.7	750	112	<1
4-79	July 20	364	503	60	20	7.6	619	77	<1
6-79	July 20	700	2060	165	106	7.2	2100	480	2
8-79	July 20	360	1550	325	7	7.5	541	92	<1
10-79	July 20	258	317	13	11	7.3	520	42	<1
11-79	July 20	280	1400	270	6	7.4	520	29	<1
13-79	July 20	392	266	34	23	7.3	750	150	<1
1-80	July 20	404	464	120	5	7.3	650	35	<1
2-80	July 20	336	306	29	17	7.3	620	59	<1
9-80	July 20	352	994	53	2	7.4	621	32	<1
K-70	July 14	272	216	<.01	22	7.6	530	57	<1
K-71	July 14	332	246	<.01	24	7.5	650	76	<1
1-67	Aug. 12	232	189	17	27	7.3	490	40	<1
5-76	Aug. 12	444	615	34	26	7.1	750	84	<1
8-76	Aug. 12	344	485	27	5	7.4	570	40	<1
1-79	Aug. 12	392	280	39	36	7.3	760	114	<1
3-79	Aug. 12	432	344	49	21	7.3	800	120	<1
4-79	Aug. 12	396	296	16	24	7.3	720	78	<1
6-79	Aug. 12	920	1190	103	108	7.2	2050	490	<1
8-79	Aug. 12	336	1650	244	30	7.5	570	120	1
10-79	Aug. 12	328	411	20	14	7.1	580	55	1
11-79	Aug. 12	324	634	101	7	7.5	500	45	2
13-79	Aug. 12	408	241	12	24	7.4	740	130	<1
1-80	Aug. 12	392	355	48	4	7.2	630	28	<1
2-80	Aug. 12	352	260	13	18	7.3	500	52	<1
9-80	Aug. 12	408	579	46	2	7.3	630	29	<1
K-70	Aug. 12	---	---	---	---	---	---	---	<1
K-71	Aug. 12	---	---	---	---	---	---	---	<1
1-67	Sep. 16	214	192	20	25	8.0	485	40	1
5-76	Sep. 16	358	548	39	--	--	--	69	1
8-76	Sep. 16	328	437	20	5	8.0	620	40	<1
1-79	Sep. 16	354	954	231	35	7.7	810	125	1
3-79	Sep. 16	410	354	87	26	7.7	790	125	1
4-79	Sep. 16	376	304	24	25	7.6	760	86	<1
6-79	Sep. 16	460	1130	116	111	7.2	2250	495	7
8-79	Sep. 16	278	840	194	7	7.4	600	103	1
10-79	Sep. 16	256	340	14	12	7.1	600	42	2
11-79	Sep. 16	260	1280	90	12	7.5	560	42	2
13-79	Sep. 16	364	238	11	22	8.1	770	145	<1
1-80	Sep. 16	362	352	88	4	7.6	640	31	<1
2-80	Sep. 16	356	293	6	19	7.6	620	56	3
9-80	Sep. 16	288	440	23	2	7.8	580	34	<1
K-70	Sep. 16	268	210	.02	22	8.3	530	49	<1
K-71	Sep. 16	304	237	<.01	23	7.8	600	65	<1

southwest of OW 13-79, and possibly east of K-71 with yields of about $3.8 \times 10^{-3} \text{ m}^3/\text{s}$; and (c) the possibility of intercepting ground-water flow from the east by means of deepened recharge canals around the collectors. Option (a) has been successfully implemented, (c) has been attempted and found not feasible for reasons outlined in IWC (1980), and (b) is discussed in the following paragraphs.

Table 1 shows chemical data for July, August, and September 1981 of the Forwell site, supplied by the Regional Municipality of Waterloo. These data indicate phenol concentrations below 1 ppb around OW 13-79, suggesting that this area has not

continuously survived as a potential contaminant source to the collectors. Generally, phenol concentrations are within treatable limits in the short term, and induced water at collector wells falls within the Ministry of Environment's permissible criteria for public drinking-water supplies. Present data also indicate that substantial phenol concentrations have not arrived at the collectors as expected from the times of arrival estimated by IWC (1980). This may be due to attenuation as well as early implementation of some of the corrective measures suggested by IWC (1980). Furthermore, the cone of influence of K-71 (Figure 7) is restricted and does not significantly

affect the contaminated centers. This would mean that contaminant migration from the centers is controlled by the naturally slow ground-water movement.

In the long term, however, as seepage from the upper aquifer through the intermediate confining layer advances, arrival of high-phenol concentrations at the collectors is anticipated especially from the lagoon area (around OW 6-79). The need for a protective measure is therefore apparent.

THE HYDRAULIC TRAP

On the basis of the anticipated pollution, a hydraulic trap is designed in the form of a purge well at OW 9-80. The trap employs the principles of flow net construction (Walton, 1970; Freeze and Cherry, 1979). The trap location was chosen for the following reasons: (1) recommendation by IWC (1980); (2) flowlines from the contaminated ponds around OW 6-79 pass through this zone to the collectors (Figure 9); (3) the authors observed that discharged water from OW 9-80 was odorous and grey during a sampling session by staff of the Regional Municipality of Waterloo, signifying some level of contamination at this point. The trap could be located east of OW 9-80, but any contaminants already downgradient would be free from the trap and could be expected to reach K-71 eventually.

To complete the trap design, pumping in the aquifer model described earlier was replaced by three real wells at the collector, each pumping at one-third the normal rate of operation at K-71. The equivalent "image wells" were placed at 304 m to the west as earlier suggested by the model. The model was then run several times with varying discharge rates at OW 9-80. Starting with a discharge rate of $7.6 \times 10^{-4} \text{ m}^3/\text{s}$ and increasing in steps of $7.6 \times 10^{-4} \text{ m}^3/\text{s}$, a limiting rate of $6.1 \times 10^{-3} \text{ m}^3/\text{s}$ was found to produce the drawdown cone necessary to divert all flowlines from the center of contamination into a sink (Figure 10). This waste water may be discharged into the Grand River downstream from K-71. Should the need arise, a lower capacity purge well may be sited northeast of OW 1-80 and west of OW 13-79. At least one more observation well is needed in this area for this design. Since the influent lower reach of the creek is presently contained by engineering works, the proposed trap at OW 9-80 would be sufficient to the south of the site. In terms of efficiency, cost, and practicability, this corrective measure is considered the most suitable of all the measures proposed by IWC (1980).

SUMMARY

The ground-water system in the vicinity of the old Breslube disposal site, which lies to the east of the Forwell collector-well K-71 was simulated using a two-dimensional finite-element model. The model was calibrated with the aid of a near-steady-state drawdown cone which resulted from a field pumping test. In order to simplify the problem significantly, and to obtain realistic results simultaneously, the image-well theory was incorporated into the model.

The calibrated model showed that the Forwell Aquifer behaves as though it has boundaries beyond the cone of influence of pumping on one side and has a perfect recharge line source on the other side, 152 m west of K-71.

The predictive simulation which followed indicated that a pumping well in the position of OW 9-80 with a constant discharge rate of at least $6.1 \times 10^{-3} \text{ m}^3/\text{s}$, would divert all of the water moving from the contamination source for onward discharge to the Grand River downstream from K-71.

As the proposed trap would be operated on

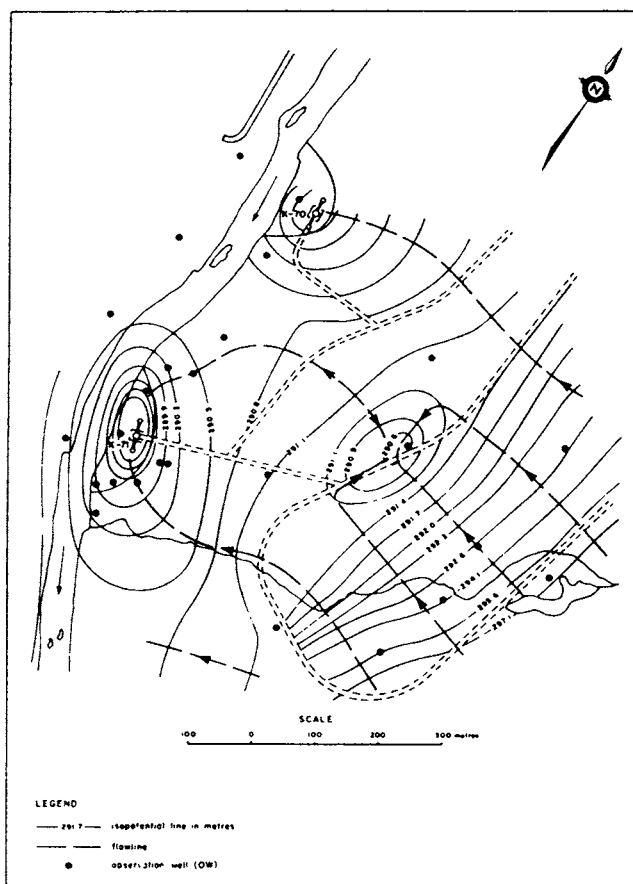


Fig. 10. Flow net with hydraulic trap.

purely physical rather than chemical principles, it is viewed as a relatively simple and inexpensive, yet important, tool to protect the Forwell collector well from contamination.

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APPENDIX 3

**NUMERICAL SIMULATIONS TO INVESTIGATE
MOISTURE-RETENTION CHARACTERISTICS
IN THE DESIGN OF OXYGEN-LIMITING COVERS
FOR REACTIVE MINE TAILINGS**

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Numerical simulations to investigate moisture-retention characteristics in the design of oxygen-limiting covers for reactive mine tailings

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Acid generation in reactive mine tailings is an oxidation process that is dependent on availability of molecular oxygen. As a consequence of the diffusion coefficient of oxygen being several orders of magnitude higher in air than in water, influx of atmospheric oxygen into a material at depth can theoretically be minimized by maintaining a protective cover layer at high moisture content. Such oxygen-limiting covers are generally of finer texture than the material being protected. A numerical model was used to investigate the importance of moisture-retention characteristics in the transient drainage of such two-layer systems. The results show that the effectiveness of a material as a moisture-retaining cover is dependent on the magnitude of its air-entry value. The thickness of the cover maintained at full saturation after prolonged drainage also depends on the pressure head at which the underlying material approaches residual saturation.

Key words: geologic covers, tailings, numerical simulations, air-entry value, residual saturation, textural layering.

La génération d'acide dans les résidus miniers réactifs résulte d'un processus d'oxydation qui est dépendant de la disponibilité d'oxygène. Comme conséquence du fait que le coefficient de diffusion de l'oxygène est plusieurs ordres de grandeur plus élevé dans l'air que dans l'eau, l'influx d'oxygène atmosphérique dans un matériau en profondeur peut être minimisé théoriquement en maintenant une couche protectrice de recouvrement à forte teneur en eau. De tels recouvrements limitant l'influx d'oxygène sont généralement d'une texture plus fine que le matériau à protéger. Un modèle numérique a été utilisé pour étudier l'importance des caractéristiques de rétention d'eau sur le drainage transitoire de tels systèmes bicouches. Les résultats démontrent que l'efficacité d'un matériau comme recouvrement hydrophile dépend de l'amplitude de la valeur d'entrée d'air. L'épaisseur d'un recouvrement qui reste complètement saturé après un drainage prolongé dépend également de la charge de pression à laquelle le matériau sous-jacent s'approche de la saturation résiduelle.

Mots clés : recouvrements géologiques, résidus miniers, simulations numériques, valeur d'entrée d'air, saturation résiduelle, couches de différentes textures.

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Introduction

Nicholson *et al.* (1989) discussed the hydraulic principles involved in the use of fine-textured materials as protective covers for reactive mine tailings. Using schematics and assuming static flow conditions, they demonstrated how fine-textured materials could remain at high moisture content above relatively coarser granular materials, even when the water table is at some arbitrary depth, far from the ground surface. The authors concluded that such a layered system would effectively reduce the influx of oxygen, thereby inhibiting oxidation of the underlying sulphide-bearing tailings. They showed that a necessary requirement to maintaining a cover material in a fully saturated state after prolonged drainage is that the magnitude of the air-entry value (AEV) be greater than or equal to the sum of the cover thickness and the magnitude of the pressure head at which the underlying coarse layer approaches the residual moisture content. Although the authors suggested that the base of the fine cover layer represents a "drip surface," it is shown here to be a limiting condition.

Nicholson *et al.* (1989) recognized that under conditions of static equilibrium, the cover layer would indeed drain. It was the contention of the authors, however, that as the

underlying coarse material drained such that the residual moisture content was approached, the hydraulic conductivity would become so small that further drainage would be exceedingly slow. As a result, the pressure head in the coarse material would be essentially constant and at a value corresponding to the residual moisture content. Though far from hydraulic equilibrium, for practical purposes and over time scales corresponding to the interval between rainfall events, the flow system could be considered static. Though critical to the model presented by Nicholson *et al.*, it should be noted that the occurrence of "static" nonequilibrium pressure-head profiles in coarse materials under conditions of prolonged drainage has not been confirmed.

Discussing the paper by Nicholson *et al.* (1989), Barbour (1990) used steady-state flow relationships to analyse a two-layer system. Unlike the work of Nicholson *et al.*, dynamic equilibrium conditions were assumed. Barbour concluded that the analysis of Nicholson *et al.* (1989) placed unnecessary restrictions on the moisture-retention characteristics of the cover material. The analysis also indicated that for the materials selected, the moisture-content profile that develops within the cover layer may be quite variable and dependent on the magnitude of water flux (in the form of infiltration) across the ground surface. Although Nicholson *et al.* (1990) clarified the concerns raised by Barbour, they also indicated the limitations of the static (Nicholson *et al.* 1989) and

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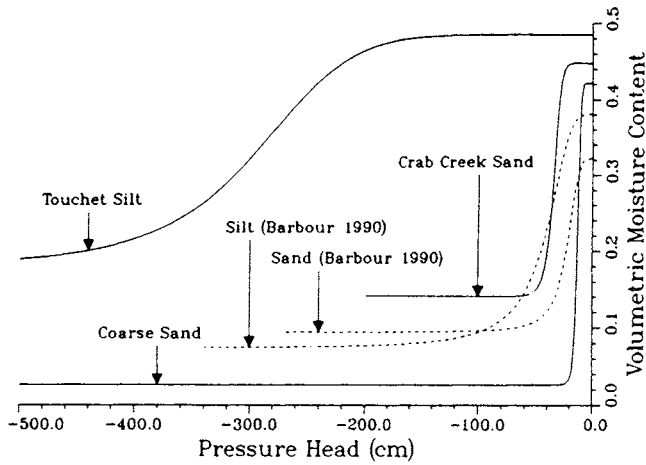


FIG. 1. Moisture-retention characteristics of the selected materials.

steady-state (Barbour 1990) approaches to the analysis of the problem. It was further indicated that a transient analysis of drainage was necessary to demonstrate the anticipated behaviour. Consideration of drainage separately (with no infiltration) would provide a conservative analysis. The objective of this paper is to demonstrate the feasibility of the concept introduced by Nicholson *et al.* (1989) using a transient numerical model and to show that transient disequilibrium is the basis for moisture retention in fine cover layers. More specifically, the purpose is to show numerically that "static" nonequilibrium conditions would prevail in the coarse layer for prolonged periods of time, such that the finer cover material would not drain.

Methodology

A one-dimensional, finite-element, saturated-unsaturated flow model (Abdul 1985) was applied to the problem of drainage through a two-layer vertical profile. The program was originally developed for two-dimensional, homogeneous, anisotropic, variably saturated, and hysteretic flow in slightly compressible porous media. The governing equation applicable to this study is somewhat simpler and is of the form

$$[1] \quad K_s k_r(\psi) \frac{\partial}{\partial z} \left(\frac{\partial \psi}{\partial z} + 1 \right) = [C(\psi) + S(\psi)S_s] \frac{\partial \psi}{\partial t}$$

where K_s is the saturated hydraulic conductivity (LT^{-1}), k_r is the relative hydraulic conductivity ($0 \leq k_r \leq 1$), C is the specific moisture capacity (L^{-1}), S is the degree of saturation (normalized moisture content), S_s is the specific storage (L^{-1}), ψ is the pressure head (L), z is the coordinate in the vertical direction (L), and t is time (T).

To accommodate layering, the original version of the program was modified to allow for variation of soil properties with location. Specific storage was evaluated using

$$[2] \quad S_s = \rho g(a + bn)$$

where ρ is the density of water, g is the acceleration owing to gravity, a is the compressibility of the soil material, b is the compressibility of water, and n is the porosity.

Freeze and Cherry (1979) gave the value for b and estimates of a for different materials. Values of compressibility used were 4.4×10^{-10} , 3.3×10^{-8} , and

$1 \times 10^{-7} \text{ m}^2/\text{N}$ for water, sand, and silt, respectively. For the simulations of this study, changes in storage caused by compressibility effects were extremely small, and thus the term could have been neglected with no perceptible change in the results.

Three sets of simulations were conducted, involving five different porous media. These included (i) the "silt" and "sand" used by Barbour (1990), (ii) Touchet silt loam overlying a medium sand (Crab Creek sand described by Brooks and Corey 1964), and (iii) Touchet silt loam overlying a coarse sand.

Moisture-retention characteristics of the different materials are shown in Fig. 1. The relative hydraulic conductivity for each porous medium was calculated from the corresponding moisture-retention curve using the method of Mualem (1976), as suggested by van Genuchten (1980), such that the moisture content (θ) at any arbitrary pressure head was given by

$$[3] \quad \theta(\psi) = \left[(\theta_s - \theta_r) \left(\frac{1}{1 + (\alpha |\psi|)^q} \right)^p \right] + \theta_r \quad \psi \leq 0$$

and the relative hydraulic conductivity was calculated as

$$[4] \quad k_r(\psi) = \frac{[1 - (\alpha |\psi|)^{q-1} [1 + (\alpha |\psi|)^q]^{-p}]^2}{[1 + (\alpha |\psi|)^q]^{\frac{p}{2}}}$$

where θ_r is the residual moisture content, θ_s is the saturated moisture content, and α and q are the curve-fitting parameters (α has a dimension L^{-1} and

$$[5] \quad p = 1 - \frac{1}{q} \quad (0 < p < 1, q > 1)$$

The parameter α is a measure of the reciprocal of the AEV for the material and q relates to the maximum slope of the moisture-retention curve. Table 1 contains a summary of the hydraulic and the curve-fitting parameters for each material. In [1] and [4], the hydraulic conductivity at a specified pressure head (or moisture content) is assumed to be the product of the hydraulic conductivity at saturation and the relative hydraulic conductivity, such that the relative hydraulic conductivity attains unity as the moisture content approaches its saturated value and becomes zero at residual moisture content.

Each layered system consists of 250 cm of the coarse-grained material overlaid by 100 cm of a finer cover material. The choice of this geometry was a deliberate attempt to be consistent with the system discussed by Barbour (1990) and Nicholson *et al.* (1990). Furthermore, Nicholson *et al.* (1989) had shown that the effectiveness of a cover material as a barrier to influx of oxygen increases appreciably within the first metre of cover thickness, beyond which it does not change much. Other simulations (not shown here), with more than 250 cm of underlying coarse material, gave results that are consistent with the discussion that follows.

The initial condition considered the entire profile to be saturated, with the water table at the surface. The boundary conditions include zero flux across the top boundary and a time-dependent pressure head at the bottom which, in effect, lowered the water table linearly from the top of the profile to the bottom over the 1st h of the simulation period. This boundary was used to relax the constraint on the numerical model caused by large and sudden changes in the boundary condition. Within the time frame of the simula-

TABLE 1. Summary of the hydraulic and curve-fitting parameters for the selected materials

Material	AEV (cm)	θ_r	θ_s	K_s (cm/min)	α (cm ⁻¹)	q
Silt*	10.0	0.074	0.381	0.045	0.028	3.60
Sand*	8.0	0.095	0.322	0.331	0.050	4.05
Touchet silt	165.0	0.18	0.485	0.035	0.004	7.05
Crab Creek sand	24.0	0.141	0.448	0.431	0.029	10.21
Coarse sand	8.0	0.026	0.422	7.80	0.077	9.74

NOTE: α and q are curve-fitting parameters in the van Genuchten (1980) model; all other parameters are measurable properties of the porous media.

* As presented by Barbour (1990).

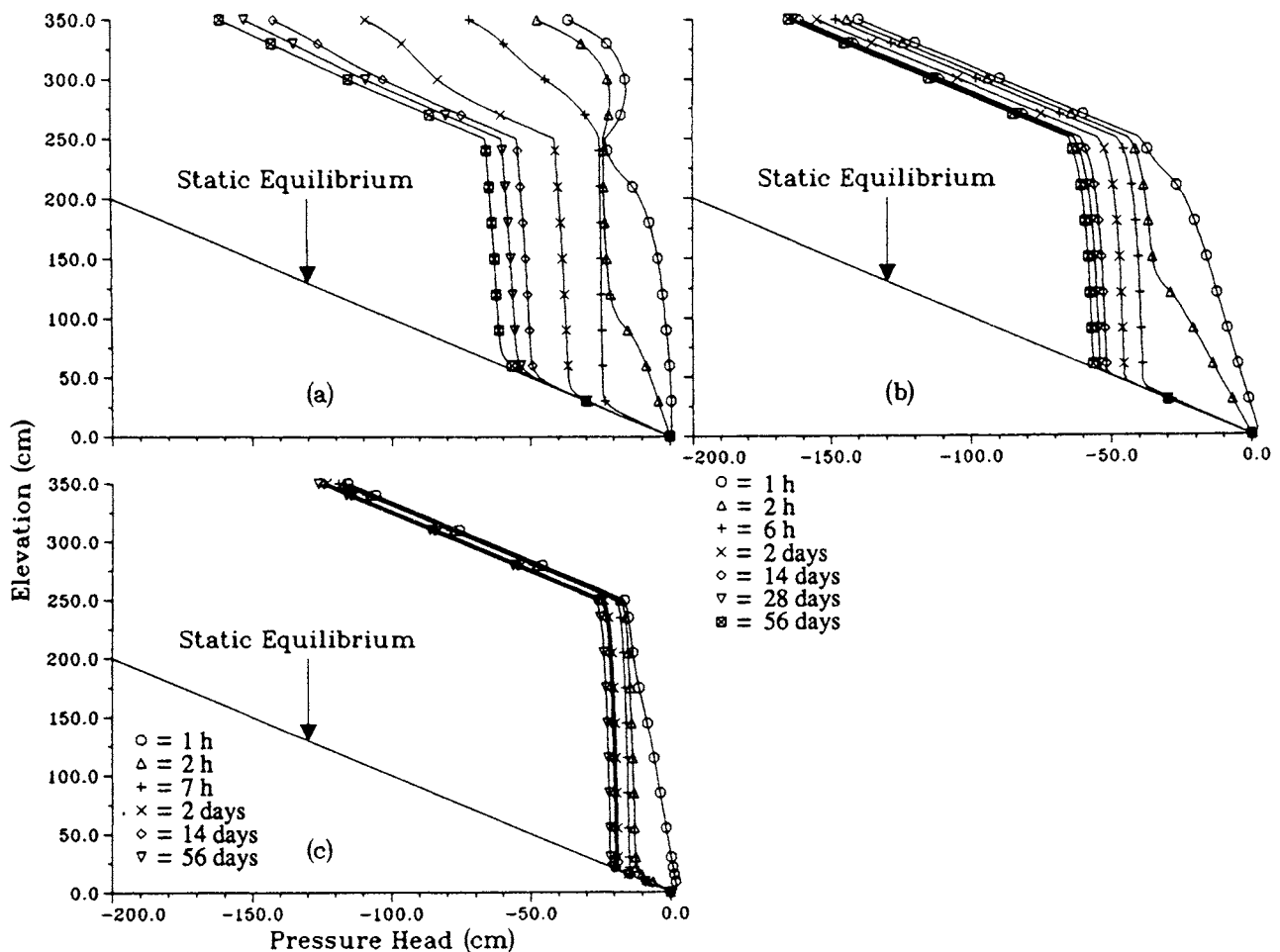


FIG. 2. Variation in pressure head with elevation at selected times. (a) "Silt" overlying "sand" (Barbour 1990). (b) Touchet silt overlying a medium sand. (c) Touchet silt overlying a coarse sand.

tions (56 days), this boundary condition is physically equivalent to an "instantaneous" lowering of the water table to the base of the profile. Variations in pressure head, total hydraulic head, and degree of saturation were tabulated for specified elevations over a period of 56 days.

Results and discussion

The results are summarized in Figs. 2-4. Because the water table was initially at the top of the column, an increasingly positive (hydrostatic) pressure head profile would extend

below the surface. To reduce the x -axes and because late-time data are of greatest relevance, only times corresponding to negative pressure head profiles are shown. The graphs are plotted for selected times to show the general trends of the hydraulic response.

The pressure-head profiles for the three pairs of soil materials (Figs. 2a-2c) changed rapidly during early time and, in all cases, appear to be approaching a static condition by 14 days. Relatively small changes occurred between 14 days and the conclusion of the simulations at 56 days. The final profiles are very similar for all pairs of soil materials. In

NOTES

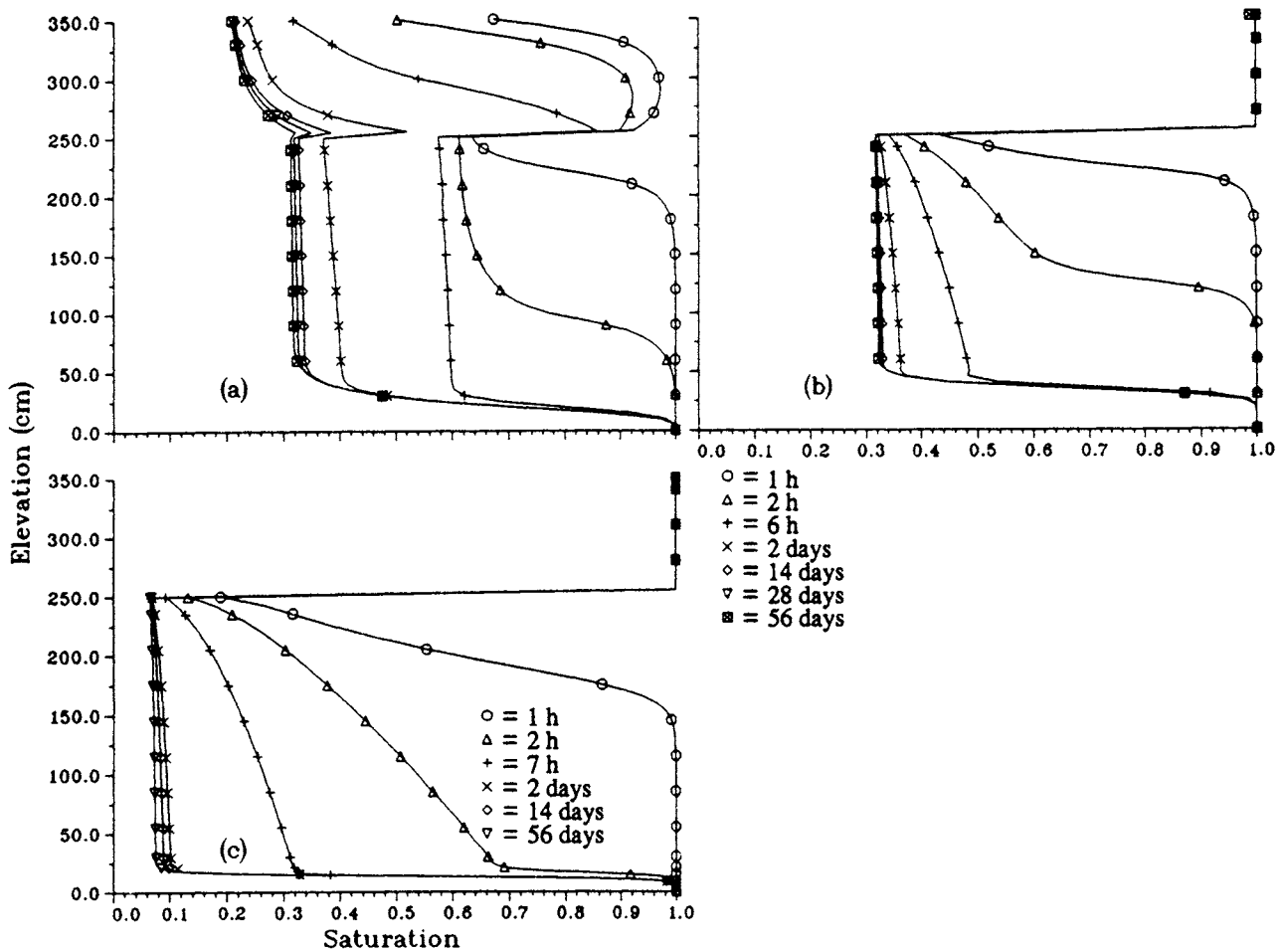


FIG. 3. Variation in saturation with elevation at selected times. (a) "Silt" overlying "sand" (Barbour 1990). (b) Touchet silt overlying a medium sand. (c) Touchet silt overlying a coarse sand.

particular, within the cover layer, which remains saturated or at a relatively high moisture content, the pressure head approaches the 1:1 hydraulic equilibrium condition. For a distance below the cover, the pressure head is almost constant and is close to the pressure head at which the moisture content approaches the residual value for the respective coarse-layer materials (Fig. 1). At greater depth, as the water table is approached, the pressure-head profile again approaches the 1:1 hydrostatic condition. Although the final profiles appear to be approaching a static condition, they are far from the static equilibrium condition indicated on each graph. This is a consequence of the low value of relative hydraulic conductivity when moisture content approaches the residual value.

The results of these simulations can be extended to address the situation that might lead to a zero pressure head (i.e., atmospheric) at the interface. The pressure head at the interface between the medium-size material and the cover changed from about -40 cm at 1 h to about -65 cm at 56 days (Fig. 2b). For the case of a coarse underlying material, the pressure head at which the residual saturation is first approached is about -10 cm (Fig. 1). Furthermore, the pressure head at the interface dropped only marginally throughout the duration of the simulation (Fig. 2c), keeping the interface pressure head at values more positive than -30 cm at 56 days. One can envision coarser materials with

less negative pressure head values at residual saturation, resulting in an interface pressure head that could practically be zero. It is therefore suggested that a condition of "drip" surface at the interface would be an end member of the continuous spectrum, satisfied only by a very coarse underlying material.

The changes in saturation for the three cases simulated are given in Fig. 3. For the materials considered by Barbour (1990), the degree of saturation in the sand declines more rapidly than in the silt (Fig. 3a). Nevertheless, even at a time of 2 h, the entire cover layer was at a water content less than saturation, which would substantially reduce the cover's effectiveness as an oxygen barrier. Thus, although Barbour showed that the moisture content could be increased by application of a constant flux, under natural conditions, the cover material considered by Barbour would be an ineffective barrier after only a few hours of redistribution and drainage following precipitation events.

The saturation profiles for the Touchet silt over Crab Creek sand are substantially different (Fig. 3b). In particular, although the sand drained rapidly, the silt remained fully saturated over its entire thickness for almost the entire duration of simulation. This observation is readily explained by reference to the pressure-head profiles. The maximum negative pressure head at the bottom of the silt layer is about -65 cm, corresponding to the pressure head at which the

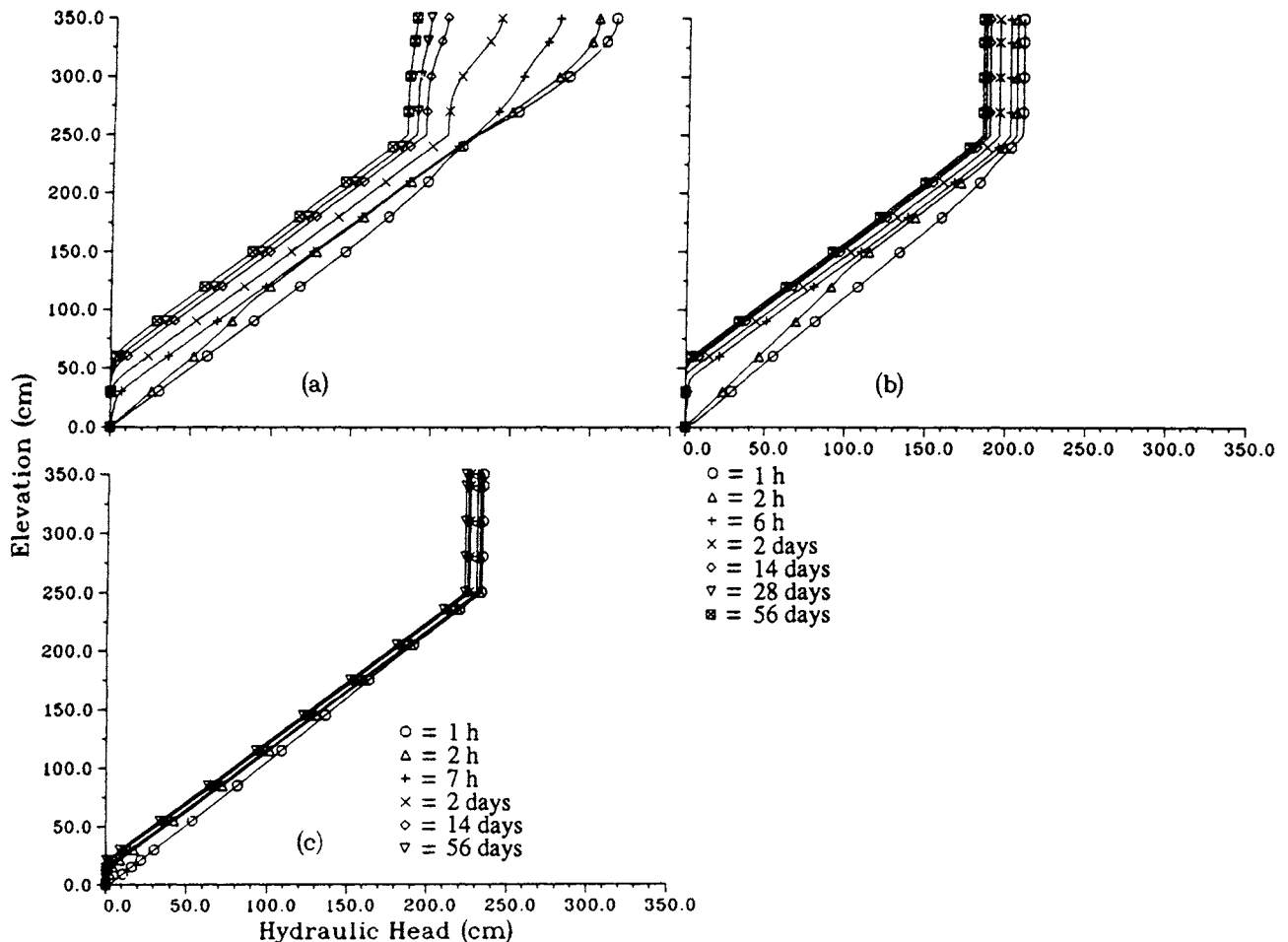


FIG. 4. Variation in hydraulic head with elevation at selected times. (a) "Silt" overlying sand (Barbour 1990). (b) Touchet silt overlying a medium sand. (c) Touchet silt overlying a coarse sand.

underlying sand approaches its residual moisture content value (Fig. 1). The maximum negative pressure head of about -165 cm occurs at the surface of the cover, reflecting an equilibrium pressure head distribution in the cover. Thus at no point in the cover layer does the pressure head significantly exceed the AEV of the Touchet silt material (-165 cm, Fig. 1). The silt therefore remains saturated. For the case of Touchet silt overlying coarse sand, the silt remained fully saturated over its entire thickness throughout the duration of the simulation (Fig. 3c). In this case, the maximum negative pressure at the base of the silt layer is only about -25 cm, which again corresponds to the pressure head at which the coarse sand approaches the residual moisture content (Fig. 1).

The hydraulic-head profiles for each soil pair are shown in Fig. 4. For both cases where the Touchet silt is the cover material (Figs. 4b and 4c), there is a negligible hydraulic gradient across the cover layer throughout the duration of simulation. This is consistent with the static equilibrium pressure head profiles discussed previously. Clearly, if there is no hydraulic gradient across the cover layer, there can be no flow of water across the layer. In the absence of a surface flux, as assumed in the present simulations, this implies that there is no drainage of the surface layer. This is consistent with the fact that the magnitude of the pressure head did not exceed the AEV of the silt. In contrast with the cover

layer, the value of hydraulic gradient in the underlying material is close to unity at all times in the zones at residual saturation. Hence drainage would proceed at the rate of the prevailing hydraulic conductivity within the drained zone, diminishing with time as the degree of saturation decreases. At late time, the profiles become almost static, though far from equilibrium, as a result of slow drainage caused by the very low values of hydraulic conductivity. The materials analysed by Barbour (1990) exhibit profiles across the cover layer that are significantly different from other pairs of material simulated, particularly at early time when the hydraulic gradient is appreciable (Fig. 4a) while saturation is high (Fig. 2a). Under these circumstances, the relative hydraulic conductivity (k_r) would have a significant magnitude and drainage of the cover would be inevitable.

Conclusions

The numerical results showed that over periods of prolonged drainage the pressure head in the underlying coarse layer approached a constant "static" value corresponding to the pressure head at which the coarse material approached residual saturation. As a consequence, the results demonstrated that it is hydraulically possible to maintain a fully saturated layer of fine-texture material above a coarse material, even though the water table may be far from the ground

surface. Neglecting water losses by evapotranspiration and for an appropriate choice of cover material with an appropriate thickness, no infiltration would be necessary to maintain a fully saturated cover layer. Two fundamental characteristics are important in assessing what thickness of a particular material can be maintained fully saturated. The first is the AEV of the cover layer. The second characteristic is the pressure head at which the underlying material approaches residual saturation, in as much as this determines the pressure head at the interface. The thickness of the cover layer that would remain saturated after prolonged drainage and redistribution would be the difference in the magnitude of AEV of the cover material and the magnitude of the pressure head at the interface.

Though the results of the numerical study support the model of Nicholson *et al.* (1990), experimental verification is required. It is also recognised that the simulations do not address all of the practical design considerations for fine-grained covers. In particular, hysteretic effects caused by alternate cycles of wetting and drying conditions, reduced moisture content caused by evapotranspiration, and the effects of freezing and thawing on the integrity of the cover are important questions that need to be addressed. Further laboratory and modelling studies are in progress to better define the limitations of the concept. Preliminary results of the laboratory experiments show trends that are consistent with the discussion above.

Acknowledgements

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APPENDIX 4

WCGR/IGR SOFTWARE LIST

(Can be obtained directly from

WCGR/IGR or through:

Dr. Festus Akindunni

Beak Consultants Limited

14 Abacus Road

Brampton, Ontario, Canada L6T 5B7)

IGR Software List – December 11, 1991

BLOB3D

Description: 3-D, transient solute transport with a parallelepiped source. Finite thickness medium. Constant, uniform groundwater velocity. Computes concentration of solute at any time and distance from source. Can handle source or solute decay. Can handle solute retardation.

Solution technique: Analytical.

Cost: \$ 150

Programming language: Fortran 77

Documentation: Descriptive comments interspersed with the source code.

Distribution notes: The program source code, example data sets and output are distributed as machine readable files on an IBM compatible floppy disk (5.25 or 3.5 inch disks are available). The user can inspect and modify the source code as desired.

System Requirements: Any computer with a Fortran 77 compiler. NOTE: Ability to read an IBM formatted diskette is required.

CFEMTRAN

Description: 2-D, transient solute transport in cross-section. Computes concentration of solute by solving the advection-dispersion equation. Mesh generation option for rectangular grids. Can also read a manually generated grid. Groundwater velocities are element-wise variable and can be read directly from a FLONETS output file. Can handle solute decay and retardation.

Solution technique: Numerical, Galerkin finite-element approach, matrix solution by Cholesky decomposition method.

Cost: \$ 1000

Programming language: Fortran 77

Documentation: Descriptive comments interspersed with the source code.

Distribution notes: The program source code, example data sets and output are distributed as machine readable files on an IBM compatible floppy disk (5.25 or 3.5 inch disks are available). The user can inspect and modify the source code as desired.

System Requirements: A computer with sufficient memory for handling finite-element programs (640 Kb is recommended) and a Fortran 77 compiler. NOTE: Ability to read an IBM formatted diskette is required.

CGAQUFEM

Description: 2-D, transient groundwater flow in plan-view. Computes distribution of heads and groundwater velocities. Confined, unconfined or mixed aquifer. Can handle areal recharge when unconfined (or leakage through an aquitard from a water table aquifer if confined). Aquifer and aquitard thickness and hydraulic conductivity, initial head, water table head, recharge and pumping (or injection) rates are node-wise variable.

Solution technique: Numerical, Galerkin finite-element approach, matrix solution by incomplete Cholesky decomposition and conjugate-gradient acceleration for efficiency. Solver reduces core storage requirements significantly for large problems.

Cost: \$ 1000

Programming language: Fortran 77

Documentation: Descriptive comments interspersed with the source code.

Distribution notes: The program source code, example data sets and output are distributed as machine readable files on an IBM compatible floppy disk (5.25 or 3.5 inch disks are available). The user can inspect and modify the source code as desired.

System Requirements: A computer with sufficient memory for handling finite-element programs (640 Kb is recommended) and a Fortran 77 compiler. NOTE: Ability to read an IBM formatted diskette is required.

CRAFLUSH

Description: 2-D, transient solute transport in a series of parallel fractures. Can handle diffusion of solute into matrix. Computes concentration of solute at any time and distance from source.

Solution technique: Analytical.

Cost: \$ 350

Programming language: Fortran 77

Documentation: Descriptive comments interspersed with the source code.

Distribution notes: The program source code, example data sets and output are distributed as machine readable files on an IBM compatible floppy disk (5.25 or 3.5 inch disks are available). The user can inspect and modify the source code as desired.

System Requirements: Any computer with a Fortran 77 compiler. NOTE: Ability to read an IBM formatted diskette is required.

FLONETS

Description: 2-D, steady-state groundwater flow in cross-section. Computes distribution of heads, stream functions and groundwater velocities. Mesh generation option for rectangular grids (can seek the water table in this case). Can also read a manually generated grid. Vertical and horizontal hydraulic conductivity, porosity and principal direction angle are element-wise variable.

Solution technique: Numerical, Galerkin finite-element approach, matrix solution by Cholesky decomposition method.

Cost: \$ 500

Programming language: Fortran 77

Documentation: Descriptive comments interspersed with the source code and a short read.me file on the distribution disk. Two published papers which discuss (1) the mathematical theory and (2) a practical application of an earlier version of the program to the Borden plume.

Distribution notes: The program source code, two example data sets and output and brief documentation are distributed as machine readable files on an IBM compatible floppy disk (5.25 or 3.5 inch disks are available). The user can inspect and modify the source code as desired.

System Requirements: A computer with sufficient memory for handling finite-element programs (640 Kb is recommended) and a Fortran 77 compiler. NOTE: Ability to read an IBM formatted diskette is required.

FRACTRAN

Description: A 2-D cross-sectional model of groundwater flow and contaminant transport in a discretely fractured, porous medium. Fractures are represented by line elements while matrix blocks are represented by rectangular elements. The program computes both the steady-state flow solution and the transient evolution of a contaminant plume. Groundwater flow, and advective and diffusive contaminant transport

within the porous media matrix blocks is rigorously treated. Retardation and first-order decay of the contaminant can be simulated. The algorithm makes use of the LTG scheme which does not require timestepping when evaluating the solution at any future time and permits coarser grids than conventional finite-element models. A separate preprocessor program is provided for ease in assigning fracture and porous media properties within zones having different physical properties. The model also has the option to solve for flow and transport in a non-fractured porous medium.

Solution technique: Numerical, Laplace Transform Galerkin(LTG) finite-element approach, second-order ILU preconditioned iterative solver with ORTHOMIN acceleration.

Cost: \$ 2500

Programming language: Fortran 77

Documentation: A comprehensive user's manual and descriptive comments interspersed with the source code. Several example problem data files are supplied.

Distribution notes: The PREFRAC, FRACTRAN, POSTFRAC and FPLOTT executable and source codes, example data sets and output are distributed as machine readable files on an IBM compatible floppy disk (5.25 or 3.5 inch disks are available).

System Requirements: Executable code is provided for IBM-compatible 386 based machines. Source code is provided which can be compiled with any suitable Fortran 77 compiler. Plotting routines are provided for 386 based machines and VMS machines running DISSPLA. NOTE: Ability to read an IBM formatted diskette is required.

HPATCH3D

Description: 3-D, transient solute transport with a horizontal patch source which can be located at any depth in the aquifer. Finite thickness medium. Constant, uniform groundwater velocity. Computes concentration of solute at any time and distance from source. Can handle source or solute decay. Can handle solute retardation.

Solution technique: Analytical.

Cost: \$ 150

Programming language: Fortran 77

Documentation: Descriptive comments interspersed with the source code.

Distribution notes: The program source code, example data sets and output are distributed as machine readable files on an IBM compatible floppy disk (5.25 or 3.5 inch disks are available). The user can inspect and modify the source code as desired.

System Requirements: Any computer with a Fortran 77 compiler. NOTE: Ability to read an IBM formatted diskette is required.

LINE2D

Description: 2-D, transient solute transport with a vertical line source at $x=0$. Finite thickness medium. Constant, uniform groundwater velocity. Computes concentration of solute at any time and distance from source. Can handle source or solute decay. Can handle solute retardation.

Solution technique: Analytical.

Cost: \$ 150

Programming language: Fortran 77

Documentation: Descriptive comments interspersed with the source code.

Distribution notes: The program source code, example data sets and output are distributed as machine readable files on an IBM compatible floppy disk (5.25 or 3.5 inch disks are available). The user can inspect and modify the source code as desired.

System Requirements: Any computer with a Fortran 77 compiler. NOTE: Ability to read an IBM formatted diskette is required.

LTGPLAN

Description: A quasi 3-D model of contaminant transport in a system consisting of an optional layered aquitard overlying an aquifer. The aquifer may be semi-confined, unconfined or of mixed type. Uniform groundwater fluxes can be assigned or variable fluxes can be imported from a separate flow solution. Contaminant movement in the aquitard is assumed to be vertical and is coupled (through the contaminant flux at the aquifer/aquitard interface) to a 2-D areal transport model for the aquifer. A 1-D finite element model is used to calculate the contaminant flux entering the aquifer and a 2-D triangular finite-element model is used to compute the aquifer concentrations. Numerous sources, with varying strengths and durations, can be located anywhere in the aquitard or on the aquifer surface. Retardation and first-order decay of the contaminant can be simulated. The aquitard layering may be different under each source area, allowing the user to simulate changes in stratigraphy due to the emplacement of the source. The program computes concentration versus time at the aquifer node points. The algorithm makes use of the LTG scheme which does not require timestepping when evaluating the solution at any future time and permits coarser grids than conventional finite-element models.

Solution technique: Numerical, Laplace Transform Galerkin(LTG) finite-element approach, ILU pre-conditioned, iterative solver with ORTHOMIN acceleration.

Cost: \$ 1000

Programming language: Fortran 77

Documentation: Descriptive comments interspersed with the source code portion of LTGPLAN. An example problem with data files is supplied.

Distribution notes: The LTGPLAN executable code, a portion of the LTGPLAN source code, INVERT postprocessor executable code, example data sets and output are distributed as machine readable files on an IBM compatible floppy disk (5.25 or 3.5 inch disks are available).

System Requirements: Executable code is available for most commonly used systems including those running VAX Fortran, 80386's and Unix-based machines. NOTE: Ability to read an IBM formatted diskette is required.

OGATA

Description: 1-D, transient solute transport. Computes concentration and flux of solute at any time and distance from source. Can handle solute retardation. Identical to SUPER1D except it can't handle time-variant source.

Solution technique: Analytical. Ogata-Banks solution.

Cost: \$ 50

Programming language: Fortran 77

Documentation: Descriptive comments interspersed with the source code.

Distribution notes: The program source code, example data sets and output are distributed as machine readable files on an IBM compatible floppy disk (5.25 or 3.5 inch disks are available). The user can inspect and modify the source code as desired.

System Requirements: Any computer with a Fortran 77 compiler. NOTE: Ability to read an IBM formatted diskette is required.

ORTHOFEM

Description: Subroutines implementing the iterative, preconditioned conjugate gradient and ORTHOMIN methods for solving banded or sparse matrix equations. The conjugate gradient acceleration technique is appropriate for symmetric matrices, while ORTHOMIN acceleration is applicable for asymmetric matrices. Preconditioning of the coefficient matrix is by first-order, incomplete lower-upper (ILU) factorization. The subroutines are designed for efficient incorporation into finite-element programs with any arbitrary element type. Modifications may need to be made to accommodate either mixed element types of the same dimensionality or finite-difference programs.

Solution technique: Numerical.

Cost: \$ 400

Programming language: Fortran 77

Documentation: A short manual outlining the theory, summarizing the algorithms and describing the steps necessary for incorporating the subroutines into a finite-element code. An example implementation is outlined. Descriptive comments are interspersed with the source code.

Distribution notes: The subroutine source code is distributed as machine readable files on an IBM compatible floppy disk (5.25 or 3.5 inch disks are available). The source code may be modified and customized as necessary to be compatible with the user's main program.

System Requirements: Any computer with a Fortran 77 compiler. NOTE: Ability to read an IBM formatted diskette is required.

PATCH3D

Description: 3-D, transient solute transport with a vertical patch source at $x=0$. Finite thickness medium. Constant, uniform groundwater velocity. Computes concentration of solute at any time and distance from source. Can handle source or solute decay. Can handle solute retardation.

Solution technique: Analytical.

Cost: \$ 150

Programming language: Fortran 77

Documentation: Descriptive comments interspersed with the source code.

Distribution notes: The program source code, example data sets and output are distributed as machine readable files on an IBM compatible floppy disk (5.25 or 3.5 inch disks are available). The user can inspect and modify the source code as desired.

System Requirements: Any computer with a Fortran 77 compiler. NOTE: Ability to read an IBM formatted diskette is required.

RCRACK

Description: 2-D, radially symmetric, transient solute transport along a single fracture. Can handle diffusion of solute into matrix. Computes concentration of solute at any time and distance from source.

Solution technique: Analytical.

Cost: \$ 150

Programming language: Fortran 77

Documentation: Descriptive comments interspersed with the source code.

Distribution notes: The program source code, example data sets and output are distributed as machine readable files on an IBM compatible floppy disk (5.25 or 3.5 inch disks are available). The user can inspect and modify the source code as desired.

System Requirements: Any computer with a Fortran 77 compiler. NOTE: Ability to read an IBM formatted diskette is required.

SUPER1D

Description: 1-D, transient solute transport. Computes concentration and flux of solute at any time and distance from source. Source strength can vary with time. Can handle solute retardation.

Solution technique: Analytical. Ogata-Banks solution with superposition to handle time-variant source.

Cost: \$ 50

Programming language: Fortran 77

Documentation: Descriptive comments interspersed with the source code.

Distribution notes: The program source code, example data sets and output are distributed as machine readable files on an IBM compatible floppy disk (5.25 or 3.5 inch disks are available). The user can inspect and modify the source code as desired.

System Requirements: Any computer with a Fortran 77 compiler. NOTE: Ability to read an IBM formatted diskette is required.

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CROSSFLO

Description: 2-D, steady-state groundwater flow in cross-section. Menu-driven, graphical interface for all steps of problem solution including mesh generation (for simple layered grids), data input and plotting of results. (can seek the water table in the upper layer). Computes distribution of heads, stream functions and groundwater velocities.

Vertical and horizontal hydraulic conductivity, porosity and principal direction angle are element-wise variable.

Solution technique: Numerical, Galerkin finite-element approach, matrix solution by Cholesky decomposition method.

Cost: \$ 2000

Programming language: GFA-BASIC

Documentation: Comprehensive 60-page User's Manual with a chapter on model verification and illustrative examples. Two published papers which discuss (1) the mathematical theory and (2) a practical application of an earlier version of the program to the Borden plume.

Distribution notes: The program *executable* code and example data sets are distributed as machine readable files on an Atari formatted 3.5 inch floppy disk. Copies of the source are *not* distributed.

System Requirements: An Atari ST computer with sufficient memory for handling finite-element programs (1040 Kb is recommended).

GRID BUILDER

Description: 2-D, triangular element mesh generator. Interactive, menu-driven, graphical interface. Can generate a completely irregular mesh with internal subdivisions. Can refine any subset of elements. Zoom feature facilitates extremely detailed refinement. Up to 32000 elements, 16000 nodes capacity (with 4 Mb of RAM). Built-in node-numbering scheme for bandwidth optimization. Flexible I/O routines allow export of grid data to any 2-D triangular finite element model (which uses triangular elements) or import of the user's existing grids.

Cost: \$ 2000

Programming language: FTN77/386 (University of Salford Fortran 77 compiler). Inter-acter graphics subroutine library (Interactive Software Limited)

Documentation: Comprehensive User's Manual with a step-by-step hands-on demonstration exercise. Extensive, context-sensitive, on-line help screens.

Distribution notes: The program *executable* code and example data sets are distributed as machine readable files on an IBM formatted floppy disk (5.25 or 3.5 inch disks are available). Copies of the source are *not* distributed. The FTN77/386 run-time disk is distributed free-of-charge as part of the package.

System Requirements: An IBM compatible 80386 microcomputer with Microsoft compatible mouse, VGA card and monitor (colour recommended), hard disk, 2 Mb RAM (4 Mb recommended). An HP-GL compatible plotter is supported and recommended.