NAPL IN BEDROCK BENEATH THE NIAGARA RIVER

ASSESSMENT OF HUMAN ENDANGERMENT

S-Area Remedial Program

May 1989
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CONESTOGA-ROVERS & ASSOCIATES

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1.0 INTRODUCTION

Pursuant to the S-Area Stipulation and Judgment Approving Settlement Agreement ("Settlement Agreement") Addendum I, Subparagraph B(6)(b), Occidental (OCC) was required to assess "whether non-aqueous phase chemicals have migrated from the Landfill Site into the Bedrock beneath the Niagara River, and, if so, ... the extent, if any, of human endangerment by such non-aqueous phase chemicals."

OCC previously submitted a report to EPA/State entitled "Assessment of the Extent of APL/NAPL Migration From the S-Area In the Lockport Bedrock" ("APL/NAPL Bedrock Migration"), in which it was concluded that non-aqueous phase chemicals ("NAPL") from the Landfill Site had migrated into the bedrock beneath the River. The present report supplements the prior submission with a further assessment of the extent, if any, of human endangerment caused by such chemicals.

In completing the above assessment, the following topics were specifically addressed:

1. Groundwater hydraulics in the bedrock beneath the Niagara River.
2. Extent of non-aqueous phase chemical migration from the Landfill Site into the bedrock beneath the Niagara River.
3. Flux of chemicals from the NAPL plume beneath the Niagara River.
4. Chemical migration pathways.
5. Points of chemical exposure.
6. Assessment of human endangerment.

2.0 GROUNDWATER HYDRAULICS IN THE BEDROCK BENEATH THE NIAGARA RIVER

2.1 OVERVIEW

The waterbearing characteristics of the bedrock beneath S-Area have previously been discussed in the APL/NAPL Bedrock Migration Report. That assessment focused only on the waterbearing characteristics of the bedrock formations which comprise the Lockport and Upper-Clinton Groups. The purpose of the following discussion is to relate the localized groundwater movement below the S-Area to the regional bedrock hydrogeology presented by Novakowski and Lapcevic (1988). The paper by Novakowski and Lapcevic (1988) is contained in Appendix A.

2.2 BEDROCK GEOLOGY

The bedrock stratigraphy in the vicinity of the S-Area has been compiled from data obtained from 20 deep bedrock wells, 26 shallow bedrock wells, and 35 historical bedrock installations. These investigations were confined to all formations above the Rochester Shale of the Clinton Group. A typical north-south cross-section through S-Area is presented in Figure 2.1. The stratigraphic sequence of bedrock formations encountered in descending order is Oak Orchard, Eramosa, Goat Island and Gasport Formations of the Lockport Group, and the Decew and Rochester Formations of the Clinton Group. The bedding planes were observed to slope southward at an approximate slope of 0.6 per cent, (See APL/NAPL Bedrock Migration Report). Figure 2.2 presents a generalized stratigraphic section at Niagara

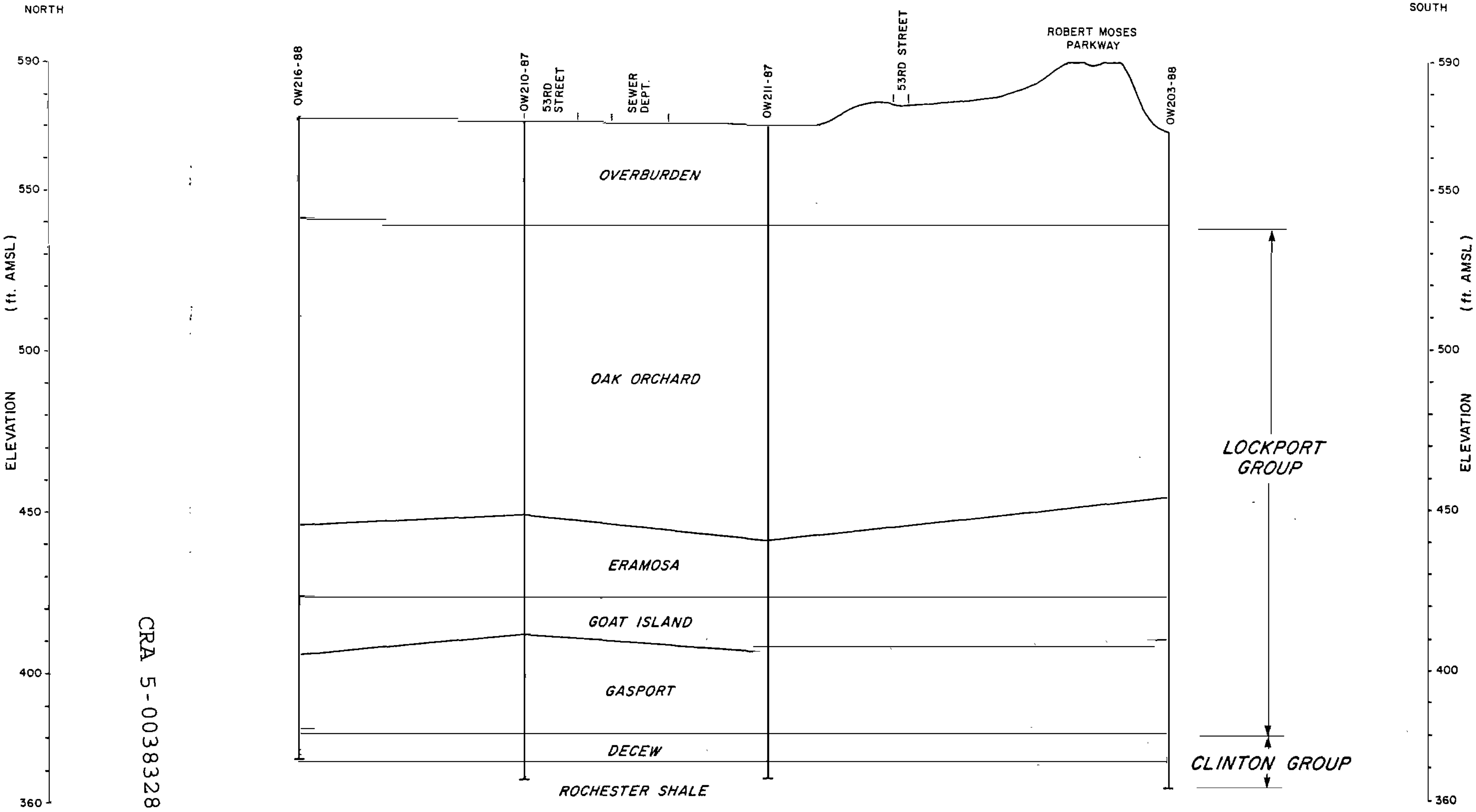

figure 2.1

TYPICAL NORTH – SOUTH CROSS – SECTION THROUGH LOCKPORT AND UPPER CLINTON GROUPS

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SYSTEM		GROUP	FORMATION	MEMBER	THICKNESS (feet)	DOMINANT LITHOLOGY	DESCRIPTION
SILURIAN	UPPER	SALINA	Bertie		45*	Dolostone	massive to laminated, finegrained, dark to light gray, fossiliferous
			Camillus		80 - 100*	Shale	green unfossiliferous, occ. dolomite, anhydrite, siltstone
			Syracuse		100*	Shale & Dolostone	gray, fossiliferous, occ. dolomite, anhydrite, halite
			Vernon		200*	Shale	massive, poorly stratified, green, occ. dolomite, halite
	MIDDLE	LOCKPORT	Oak Orchard/ Guelph		120 - 140	Dolostone	med. to thick-bedded, med. grained, brownish to dark gray, bituminous, occ. cherty, stromatolitic
			Eramosa		7 - 34	Dolostone	v. fine grained, crystalline, gray to brownish gray, occ. chert nodules, shale partings
			Goat Island		16 - 52	Dolostone	massive, fine grained, crystalline, light to dark gray, chert beds, shale bed at upper contact
			Gasport		15 - 45	Limestone & Dolostone	fine to med. grained, semicrystalline, crinoidal, light to med. gray, vuggy
		CLINTON	Decew		5 - 13	Dolostone	fine grained, crystalline, argillaceous, med. to dark gray, shaly partings
			Rochester		55 - 60	Shale & Limestone	thin-bedded, dark gray, calcareous shale, numerous gray limestone interbeds
			Irondequoite		6 - 12	Limestone	med. bedded, fine to med. grained, light to med. gray, crystalline, fossiliferous
			Reynales	Rockway	10	Dolostone	weakly laminated, finegrained, buff to gray, lithographic, occ. shale partings
				Meritton	0 - 3	Limestone	medium grained, crystalline, buff to gray, may be absent
				Hickory Corners	0 - 5	Limestone	thin-bedded, coarse to med. grained, crystalline, dark gray, bioclastic, argillaceous
			Neahga		5	Shale	platy to fissile, soft, dark greenish gray, minor gray limestone
			Thorold		2 - 9	Sandstone	fine to v. fine grained, hard, quartz rich, light gray, silica cement
	LOWER	MEDINA	Grimsby		42 - 55	Sandstone & Shale	fine grained, red (hematitic) sandstone with shale interbeds grading downwards to dominant shale with sandstone interbeds
			Power Glen		34 - 48	Shale & Siltstone	laminated, fissile, sandy calcareous shale, with fine grained sandstone interbeds
			Whirlpool		15 - 28	Sandstone	fine to med. grained, hard, cross bedded, gray to white, thin shaly partings, silica cement
ORDOVICIAN	UPPER		Queenston		700 - 1200	Mudstone & Shale	med. bedded, low fissility, random partings, hematitic, uniform, laterally extensive, reddish brown, locally grayish green (reduced by groundwater), extensively fractured and jointed.

SOURCES:
Fisher (1970)
Fisher (1977)
Johnson (1964)
Kilgour (1966)
Liberty (1971)
Richard (1966, 1975)
Zenger (1975)

〰〰〰 Represents erosional unconformity

NOTE: Thickness represents measured thicknessess in Niagara Area.
* Thickness is entire unit stratigraphic thickness since not exposed at Niagara Falls

figure 2.2

GENERALIZED STRATIGRAPHIC SECTION
NIAGARA FALLS
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Falls, while detailed stratigraphic information and descriptions of each bedrock formation are found in the Information Summary Report, Section 9.4.1.

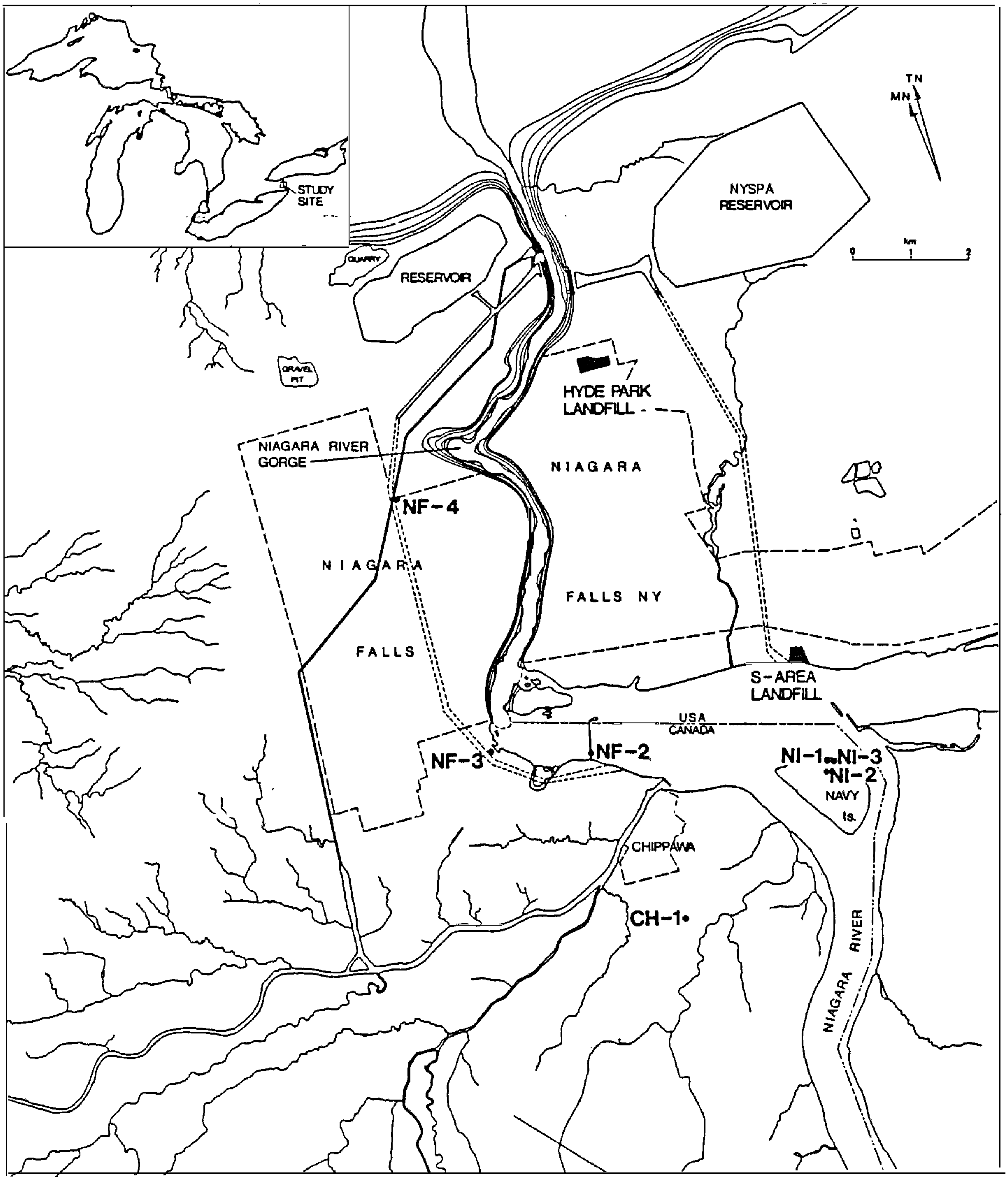
The investigation conducted by Novakowski and Lapcevic (1988) consisted of the installation and sampling of seven boreholes distributed around the Niagara Falls area, as shown in Figure 2.3. All boreholes in that study penetrated to below Lake Ontario water levels. Interestingly two of the boreholes were inclined holes (NI-1 and NI-2 on Navy Island), specifically designed for identification of vertical fractures.

The core logs and borehole geophysical measurements from the Novakowski and Lapcavic investigation were consistent with the stratigraphy and descriptions given in Figure 2.2.

2.3 BEDROCK WATERBEARING UNITS

The waterbearing characteristics of the bedrock in the vicinity of S-Area have been assessed in Chapter 5.0 of the APL/NAPL Bedrock Migration Report .

In summary, waterbearing zones were encountered in virtually all bedrock formations; however, hydraulic testing indicated that the following three distinct strata had a higher frequency of waterbearing occurrence:



SOURCE:
NOVAKOWSKI AND LAPCEVIC, 1988

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figure 2.3

BOREHOLE LOCATIONS

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a) the top 30 feet of the Oak Orchard Formation (Bedrock Upper Unit),
b) between 60 to 90 feet into the bedrock surface (Bedrock Second Unit),
c) and the Goat Island Formation (Bedrock Third Unit).

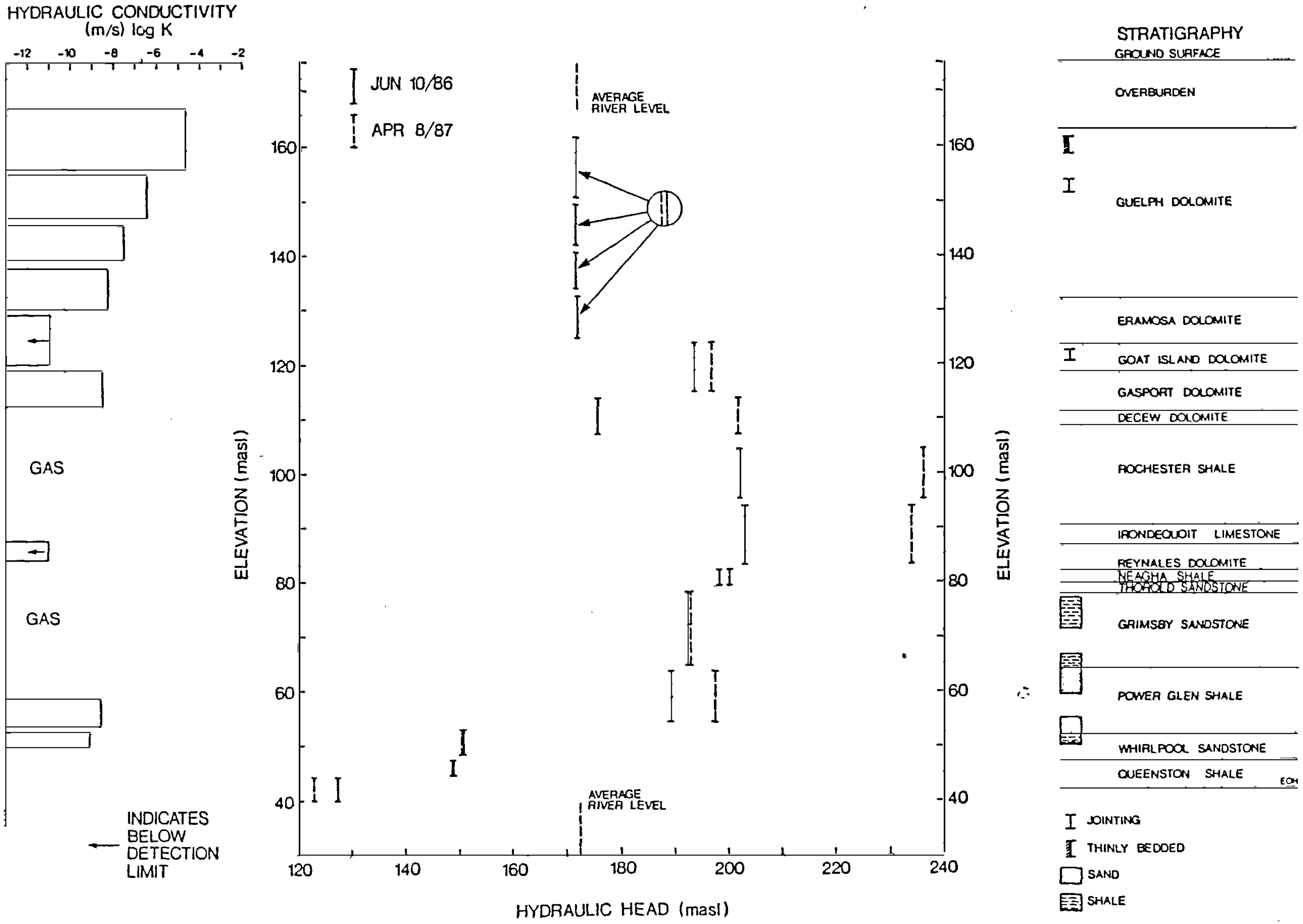
Novakowski and Lapcevic (1988) confirmed the presence on a regional scale of the upper waterbearing unit of the Oak Orchard Formation. They described this unit as:

> "A weathered zone about 4-5 m thick... characterized by frequent bedding plane partings (fractures) 2-3 cm apart that have been subjected to considerable dissolution"

Novakowski and Lapcevic (1988) also note that vertical fractures interconnect most of the bedding plane fractures within this upper weathered zone.

Although there was no regional indication of the Bedrock Second Unit identified in the vicinity of S-Area, the Novakowski and Lapcevic (1988) data indicates that this zone does extend at least south to Navy Island. The hydraulic conductivity measurements for borehole NI-2 are shown in Figure 2.4. It is noted that the high hydraulic conductivity zone that extends from the top of the Lockport Group (Guelph Formation) to the top of the Eramosa Formation indicates the possibility of the Bedrock Second Unit.

The Goat Island Formation, which is highly fractured, was identified by Novakowski and Lapcevic (1988) to be present throughout the region as it correlated well between boreholes.



SOURCE:
NOVAKOWSKI AND LAPCEVIC, 1988

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figure 2.4
BOREHOLE INFORMATION FOR NI – 2
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In the OCC investigation of the waterbearing zones within the bedrock below S-Area, the Decew Formation, which is the upper member of the Clinton group, was determined to be a non-waterbearing zone or a gas production zone, (See Section 5.1 of the APL/NAPL Bedrock Migration Report). On the regional scale, this unit was not identified.

A fourth strata (Decew) beneath the Goat Island Formation was not tested sufficiently by Novakowski and Lapcevic (1988) to allow for a thorough hydraulic characterization. As discussed in Section 4.2, this formation was assumed to have the same hydraulic characteristics as the Goat Island Formation even though a waterbearing interval was not identified. This formation will be referenced hereinafter as the Bedrock Fourth Unit.

Novakowski and Lapcevic (1988) discuss two other distinct groundwater flow regimes: one in the Clinton - Upper Cataract Groups and Lower Queenston Formation, and the other in the Lower Cataract Group Upper Queenston Formation. They suggest, based on geochemical and permeability information, that there has been little groundwater migration since pre-Pleistocene time. This indicates that there is little, if any, mixing between these two flow regimes and the flow regime within the Lockport Group.

2.4 BEDROCK GROUNDWATER MOVEMENT

Within the Lockport flow regime, which encompasses the four hydraulic units identified in Section 2.3 present at S-Area, the groundwater flow on the regional scale is toward the Niagara Gorge.

Based on the hydraulic head data provided by Novakowski and Lapcevic (1988) for each major lithologic unit in each borehole, the groundwater flow beneath the Niagara River adjacent to S-Area is in general to the northwest. This regional groundwater movement is consistent with the northwest groundwater flow observed at S-Area, which is controlled by the weathered fracture zones which are laterally interconnected.

Novakowski and Lapcevic (1988) estimate a hydraulic gradient from Navy Island toward the Gorge of about 4×10^{-4} ft/ft; however, there is insufficient spatial distribution of data to construct a regional potentiometric surface.

Groundwater levels in the upper bedrock are controlled by recharge from the Niagara River through major fracture zones. Novakowski and Lapcevic (1988) confirmed this observation by reporting that the hydraulic head in the Oak Orchard formation is fairly uniform, indicating good hydraulic communication. Therefore, a vertical downward gradient exists between the Niagara River and Lockport Group.

On the regional scale, the Clinton Group which underlies the Lockport Group is over-pressured with respect to the Lockport Group and thus produces an upward vertical gradient. The presence of this upward gradient occurs at a considerable distance from the Gorge. Novakowski and Lapcevic (1988) suggest that this occurs between NF-2 and NI-2, thereby indicating that in the bedrock beneath the Niagara River adjacent to S-Area, the vertical gradient below the Lockport Group is upward.

In summary, within the bedrock beneath the Niagara River adjacent to S-Area, the groundwater flow generally can be described as:

- a horizontal flow in the Lockport Group to the northwest,
- a vertical downward flow from the Niagara River into the Lockport Group,
- a vertical upward flow between the Clinton and Lockport Groups.

Any NAPL that has migrated southward in the bedrock beyond the shoreline of the Niagara River within the Lockport Group would be impacted by the above groundwater hydraulic conditions as well as the other forces described in Section 3.0. In addition, the downward hydraulic gradient from the Niagara River into the Lockport Group would ensure that groundwater from the bedrock would not move upward and enter the Niagara River through the river bottom.

In addition, the potential for groundwater migration below the Lockport Group is slight, since an upward vertical gradient exists and the vertical fracture network within the Clinton Group is limited (Novakowski and Lapcevic, 1988).

The extent to which the NAPL has migrated beyond the shoreline of the Niagara River is addressed in the following chapter.

3.0 EXTENT OF NAPL MIGRATION IN THE BEDROCK BENEATH THE NIAGARA RIVER

The findings to date demonstrate that while some NAPL has migrated southward beyond the shoreline of the Niagara River through the bedrock, the migration of NAPL southward remains relatively close to the shoreline (the APL/NAPL Bedrock Migration Report). This conclusion is based in part on the following:

i) At the Hyde Park Landfill, where the lateral extent of NAPL migration has been defined, the NAPL migration through the Lockport bedrock formation was determined to be on the order of 1600 feet. The Hyde Park conditions, including overburden and bedrock stratigraphy, NAPL characteristics and methods of liquid waste placement are similar to the conditions at the S-Area; and

ii) As NAPL migrates, its volume is continually depleted by the residual NAPL saturation retained in the pore space and fracture networks.

This conclusion is consistent with an EPA modeling study of migration of S-Area NAPL under the Niagara River. The results of the study were presented in the paper entitled "Simulation of Three-Dimensional Flow of Immiscible Fluids Within and Below the Unsaturated Zone" (Faust et al, 1988). The Faust report concluded that S-Area NAPL may have migrated southward from S-Area as far as 450 feet beyond the Niagara River shoreline during a travel time of 30.8 years (Appendix B). The limited extent of NAPL presence in the bedrock beneath the Niagara River as modeled by Faust et al (1988) substantiates the above conclusion.

4.0 FLUX OF CHEMICALS FROM THE NAPL PLUME BENEATH THE NIAGARA RIVER

4.1 GROUNDWATER FLOW ROUTES AND DISCHARGE BOUNDARIES

The first step in estimating the bedrock chemical flux in the groundwater from the NAPL plume beneath the Niagara River (Chemical Flux) is to estimate the groundwater flow routes and flow rates for the hydrogeologic units. Once the flow rates are determined, the chemical analytical results from the RRT Studies Chemical Monitoring Program (Study Chemical Program) can be used to calculate the chemical flux estimates for those hydrogeologic units that provide significant pathways from the source (NAPL plume beneath the Niagara River) to the discharge boundary.

As discussed in Section 2.3, the bedrock hydrogeologic units of concern as encountered with depth from the surface, are:

i) Bedrock Upper Unit,
ii) Bedrock Second Unit
iii) Bedrock Third Unit
iv) Bedrock Fourth Unit

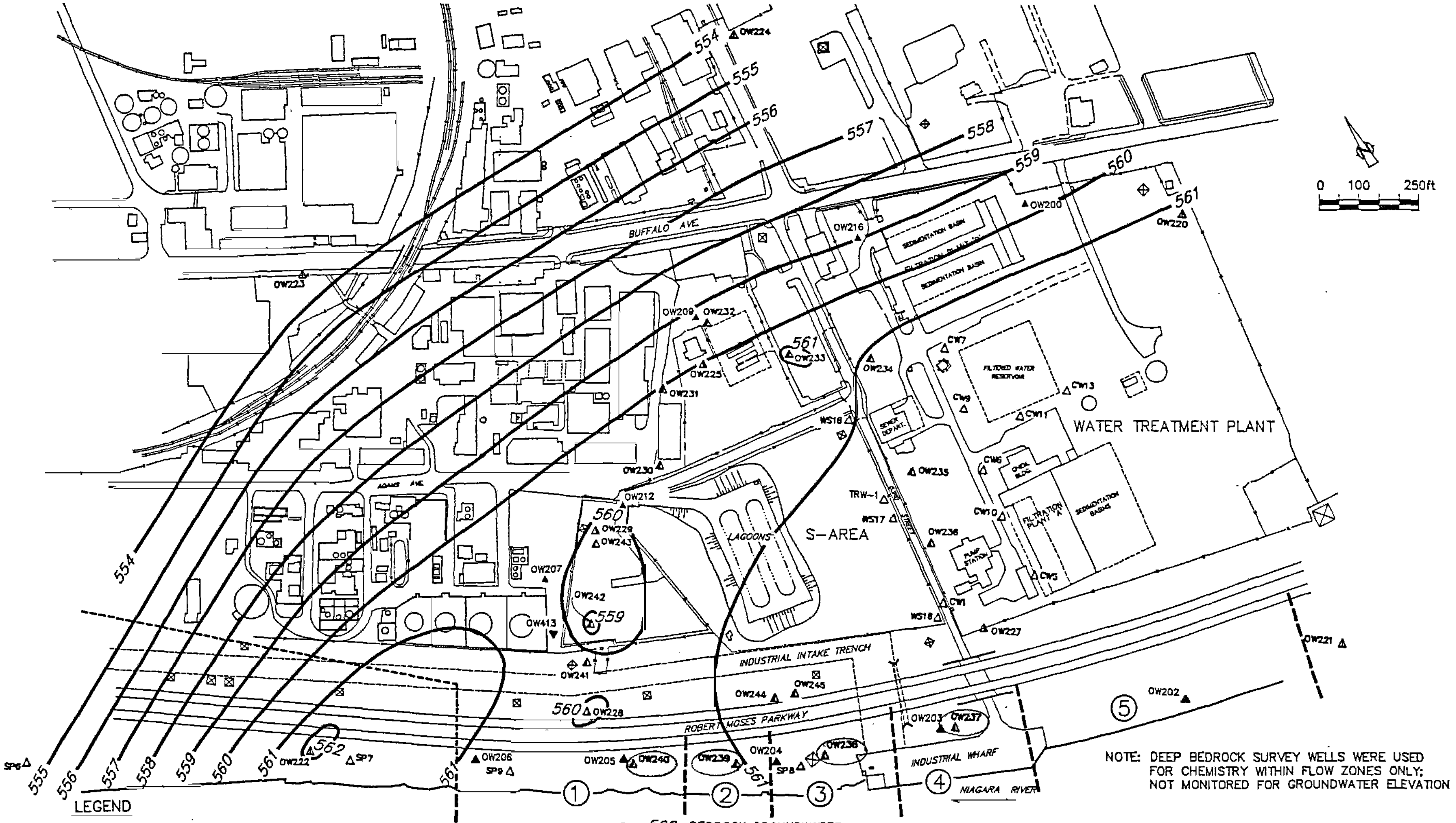
To estimate the groundwater flow in the bedrock waterbearing units, the following assumptions and procedures were used:

i) It was assumed that groundwater migration through the NYSPA grout curtain wall would be minimal.

ii) The discharge boundary was set along the shoreline, extending from the NYSPA grout curtain wall to approximately 800 feet beyond the industrial wharf. The boundary was assumed to be the same for all four waterbearing units as represented in Figures 4.1, 4.2, 4.3 and 4.4 with the zones delineated by dashed lines perpendicular to the shoreline.

The groundwater level data was plotted for the Upper, Second and Third Bedrock Units using the most complete data sets available (see Figures 4.1 to 4.3, respectively). The data of April 18, 1988 (see Table 4.1) was used for the Bedrock Upper Unit. For the Bedrock Second Unit, only one data set is available, the one collected during construction of the bedrock survey wells (see Table 4.2). The data set for the Bedrock Third Unit collected during construction of bedrock survey wells contains more data points than the data set of April 18, 1988 since, during the early stages of the bedrock survey well construction, site-specific detail was not available as to where the lowest waterbearing interval above the Rochester Formation would occur. Consequently, many of the lowest waterbearing intervals were grouted in the belief that another waterbearing interval would be encountered at greater depth. Since the bedrock survey well groundwater level data provided a better areal distribution than the April 18, 1988 data, the survey data was used to draw the flow zones for the Bedrock Third Unit. The April 18, 1988 data confirm the general pattern of groundwater flow interpreted from the survey data. Gas was encountered in the Bedrock Fourth Unit and thus, the groundwater level data available for it is limited and suspect as discussed in Section 4.2. The diagram for this unit (see Figure 4.4) illustrates only the

NOTE: REVISED CONTOURS IN VICINITY OF SP9 (JUNE 8, 1988)



NOTE: DEEP BEDROCK SURVEY WELLS WERE USED FOR CHEMISTRY WITHIN FLOW ZONES ONLY; NOT MONITORED FOR GROUNDWATER ELEVATION

LEGEND

REMEDIAL INVESTIGATION WELLS

- ▼ BEDROCK - NIAGARA PLANT SDCP
- ◬ BEDROCK - CHEMICAL
- ◬ BEDROCK - HYDRAULIC GRADIENT
- ◬ BEDROCK - TRACER
- ▲ BEDROCK - SURVEY

HISTORICAL WELLS

- △ BEDROCK
- ⬭ BEDROCK RRT STUDY WELLS

- —560 BEDROCK GROUNDWATER CONTOUR (APRIL 18, 1988)
- - - - - NYSPA GROUT CURTAIN
- — — FLOW ZONE BOUNDARY
- ① FLOW ZONE DESIGNATION

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figure 4.1

BEDROCK FLOW ZONES
BEDROCK UPPER UNIT
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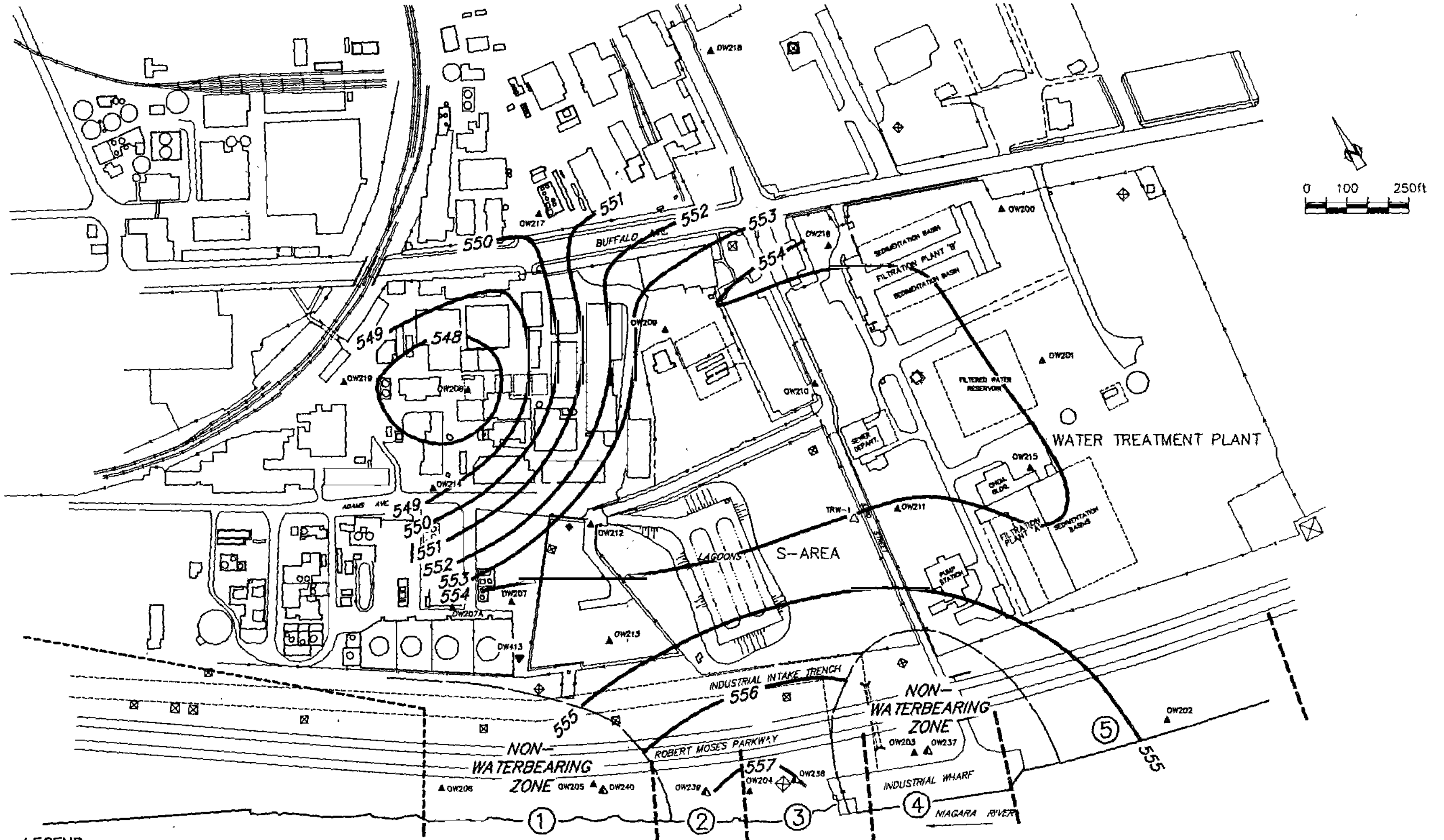

LEGEND

REMEDIAL INVESTIGATION WELLS
- ▼ BEDROCK - NIAGARA PLANT SDCP
- △ BEDROCK - CHEMICAL
- △ BEDROCK - HYDRAULIC GRADIENT
- △ BEDROCK - TRACER
- ▲ BEDROCK - SURVEY

HISTORICAL WELLS
- △ BEDROCK

552 BEDROCK GROUNDWATER CONTOUR (SURVEY DATA)

FLOW ZONE BOUNDARY

① FLOW ZONE DESIGNATION

NYSPA GROUT CURTAIN

figure 4.2

BEDROCK FLOW ZONES
BEDROCK SECOND UNIT
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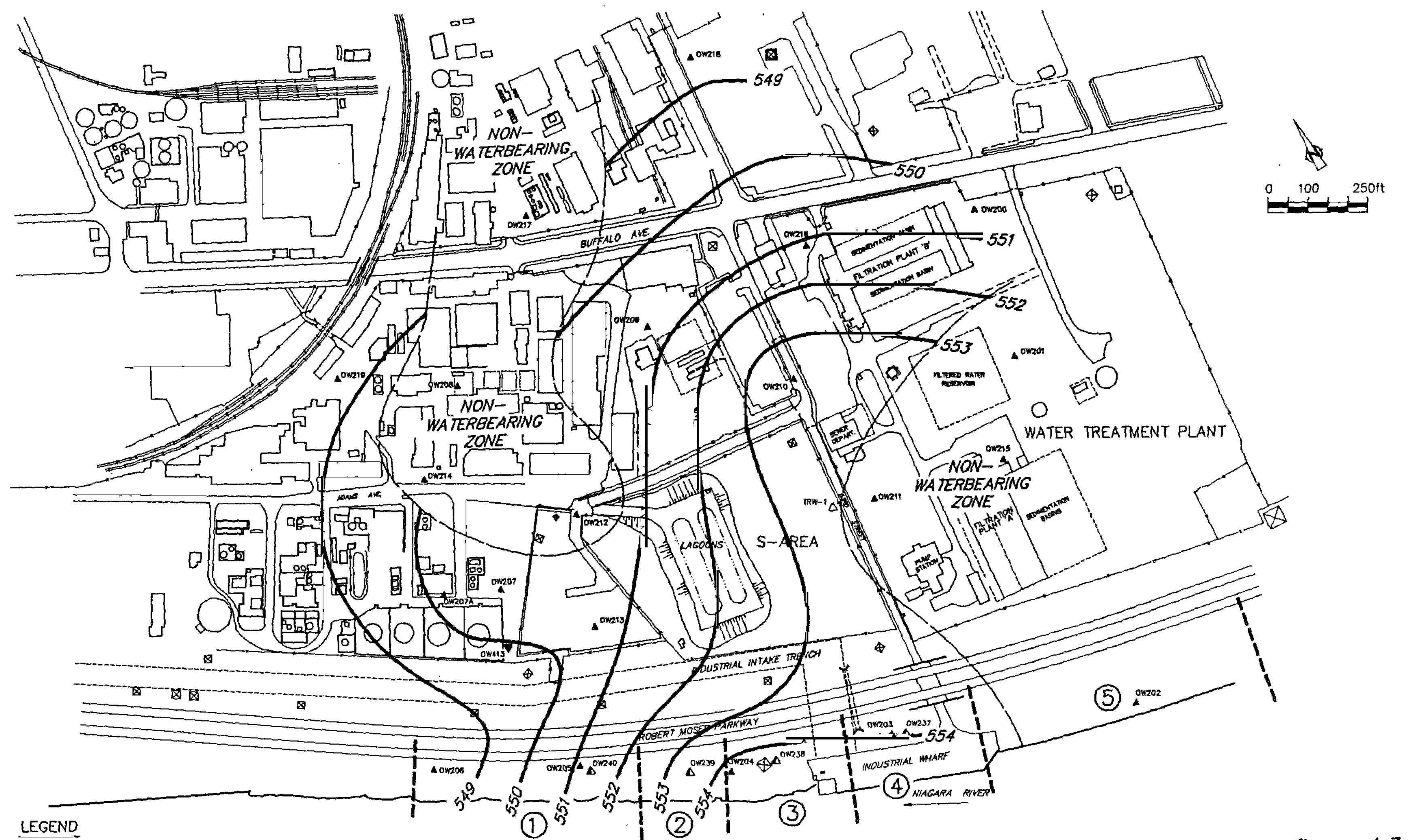

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REMEDIAL INVESTIGATION WELLS

▼	BEDROCK - NIAGARA PLANT SDCP
⚠	BEDROCK - CHEMICAL
▲	BEDROCK - HYDRAULIC GRADIENT
△	BEDROCK - TRACER
▲	BEDROCK - SURVEY

HISTORICAL WELLS

△ BEDROCK

—552	BEDROCK GROUNDWATER CONTOUR (SURVEY DATA)
— — —	FLOW ZONE BOUNDARY
①	FLOW ZONE DESIGNATION

figure 4.3

BEDROCK FLOW ZONES
BEDROCK THIRD UNIT
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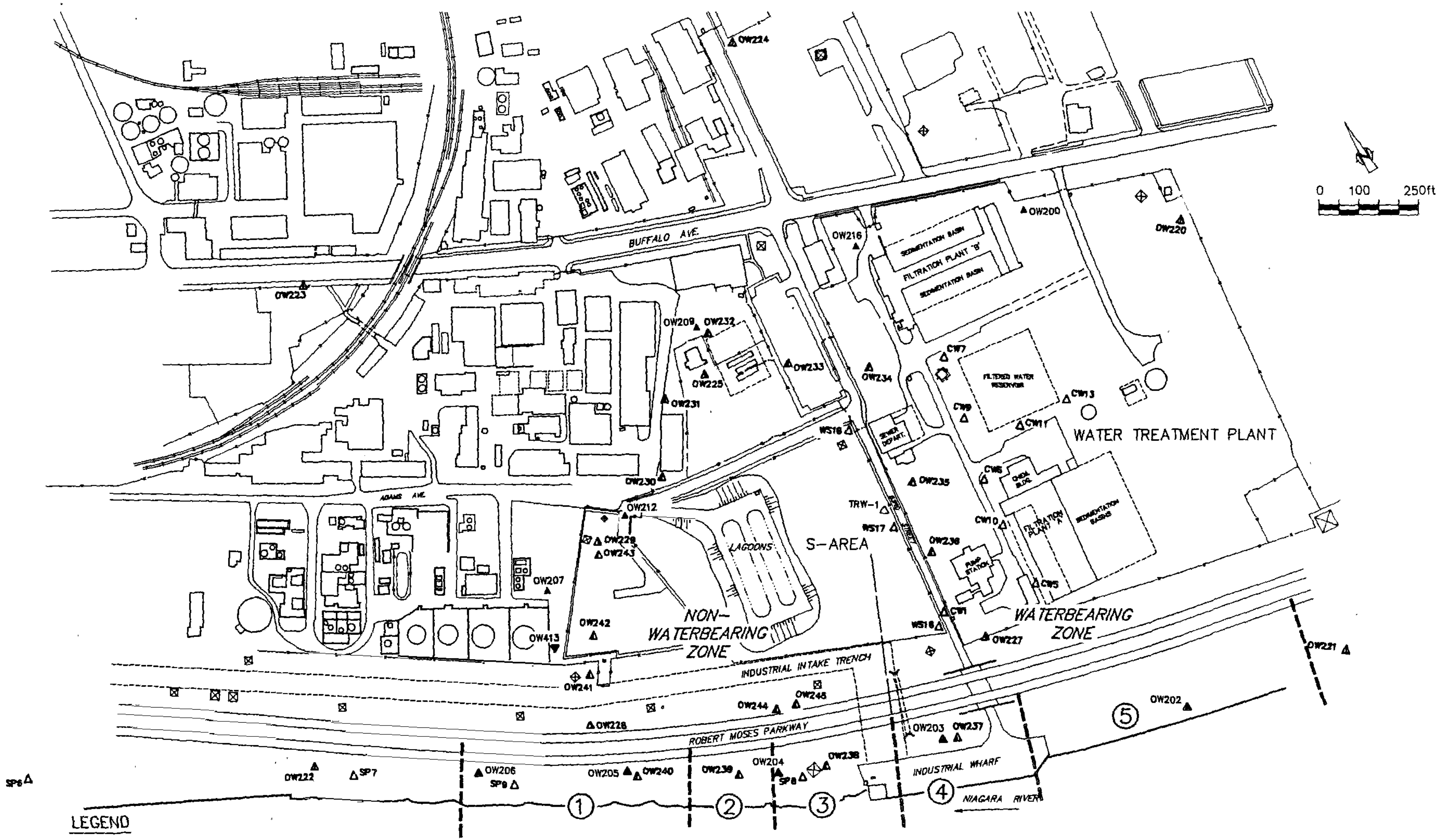

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REMEDIAL INVESTIGATION WELLS

- ▼ BEDROCK - NIAGARA PLANT SDCP
- ◬ BEDROCK - CHEMICAL
- △ BEDROCK - HYDRAULIC GRADIENT
- △ BEDROCK - TRACER
- ▲ BEDROCK - SURVEY

HISTORICAL WELLS

- △ BEDROCK

— — — FLOW ZONE BOUNDARY

① FLOW ZONE DESIGNATION

figure 4.4

BEDROCK FLOW ZONES
BEDROCK FOURTH UNIT
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TABLE 4.1

WATER ELEVATIONS - BEDROCK WELLS
S-AREA/WATER TREATMENT PLANT/NIAGARA PLANT

Bedrock Wells	*Reference Elevations*	*Dec. 24/87*	*Jan. 5-8/88*	*Feb. 8-9/88*	*April 18/88*	*Minimum*	*Maximum*
S-Area RI Wells							
(Deep Bedrock)							
OW202	571.42	--	--	--	--	--	--
OW206	575.25	--	550.71	549.43	552.76	549.43	552.76
OW209	570.79	--	552.23	551.44	554.32	551.44	554.32
OW210	571.06	--	550.55	546.32	553.59	546.32	553.59
OW212	569.97	--	548.70	--	551.71	548.70	551.71
OW214	569.55	--	550.47	552.10	553.00	550.47	553.00
OW215	574.68	--	547.00	547.73	551.53	547.00	551.53
OW216	572.05	--	--	--	553.77	553.77	553.77
OW217	572.02	--	--	--	555.23	555.23	555.23
OW218	573.88	--	--	--	550.70	550.70	550.70
OW219	568.21	--	--	--	552.28	552.28	552.28
(Shallow Bedrock)							
OW220	572.39	559.90	559.84	559.80	561.27	559.80	561.27
OW221	570.11	560.50	559.74	559.99	561.55	559.74	561.55
OW222	571.34	561.40	561.36	561.28	562.41	561.28	562.41
OW223	570.71	--	--	--	553.66	553.66	553.66
OW224	573.90	--	--	--	554.06	554.06	554.06
OW225	571.30	558.30	559.53	--	559.90	558.30	559.90
OW226	571.49	--	561.62	--	--	561.62	561.62
OW227	573.84	559.00	559.72	559.79	561.53	559.00	561.53

TABLE 4.1

WATER ELEVATIONS - BEDROCK WELLS
S-AREA/WATER TREATMENT PLANT/NIAGARA PLANT

Bedrock Wells	*Reference Elevations*	*Dec. 24/87*	*Jan. 5-8/88*	*Feb. 8-9/88*	*April 18/88*	*Minimum*	*Maximum*
(Shallow Bedrock)							
OW228	579.91	--	--	--	559.89	559.89	559.89
OW229	569.06	--	--	--	559.87	559.87	559.87
OW230	569.15	559.00	560.03	558.83	560.67	558.83	560.67
OW231	569.93	558.70	559.50	558.50	560.21	558.50	560.21
OW232	571.97	558.60	559.18	558.27	559.86	558.27	559.86
OW233	570.88	559.30	560.13	559.03	561.14	559.03	561.14
OW234	569.75	557.70	559.43	--	561.24	557.70	561.24
OW235	570.65	559.70	--	559.63	561.16	559.63	561.16
OW236	576.90	559.80	559.30	559.76	561.22	559.30	561.22
OW237	568.04	559.90	559.92	559.71	561.43	559.71	561.43
OW238	569.44	559.50	559.59	559.49	561.18	559.49	561.18
OW239	575.91	559.30	559.66	558.90	560.93	558.90	560.93
OW240	576.88	559.20	559.40	559.34	560.93	559.20	560.93
OW241	567.76	--	558.94	559.19	560.91	558.94	560.91
OW242	567.79	559.00	560.26	559.27	558.86	558.86	560.26
OW243	568.76	558.00	559.08	558.25	559.91	558.00	559.91
OW244	582.96	559.80	559.68	559.62	561.31	559.62	561.31
OW245	582.81	559.80	559.70	559.52	561.08	559.52	561.08

TABLE 4.1

WATER ELEVATIONS - BEDROCK WELLS
S-AREA/WATER TREATMENT PLANT/NIAGARA PLANT

Bedrock Wells	*Reference Elevations*	*Dec. 24/87*	*Jan. 5-8/88*	*Feb. 8-9/88*	*April 18/88*	*Minimum*	*Maximum*
WTP Wells *(Shallow Bedrock)*							
CW1	570.86	--	559.80	559.86	561.53	559.80	562.57
CW5	575.93	--	--	--	561.18	559.18	562.48
CW6	575.15	--	559.67	559.89	561.37	559.67	562.74
CW7	570.49	--	560.28	559.89	561.17	559.33	561.96
CW9	571.98	--	559.65	559.78	561.40	559.65	562.33
CW10	576.73	--	559.70	--	561.41	559.70	563.43
CW11	574.53	--	560.36	--	561.30	560.31	562.38
CW13	573.27	--	559.83	560.03	561.45	559.83	562.51
Niagara Plant Wells *(Shallow Bedrock)*							
SP6	568.31	--	552.36	551.29	554.43	550.30	554.91
SP7	572.64	--	560.11	560.45	561.66	560.05	562.65
SP8	569.86	--	559.45	559.57	561.23	559.45	562.45
SP9	573.85	--	558.68	558.73	560.50	558.68	568.15
WS9	571.21	--	553.88	553.92	--	553.21	557.64
WS10	570.29	--	559.14	558.64	--	558.34	560.67
WS16	572.57	--	560.92	559.94	561.21	559.94	563.81
WS17	573.31	--	560.85	559.87	561.16	559.87	562.63
WS18	573.76	--	560.09	560.03	560.93	559.92	561.90

TABLE 4.1

WATER ELEVATIONS - BEDROCK WELLS
S-AREA/WATER TREATMENT PLANT/NIAGARA PLANT

Bedrock Wells	*Reference Elevations*	*Dec. 24/87*	*Jan. 5-8/88*	*Feb. 8-9/88*	*April 18/88*	*Minimum*	*Maximum*
Niagara Plant Wells *(Shallow Bedrock) continued*							
WS19	571.41	--	561.73	558.99	--	558.99	562.45
WS20	572.08	--	558.58	558.42	--	557.93	560.42
WS21	573.31	--	554.12	--	--	553.13	556.29
WS23	572.21	--	551.83	--	--	549.16	553.78
WS28	570.18	--	--	558.00	--	545.77	569.45
WS30	571.78	--	551.93	552.61	--	551.17	559.91
WS40	572.22	--	--	--	--	551.14	554.30

Notes:

1) The following is a list of the non-functioning well installations (buried, destroyed, plugged) not presented in the table but used for stratrigraphic information WS11, WS12, WS13, WS22, WS24, WS31 and WS32.
2) The following is a list of the S-Area RI wells which were grouted to ground surface: OW200, OW201, OW204, OW205, OW207, OW208, OW211 and OW213.
3) All elevations are based on 1986 OCC Datum (Ref. Dwg. A-11-19200).

TABLE 4.2

BEDROCK SURVEY WELL STATIC WATER LEVELS
S-AREA REMEDIAL PROGRAM

Bedrock Well:	OW200		OW201	
Ground Surface:	573.8		568.9	
Bedrock Interval	*Interval Elevation*	*Static W/L Elevation*	*Interval Elevation*	*Static W/L Elevation*
A	545. 3 - 527.4	561.1	537.4 - 522.6	557.5
B	527.4 - 512.4	561.1	522.6 - 507.6	557.5
C	512.4 - 497.4	NWB	507.6 - 492.6	559.9
D	497.4 - 482.4	NWB	492.6 - 477.6	NWB
E	482.4 - 467.4	554.1	477.6 - 462.6	554.1
F	467.4 - 452.4	555.3	462.6 - 447.6	554.7
G	452.4 - 437.4	NWB	447.6 - 432.6	NWB
H	437.4 - 422.4	NWB	432.6 - 417.6	NWB
I	422.4 - 407.4	550.6	417.6 - 402.1	NWB
J	407.4 - 392.4	NWB	402.1 - 387.1	NWB
K	392.4 - 377.5	NWB	387.1 - 363.1	NWB
L	377.5 - 369.5	NWB		NWB

Notes:

WB = Waterbearing
NWB = Non-Waterbearing

TABLE 4.2

BEDROCK SURVEY WELL STATIC WATER LEVELS
S-AREA REMEDIAL PROGRAM

Bedrock Well:	OW202		OW203	
Ground Surface:	571.5		568.2	
Bedrock Interval	*Interval Elevation*	*Static W/L Elevation*	*Interval Elevation*	*Static W/L Elevation*
A	534.5 - 519.5	558.9	538.1 - 522.4	558.9
B	519.5 - 504.5	558.3	522.4 - 507.3	559.9
C	504.5 - 489.5	561.0	507.3 - 492.1	NWB
D	489.5 - 474.5	NWB	492.1 - 477.1	NWB
E	474.5 - 459.5	554.8	477.1 - 462.1	NWB
F	459.5 - 444.5	NWB	462.1 - 447.1	NWB
G	444.5 - 430.5	NWB	447.1 - 432.1	NWB
H	430.5 - 414.2	NWB	432.1 - 417.1	554.0
I	414.2 - 399.2	NWB	417.1 - 402.1	NWB
J	399.2 - 384.2	NWB	402.1 - 386.5	NWB
K	384.2 - 364.7	384.2	386.5 - 371.8	384.00

Notes:

WB = Waterbearing
NWB = Non-Waterbearing

TABLE 4.2

BEDROCK SURVEY WELL STATIC WATER LEVELS
S-AREA REMEDIAL PROGRAM

Bedrock Well:	OW204		OW205	
Ground Surface:	572.3		578.3	
Bedrock Interval	***Interval Elevation***	***Static W/L Elevation***	***Interval Elevation***	***Static W/L Elevation***
A	537.8 - 520.9	560.3	539.8 - 524.8	561.2
B	520.9 - 505.9	558.3	524.8 - 510.0	561.2
C	505.9 - 490.9	558.3	510.0 - 495.0	561.0
D	490.9 - 475.9	NWB	495.0 - 480.0	NWB
E	475.9 - 460.9	557.3	480.0 - 465.9	NWB
F	460.9 - 445.7	NWB	465.9 - 449.8	NWB
G	445.7 - 430.3	NWB	449.8 - 434.8	NWB
H	430.3 - 415.3	NWB	434.8 - 419.8	NM/WB
I	415.3 - 400.3	554.3	419.8 - 404.8	NWB
J	400.3 - 385.3	NWB	404.8 - 389.1	NWB
K	385.3 - 370.3	NWB	389.1 - 373.1	NWB
L	370.3 - 360.3	NWB	373.1 - 363.1	NWB

Notes:

NM = Not Measured
WB = Waterbearing
NWB = Non-Waterbearing

TABLE 4.2

BEDROCK SURVEY WELL STATIC WATER LEVELS
S-AREA REMEDIAL PROGRAM

Bedrock Well:	OW206		OW207	
Ground Surface:	575.1		568.8	
Bedrock Interval	*Interval Elevation*	*Static W/L Elevation*	*Interval Elevation*	*Static W/L Elevation*
A	541.9 - 529.1	557.1	540.1 - 525.1	559.8
B	529.1 - 515.5	557.1	525.1 - 510.4	558.8
C	515.5 - 499.1	554.2	510.4 - 495.4	558.5
D	499.1 - 484.1	554.2	495.4 - 480.4	NWB
E	484.1 - 469.1	NWB	480.4 - 465.4	554.9
F	469.1 - 454.1	NWB	465.4 - 450.4	NWB
G	454.1 - 439.2	NWB	450.4 - 435.4	NWB
H	439.2 - 424.1	NWB	435.4 - 420.4	NM/WB
I	424.1 - 409.1	548.1	420.4 - 404.6	551.0
J	409.1 - 394.1	548.1	404.6 - 389.6	536.1
K	394.1 - 379.1	NWB	389.6 - 370.8	GAS
L	379.1 - 369.1	NWB		

Notes:

NM = Not Measured
WB = Waterbearing
NWB = Non-Waterbearing

TABLE 4.2

BEDROCK SURVEY WELL STATIC WATER LEVELS
S-AREA REMEDIAL PROGRAM

Bedrock Well:	OW208		OW209	
Ground Surface:	567.6		571.0	
Bedrock Interval	*Interval Elevation*	*Static W/L Elevation*	*Interval Elevation*	*Static W/L Elevation*
A	542.6 - 527.6	557.9	541.0 - 526.0	560.0
B	527.6 - 512.6	NWB	526.0 - 511.0	558.1
C	512.6 - 497.6	NWB	511.0 - 496.0	NWB
D	497.6 - 482.6	NWB	496.0 - 481.0	NWB
E	482.6 - 467.6	NWB	481.0 - 466.0	553.9
F	467.6 - 452.9	546.9	466.0 - 451.0	NWB
G	452.9 - 437.4	NWB	451.0 - 436.0	NWB
H	437.4 - 422.6	NWB	436.0 - 420.6	550.8
I	422.6 - 407.6	NWB	420.6 - 405.6	NWB
J	407.6 - 392.6	NWB	405.6 - 389.6	NWB
K	392.6 - 372.6	NWB	389.6 - 372.6	NWB

Notes:

WB = Waterbearing
NWB = Non-Waterbearing

TABLE 4.2

BEDROCK SURVEY WELL STATIC WATER LEVELS
S-AREA REMEDIAL PROGRAM

Bedrock Well:	OW210		OW211	
Ground Surface:	570.6		570.6	
Bedrock Interval	*Interval Elevation*	*Static W/L Elevation*	*Interval Elevation*	*Static W/L Elevation*
A	537.1 - 524.1	558.9	539.6 - 523.2	559.0
B	524.1 - 509.1	558.8	523.2 - 510.4	560.1
C	509.1 - 494.1	NWB	510.4 - 495.6	NWB
D	494.1 - 480.3	NWB	495.6 - 480.8	NWB
E	480.3 - 463.9	552.6	480.8 - 465.6	554.1
F	463.9 - 448.9	552.6	465.6 - 449.9	NWB
G	448.9 - 433.9	NWB	449.9 - 434.9	NWB
H	433.9 - 416.6	553.8	434.9 - 421.6	NWB
I	416.6 - 401.6	553.9	421.6 - 406.6	NWB
J	401.6 - 384.6	NWB	406.6 - 391.6	NWB
K	384.6 - 367.5	NWB	391.6 - 375.2	NWB
L			375.2 - 366.6	NWB

Notes:

WB = Waterbearing
NWB = Non-Waterbearing

TABLE 4.2

BEDROCK SURVEY WELL STATIC WATER LEVELS
S-AREA REMEDIAL PROGRAM

Bedrock Well:	OW212		OW213	
Ground Surface:	570.1		568.6	
Bedrock Interval	*Interval Elevation*	*Static W/L Elevation*	*Interval Elevation*	*Static W/L Elevation*
A	541.6 - 527.5	560.0	540.1 - 525.2	NM/WB
B	527.5 - 513.2	558.6	525.2 - 509.9	NM/WB
C	513.2 - 496.7	NWB	509.9 - 494.9	561.3
D	496.7 - 481.7	NWB	494.9 - 479.9	561.3
E	481.7 - 466.7	NM/WB	479.9 - 465.4	549.6
F	466.7 - 451.7	NWB	465.4 - 449.9	554.4
G	451.7 - 436.7	NWB	449.9 - 434.9	554.6
H	436.7 - 421.1	NWB	434.9 - 419.9	NWB
I	421.1 - 406.1	NWB	419.9 - 404.9	550.4
J	406.1 - 390.1	537.0	404.9 - 389.5	NWB
K	390.1 - 370.6	NWB	389.5 - 374.5	NWB
L			374.5 - 364.5	NWB

Notes:

NM = Not Measured
WB = Waterbearing
NWB = Non-Waterbearing

TABLE 4.2

BEDROCK SURVEY WELL STATIC WATER LEVELS
S-AREA REMEDIAL PROGRAM

Bedrock Well:	OW214		OW215	
Ground Surface:	569.7		575.0	
Bedrock Interval	*Interval Elevation*	*Static W/L Elevation*	*Interval Elevation*	*Static W/L Elevation*
A	545.2 - 531.4	559.3	537.3 - 519.0	560.6
B	531.4 - 516.5	557.7	519.0 - 504.0	561.1
C	516.5 - 501.5	556.9	504.0 - 489.0	NWB
D	501.5 - 486.5	NWB	489.0 - 474.0	NWB
E	486.5 - 471.6	NWB	474.0 - 456.0	553.8
F	471.6 - 456.1	548.8	456.0 - 437.5	NWB
G	456.1 - 436.1	NWB	437.5 - 421.0	NWB
H	436.1 - 421.1	NWB	421.0 - 406.0	553.8
I	421.1 - 406.1	NWB	406.0 - 389.0	NWB
J	406.1 - 386.1	NWB	389.0 - 369.0	NWB
K	386.1 - 371.1	NWB		

Notes:

WB = Waterbearing
NWB = Non-Waterbearing

TABLE 4.2

BEDROCK SURVEY WELL STATIC WATER LEVELS
S-AREA REMEDIAL PROGRAM

Bedrock Well: OW216 OW217
Ground Surface: 572.3 572.3

Bedrock Interval	OW216 *Interval Elevation*	OW216 *Static W/L Elevation*	OW217 *Interval Elevation*	OW217 *Static W/L Elevation*
A	541.0 - 526.3	558.3	545.3 - 534.3	551.9
B	526.3 - 511.3	555.8	543.3 - 519.3	NM/WB
C	511.3 - 496.3	NWB	519.3 - 504.3	NM/WB
D	496.3 - 481.3	NWB	504.3 - 489.0	NWB
E	481.3 - 466.3	554.3	489.0 - 473.9	551.7
F	466.3 - 451.3	554.3	473.9 - 458.9	548.8
G	451.3 - 436.3	NWB	458.9 - 441.9	NWB
H	436.3 - 418.3	551.5	441.9 - 424.9	NWB
I	418.3 - 400.8	550.7	424.9 - 408.9	NWB
J	400.8 - 383.8	NWB	408.9 - 388.9	NWB
K	383.8 - 374.0	NWB	388.9 - 369.1	NWB

Notes:

NM = Not Measured
WB = Waterbearing
NWB = Non-Waterbearing

TABLE 4.2

BEDROCK SURVEY WELL STATIC WATER LEVELS
S-AREA REMEDIAL PROGRAM

Bedrock Well: OW218 / OW219

Ground Surface: 568.9 / 568.9

	OW218		OW219	
Bedrock Interval	*Interval Elevation*	*Static W/L Elevation*	*Interval Elevation*	*Static W/L Elevation*
A	547.4 - 531.3	552.1	548.0 - 532.4	555.0
B	531.3 - 515.8	550.9	532.4 - 517.8	552.2
C	515.8 - 500.8	552.1	517.8 - 502.8	552.3
D	500.8 - 486.1	551.9	502.8 - 488.3	546.5
E	486.1 - 471.1	NM/WB	488.3 - 473.3	NWB
F	471.1 - 456.1	NWB	473.3 - 458.6	548.2
G	456.1 - 441.1	549.9	458.6 - 443.5	548.5
H	441.1 - 425.5	547.4	443.5 - 427.5	NWB
I	425.5 - 405.5	NWB	427.5 - 411.5	548.2
J	405.5 - 385.5	NWB	411.5 - 395.5	NWB
K	385.5 - 375.6	NWB	395.5 - 379.5	NWB
L			379.5 - 369.7	NWB

Notes:

NM = Not Measured
WB = Waterbearing
NWB = Non-Waterbearing

division between waterbearing and non-waterbearing regions of the flux boundary. For the purposes of this study, the hydraulic characteristics in the Bedrock Fourth Unit are assumed to be identical to those in the Bedrock Third Unit.

Groundwater flow through the bedrock waterbearing units at the northern shore of the Niagara River is generally to the northwest, as shown in the upper three units (see Figures 4.1, 4.2 and 4.3) and assumed for the fourth unit. From here, the groundwater flow in the bedrock either enters the NYSPA Conduits or the Falls Street Tunnel to discharge to the Lower Niagara River. In either case, the ultimate discharge is to the Lower Niagara River.

For purposes of the risk assessment-Section 6.0, it was assumed that all flow entered the conduits, a conservative estimate, for assessing the condition at the NYSPA reservoir, since some flow does enter the Falls Street Tunnel.

4.2 GROUNDWATER FLOW RATE

The wells at the discharge boundary of the bedrock waterbearing units used to calculate the groundwater flow rate are shown on Figure 4.1.

The groundwater flow rates are calculated using the Darcy equation:

$Q = KiA$

Where: Q = Flow (L^3/T)

K = hydraulic conductivity (L/T)

i = gradient

A = cross-section area of flow (L^2)

Using the flow zones shown in Figure 4.1, the bedrock groundwater flow was calculated using the gradient and hydraulic conductivity values presented in the report entitled "Requisite Remedial Technology Study of Chemicals in the Overburden and Bedrock" ("S-Area RRT"). The hydraulic conductivity values represent regional pump test results obtained from well TRW-1 (Historical Data Base, Buffalo Avenue Plant, Volumes I-II, August 1), and coincide well with injection test results from well OW413 (See Appendix C) obtained during the Buffalo Avenue Plant SDCP. Because the hydraulic gradients are poorly defined in the vicinity of the shoreline and the data for the gradients was collected over an extended period of time, the values previously calculated in the S-Area RRT were used. The data represented in Figures 4.1, 4.2 and 4.3 indicate that the gradient values along the shoreline are one to two orders of magnitude less than these assumed values, resulting in a very conservative (i.e. high) estimated of groundwater flow and chemical flux.

Hydraulic conductivity and gradient values for the Bedrock Fourth Unit (Decew Formation) were assumed to be equal to those of the Bedrock Third Unit (Goat Island Formation) since the sparsity of data did not allow separate estimates for the Bedrock Fourth Unit to be calculated.

Water level data for the Bedrock Fourth Unit indicates water levels approximately 160 feet lower than the Bedrock Third Unit. While pump testing indicated a waterbearing interval at OW202 and OW203 in the Bedrock Fourth Unit (Decew Formation), this was actually a false indication of a waterbearing zone due to the gas release in this interval (APL/NAPL Bedrock Migration Report). Regardless, for purposes of a conservative mass flux estimate, this interval was assumed to be waterbearing.

The estimation of groundwater flow rates used the bedrock waterbearing unit thicknesses described in the S-Area RRT and are consistent with the well log data available for the shoreline area (see Figure 14, the APL/NAPL Bedrock Migration Report).

Groundwater flow estimates and parameter values are as indicated in Table 4.3.

4.3 CHEMICAL FLUX ESTIMATES

The calculated organic chemical flux at the specified boundary in the bedrock was estimated using the estimated groundwater flow and the data from the Study Chemical Program. The Study Chemical list was selected with the concurrence of the EPA/State in order to evaluate the endangerment to health. The specific boundaries selected for the chemical flux calculations are the same as the discharge boundaries used for the groundwater flow calculations. Study Chemical data from four shallow bedrock wells along the discharge boundary (see Figure 4.1) was used for the

TABLE 4.3

BEDROCK GROUNDWATER FLOW

	Flow Zone				
	1	2	3	4	5
Upper:					
K(ft/day)	113.4	113.4	113.4	113.4	113.4
Gradient	0.005	0.005	0.005	0.005	0.005
Thick (ft)	30	30	30	30	30
Length (ft)	561	227	303	333	758
Flow (cfd)	9,543	3,861	5,154	5,664	12,894
Second:					
K(ft/day)	NA	2.8	2.8	NA	2.8
Gradient	0	0.006	0.006	0	0.006
Thick (ft)	30	30	30	30	30
Length (ft)	561	227	303	333	758
Flow (cfd)	0	114	153	0	382
Third:					
K(ft/day)	2.8	2.8	2.8	2.8	NA
Gradient	0.005	0.005	0.005	0.005	0
Thick (ft)	15	15	15	15	15
Length (ft)	561	227	303	333	758
Flow (cfd)	118	48	64	70	0
Fourth:					
K(ft/day)	NA	NA	NA	2.8	2.8
Gradient	0	0	0	0.005	0.005
Thick (ft)	15	15	15	15	15
Length (ft)	561	227	303	333	758
Flow (cfd)	0	0	0	70	159

Note: 'NA' in the hydraulic conductivity (K) field and a gradient of 0 indicates that the zone is non-waterbearing in that interval.

flux calculations. This data is presented in Appendix D for wells OW240, OW239, OW238 and OW237. As no Study Chemical data was available for the second, third or fourth units, the upper unit concentrations were assumed to apply to all four levels providing a very conservative (high) estimate of chemical flux. This conclusion is based on the observed decreasing gradient of chemical concentration data measured in the bedrock with depth north of S-Area.

For purposes of this chemical flux estimation, if a parameter was not detected in the APL at a particular well above the quantitation level, it was nevertheless assigned a value of one-half of the quantification level if it had been detected at any other discharge boundary well. If a parameter was not detected in the APL at any interval above the quantitation level, it was assigned a value of zero and was not considered further. Table 4.4 presents the concentration values assigned to non-detected Study Chemicals for flux estimation.

The groundwater chemical flux estimates for the corresponding hydrogeologic units are detailed on the following tables:

Hydrogeologic Unit	*Groundwater Flow*	*Chemical Flux of Study Chemicals*
Bedrock Upper Unit	Table 4.3	Table 4.5
Bedrock Second Unit	Table 4.3	Table 4.6
Bedrock Third Unit	Table 4.3	Table 4.7
Bedrock Fourth Unit	Table 4.3	Table 4.8

TABLE 4.4

ASSIGNED VALUE FOR NON-DETECTS STUDY CHEMICALS

Study Chemical	*Quantitation Level*	*Number of Detections+*	*Assigned Vallues for Chemical Flux*
1,1-Dichloroethylene	5 ug/L	0	0 ug/L
2-Chlorophenol	10 ug/L	0	0 ug/L
2,4-Dichlorophenol	10 ug/L	0	0 ug/L
2,4,5-Trichlorophenol (2,4,5-TCP)	50 ug/L	0	0 ug/L
2,4,6-Trichlorophenol	10 ug/L	0	0 ug/L
4-Chloro-3-methylphenol	10 ug/L	0	0 ug/L
Pentachlorophenol	50 ug/L	0	0 ug/L
Phenol	10 ug/L	1	5 ug/L
Endosulfan I	10 ug/L	0	0 ug/L
Endolsulfan II	10 ug/L	0	0 ug/L
1,2,3-Trichlorobenzene (1,2,3-TCB)	7 ug/L	5	3.5 ug/L
1,2,4-Trichlorobenzene (1,2,4-TCB)	7 ug/L	5	3.5 ug/L
Hexachlorobenzene	7 ug/L	0	0 ug/L
a-Hexachlorocyclohexane (a-HCCH)	7 ug/L	2	3.5 ug/L
b-Hexachlorocyclohexane (b-HCCH)	7 ug/L	0	0 ug/L
g-Hexachlorocyclohexane (g-HCCH)	7 ug/L	0	0 ug/L
d-Hexachlorocyclohexane (d-HCCH)	7 ug/L	0	0 ug/L
Perchloropentacyclodecane (Mirex)	7 ug/L	0	0 ug/L
PCB-1248 (Arochlor 1248)	1 ug/L	1	0.5 ug/L
2,3,7,8-Tetrachlorodibenzo-p-dioxin	0.5 ng/L	0	0 ng/L
Total Tetrachlorodibenzo-p-dioxins	0.5 ng/L	0	0 ng/L
1,2,3,7,8-Pentachlorodibenzodioxin	0.5 ng/L	0	0 ng/L
Total Pentachlorodibenzodioxins	0.5 ng/L	0	0 ng/L
1,2,3,4,7,8-Hexachlorodibenzodioxin	0.5 ng/L	0	0 ng/L
1,2,3,6,7,8-Hexachlorodibenzodioxin	0.5 ng/L	0	0 ng/L
1,2,3,7,8,9-Hexachlorodibenzodioxin	0.5 ng/L	0	0 ng/L
Total Hexachlorodibenzodioxins (Total HxCDD)	0.5 ng/L	0	0 ng/L
1,2,3,4,6,7,8-Heptachlorodibenzodioxin (1,2,3,4,6,7,8-HpCDD)	0.5 ng/L	0	0 ng/L
Total Heptachlorodibenzodioxins (Total HpCDD)	0.5 ng/L	0	0. ng/L
Octachlorobenzodioxin (OCDD)	0.5 ng/L	0	0 ng/L
2,3,7,8-Tetrachlorobenzofuran	0.5 ng/L	0	0 ng/L
Total Tetrachlorodibenzofurans (Total TCDF)	0.5 ng/L	0	0 ng/L
1,2,3,7,8-Pentachlorodibenzofuran	0.5 ng/L	0	0 ng/L
2,3,4,7,8-Pentachlorodibenzofuran	0.5 ng/L	0	0 ng/L
Total Pentachlorodibenzofurans (Total PCDF)	0.5 ng/L	1	0.25 ng/L
1,2,3,4,7,8-Hexachlorodibenzofuran (1,2,3,4,7,8-HxCDF)	0.5 ng/L	0	0 ng/L
1,2,3,6,7,8-Hexachlorodibenzofuran	0.5 ng/L	0	0 ng/L
2,3,4,6,7,8-Hexachlorodibenzofuran	0.5 ng/L	0	0 ng/L
1,2,3,7,8,9-Hexachlorodibenzofuran	0.5 ng/L	0	0 ng/L

TABLE 4.4

ASSIGNED VALUE FOR NON-DETECTS
STUDY CHEMICALS

Study Chemical	*Quantitation Level*	*Number of Detections+*	*Assigned Values for Chemical Flux*
Total Hexachlorodibenzofurans (Total HxCDF)	0.5 ng/L	1	0.25 ng/L
1,2,3,4,6,7,8-Heptachlorodibenzofuran (1,2,3,4,6,7,8-HpCDF)	0.5 ng/L	2	0.25 ng/L
1,2,3,4,7,8,9-Heptachlorodibenzofuran	0.5 ng/L	0	0 ng/L
Total Heptachlorodibenzofurans (Total HpCDF)	0.5 ng/L	2	0.25 ng/L
Octachlorodibenzofuran (OCDF)	0.5 ng/L	3	0.25 ng/L
Mercury (Hg)	0.2 µg/L	0	0 µg/L

+ Total number of analyses is 5 including one duplicate analysis

* Five detections above quantitation level of which one was a duplicate with compound detected in both samples.

TABLE 4.5

CHEMICAL FLUX
BEDROCK UPPER UNIT

			Flow Zone Concentrations					
Study Chemical	***Units of Measurement***	***Quantitation Levels***	***1 (OW240)***	***2 (OW239)***	***3 (OW238)***	***4 (OW237)***	***5 (OW237)***	***Total Study Chemical Flux (lbs/day)***
Phenol	ug/L	10	5	5	110	5	5	4.54 E-2
1,2,3-TCB	ug/L	7	22.5	200	190	11	11	1.36 E-1
1,2,4-TCB	ug/L	7	130	930	1200	63	63	7.61 E-1
a-HCCH	ug/L	7	3.5	19	18	3.5	3.5	1.65 E-2
PCB-1248	ug/L	1	0.5	1	.5	.5	.5	1.28 E-3
Total PCDF	ng/L	0.5	.25	0.6	.25	.25	.25	6.64 E-7
Total HxCDF	ng/L	0.5	.25	0.8	.25	.25	.25	7.12 E-7
1,2,3,4,6,7,8 HpCDF	ng/L	0.5	.25	5.2	.25	.8	.8	2.41 E-6
Total HpCDF	ng/L	0.5	.25	6.5	.25	1.	1.	2.96 E-6
OCDF	ng/L	0.5	.25	29	.5	4.2	4.2	1.22 E-5
Zonal Groundwater Flow (cfd)			9543	3861	5154	5664	12894	
Zonal Chemical Flux (lbs/day)			9.62 E-2	2.78 E-1	4.89 E-1	2.94 E-2	6.68 E-2	9.60 E-1 (total)

TABLE 4.6

RRT CHEMICAL FLUX
BEDROCK SECOND UNIT

			Flow Zone Concentrations					
Study Chemical	*Units of Measurement*	*Quantitation Levels*	*1 (OW240)*	*2 (OW239)*	*3 (OW238)*	*4 (OW237)*	*5 (OW237)*	*Total Study Chemical Flux (lbs/day)*
Phenol	ug/L	10	5	5	110	5	5	1.20 E-3
1,2,3-TCB	ug/L	7	22.5	200	190	11	11	3.50 E-3
1,2,4-TCB	ug/L	7	130	930	1200	63	63	1.96 E-2
a-HCCH	ug/L	7	3.5	19	18	3.5	3.5	3.91 E-4
PCB-1248	ug/L	1	0.5	1	0.5	0.5	0.5	2.38 E-5
Total PCDF	ng/L	0.5	.25	0.6	.25	.25	.25	1.26 E-8
Total HxCDF	ng/L	0.5	.25	0.8	.25	.25	.25	1.41 E-8
1,2,3,4,6,7,8 HpCDF	ng/L	0.5	.25	5.2	.25	.8	.8	5.86 E-8
Total HpCDF	ng/L	0.5	.25	6.5	.25	1.	1.	7.27 E-8
OCDF	ng/L	0.5	.25	29	0.5	4.2	4.2	3.12 E-7
Zonal Groundwater Flow (cfd)			0	114	153	0	382	
Zonal Chemical Flux (lbs/day)			0	8.25 E-3	1.45 E-2	0	1.98 E-3	2.47 E-2 (total)

Note:

A zonal groundwater flow of zero (0) indicates that the zone is non-waterbearing in that interval and yields a zonal chemical flux of zero (0).

TABLE 4.7

CHEMICAL FLUX
BEDROCK THIRD UNIT

			Flow Zone Concentrations					
Study Chemical	*Units of Measurement*	*Quantitation Levels*	*1 (OW240)*	*2 (OW239)*	*3 (OW238)*	*4 (OW237)*	*5 (OW237)*	*Total Study Chemical Flux (lbs/day)*
Phenol	ug/L	10	5	5	110	5	5	5.11 E-4
1,2,3-TCB	ug/L	7	22.5	200	190	11	11	1.56 E-3
1,2,4-TCB	ug/L	7	130	930	1200	63	63	8.77 E-3
a-HCCH	ug/L	7	3.5	19	18	3.5	3.5	1.69 E-4
PCB-1248	ug/L	1	0.5	1	0.5	0.5	0.5	1.08 E-5
Total PCDF	ng/L	0.5	.25	0.6	.25	.25	.25	5.71 E-9
Total HxCDF	ng/L	0.5	.25	0.8	.25	.25	.25	6.30 E-9
1,2,3,4,6,7,8 HpCDF	ng/L	0.5	.25	5.2	.25	.8	.8	2.18 E-8
Total HpCDF	ng/L	0.5	.25	6.5	.25	1.	1.	2.66 E-8
OCDF	ng/L	0.5	.25	29	0.5	4.2	4.2	1.08 E-7
Zonal Groundwater Flow (cfd)			118	48	64	70	0	
Zonal Chemical Flux (lbs/day)			1.19 E-3	3.44 E-3	6.03 E-3	3.62 E-4	0	1.10 E-2 (total)

Note:

A zonal groundwater flow of zero (0) indicates that the zone is non-waterbearing in that interval and yields a zonal chemical flux of zero (0).

TABLE 4.8

CHEMICAL FLUX
BEDROCK FOURTH UNIT

			Flow Zone Concentrations					
Study Chemical	*Units of Measurement*	*Quantitation Levels*	*1 (OW240)*	*2 (OW239)*	*3 (OW238)*	*4 (OW237)*	*5 (OW237)*	*Total Study Chemical Flux (lbs/day)*
Phenol	ug/L	10	5	5	110	5	5	7.15 E-5
1,2,3-TCB	ug/L	7	22.5	200	190	11	11	1.57 E-4
1,2,4-TCB	ug/L	7	130	930	1200	63	63	9.01 E-4
a-HCCH	ug/L	7	3.5	19	18	3.5	3.5	5.01 E-5
PCB-1248	ug/L	1	0.5	1	0.5	0.5	0.5	7.15 E-6
Total PCDF	ng/L	0.5	.25	0.6	.25	.25	.25	3.58 E-9
Total HxCDF	ng/L	0.5	.25	0.8	.25	.25	.25	3.58 E-9
1,2,3,4,6,7,8 HpCDF	ng/L	0.5	.25	5.2	.25	.8	.8	1.14 E-8
Total HpCDF	ng/L	0.5	.25	6.5	.25	1.	1.	1.43 E-8
OCDF	ng/L	0.5	.25	29	0.5	4.2	4.2	6.01 E-8
Zonal Groundwater Flow (cfd)			0	0	0	70	159	
Zonal Chemical Flux (lbs/day)			0	0	0	3.62 E-4	8.25 E-4	1.19 E-3

Note:

A zonal groundwater flow of zero (0) indicates that the zone is non-waterbearing in that interval and yields a zonal chemical flux of zero (0).

The chemical flux in the Bedrock Upper Unit of the bedrock consists of (see Table 4.5):

- Loading due to organic chemicals measured in ppb

  = 0.96 lb/day
  - Phenol
  - 1,2,3-TCB
  - 1,2,4-TCB
  - a-HCCH
  - PCB-1248

- Loading due to organic chemicals measured in ppt

  = 1.6×10^{-5} lb/day (not including 1,2,3,4,5,6,7,8 - HpCDF since compound included in Total HpCDF)
  - Total PCDF
  - Total HxCDF
  - 1,2,3,4,6,7,8-HpCDF
  - Total HpCDF
  - OCDF

As shown on Table 4.5 the organic chemical flux in the Bedrock Upper Unit is 0.96 lbs/day. The second, third and fourth (see Tables 4.6, 4.7 and 4.8, respectively) bedrock units have significantly less organic chemical flux (2.5×10^{-2}, 1.1×10^{-2} and 1.2×10^{-3} lbs/day, respectively).

These results indicate that greater than 95 percent of the chemical flux from NAPL plume beneath the Niagara River occurs within the Bedrock Upper Unit with the Bedrock Second Unit comprising the next most significant pathway of chemical migration (3 percent). These two units (upper and second units) account for over 98 percent of the total chemical flux.

Table 4.9 summarizes the chemical flux for each Study Chemical.

TABLE 4.9

CHEMICAL FLUX SUMMARY

Study Chemical	*Total Study* Chemical Flux (lbs/day)*
Phenol	4.72 E-2
1,2,3-TCB	1.41 E-1
1,2,4-TCB	7.90 E-1
a-HCCH	1.71 E-2
PCB-1248	1.32 E-3
Total PCDF	6.86 E-7
Total HxCDF	7.36 E-7
1,2,3,4,6,7,8 HpCDF	2.50 E-6
Total HpCDF	3.07 E-6
OCDF	1.26 E-5
	9.96 E-1

* Summation of flux calcuations in each zone and each bedrock unit presented in Tables 4.5, 4.6, 4.7, & 4.8.

5.0 HUMAN EXPOSURE PATHWAYS

To evaluate the human endangerment posed by NAPL presence in the bedrock beneath the Niagara River adjacent to the S-Area landfill, it is necessary to identify the pathways which could result in potential human health exposure.

There are four such potential pathways:

1. Southward migration of the NAPL plume and APL in the bedrock to areas where the groundwater in contact with the NAPL could be pumped to the surface for human consumption.

2. Upward movement of the NAPL or APL from groundwater contact with the NAPL plume into the Niagara River where human exposure could result.

3. Northwesterly migration of APL from groundwater contact with the NAPL plume to the Falls Street Tunnel and then to the Lower Niagara River and Lake Ontario.

4. Northwesterly migration of APL from groundwater contact with the NAPL plume into the NYSPA conduits and from there to the NYSPA reservoir and the Lower Niagara River and Lake Ontario.

5.1 SOUTHWARD MIGRATION PATHWAY

Groundwater in bedrock beneath land areas south of the NAPL plume can be pumped to the surface and used as drinking water supplies or for other purposes involving human exposure. The closest such receptor areas south of the NAPL plume are Grand Island, New York, and Chippawa, Ontario, which are 0.7 miles and 1.7 miles, respectively. from the Niagara River's northern shoreline adjacent to S-Area (see Figure 2.3). Navy Island, Ontario, approximately 0.9 miles from the northern shoreline, is uninhabited. As described in Section 3.0 the NAPL will not reach these receptor areas.

Furthermore, due to the distance between the S-Area Landfill and Grand Island and Chippawa, it would be expected that even if the NAPL reached the bedrock below these areas; it would not be present in the uppermost bedrock strata. This conclusion is based on the following:

1. the upper bedrock contains considerable vertical fracturing;
2. the NAPL from the S-Area is denser than water and therefore its migration is gravity controlled; and
3. the bedrock bedding planes slope southward at a gradient of 0.6%.

Consequently, in traveling a distance in excess of 0.7 miles, the NAPL would be expected to migrate downward to the lower strata and not be in the upper bedrock strata which is the most likely source of groundwater to be pumped on either Grand Island or in Chippawa.

The APL plume generated by the NAPL plume in the bedrock beneath the Upper Niagara River will not impact the areas south of the S-Area Landfill because the direction of groundwater flow in the waterbearing zones identified beneath the River is to the northwest (see Section 2.1). The conclusions for APL movement is supported by the findings described in the report of Novakowski and Lapcevic (1988) (see Appendix A).

5.2 MIGRATION TO UPPER NIAGARA RIVER

The NAPL and APL is not expected to travel vertically upward and enter the Upper Niagara River. The vertical gradients in the bedrock are downward and the bedrock is separated from the bottom of the River by the layer of low permeable clay and till predominant throughout the entire Niagara area.

However, the river bottom immediately south of and a portion underlying the industrial wharf intake structure itself has been stripped of clay/till materials to channelize river flow into the industrial intakes and provide a foundation for the intake structure. This area lies immediately south of the NAPL plume encountered at OW204, OW203 and OW240 in the Bedrock Upper Unit.

Furthermore, the entrance area immediately south of both NYSPA conduits intakes also had the river bottom, as well as a portion of the upper bedrock removed. This area is significantly distanced from the westerly edge of the identified NAPL plume (i.e. >1,000 feet) and NAPL movement in the upper bedrock to the west is minimal as a result of the grouting undertaken by NYSPA in the upper 100 feet of bedrock. The presence of this grout curtain possibly explains why the NAPL plume migration stops so abruptly to the west. For example, NAPL was identified at OW240 but was not observed at Bedrock Survey well OW205 located approximately 25 feet further to the west, nor in any other well to the west of OW240. Due to the grouting performed, a large section of the area stripped of clay/till at the NYSPA conduit intakes has been sealed by the grouting. Since NAPL and APL are thus restricted from entering the grouted area, this area is inaccessible as a pathway for NAPL or APL flow into the River.

Regardless of the presence of the clay/till aquitard, the potential for APL or NAPL plume migration upward into the Upper Niagara River from the bedrock is exceedingly remote. As previously discussed, the hydraulic gradient is downward from the River into the upper bedrock (see Section 2.0). Thus, river water is continually recharging the bedrock in this area and areas where the clay/till have been removed are going to be the preferential pathways of recharge into the bedrock formation. Considering the high specific gravity of NAPL and downward gradient of the groundwater flow, upward flow of NAPL and APL into the Upper Niagara River would not occur.

5.3 GROUNDWATER MIGRATION TO FALLS STREET TUNNEL

The APL in the bedrock waterbearing units migrates northwest toward the Falls Street Tunnel and the NYSPA Conduits. For the exposure assessment, it is reasonable to assume that the entire chemical flux from the bedrock would ultimately migrate into the NYSPA Conduits. Although the lower two waterbearing units of the bedrock may not discharge totally into the NYSPA Conduits, the chemical flux from this APL is minor and its inclusion would be insignificant.

5.4 GROUNDWATER MIGRATION TO NYSPA CONDUITS

As discussed in Section 5.3, it is assumed for the purposes of the exposure assessment that the total chemical flux enters the NYSPA conduits. There is no direct human exposures to NYSPA Conduit water, but this water forms the total input to the NYSPA Reservoir and the chemical concentrations in the NYSPA Conduits and Reservoir would be essentially equal. For this assessment, the concentrations in the NYSPA Conduits and Reservoir were assumed to be the same.

Two types of human exposure at the NYSPA Reservoir are possible: potential consumption of fish and recreational use of the Reservoir for swimming.

Also, for the purposes of the risk assessment, the total chemical flux entering the conduits is assumed to discharge to the Lower

Niagara River and then to Lake Ontario. Exposures via fish ingestion and swimming could occur as a result of these discharges.

An additional pathway for potential human exposure is the use of Lake Ontario and Lower Niagara River water for drinking water supply by cities bordering Lake Ontario.

Finally, there is the possibility that some individuals might be exposed to a combination of some or all of the exposures described above. The scenario will be addressed in Section 6.0.

5.5 SUMMARY

NAPL in bedrock beneath the Niagara River adjacent to the S-Area landfill is not expected to migrate to bedrock beneath receptor areas to the south. Thus, APL cannot be withdrawn for human exposure in these areas. Because vertical gradients of NAPL and APL migration are downward in this area where the NAPL plume is located in the bedrock, the NAPL and APL plume will not move upward and impact the Upper Niagara River.

The APL generated by the NAPL plume in the bedrock will migrate northwest. Substantially all of this APL plume will discharge to the NYSPA Conduits and Reservoir and eventually discharge to the Lower Niagara River and Lake Ontario. There is potential human exposure to chemicals in this APL plume via the following:

- ingestion of fish taken from the NYSPA Reservoir, Lower Niagara River and Lake Ontario;
- swimming in the NYSPA Reservoir, Lower Niagara River and Lake Ontario; and
- ingestion of drinking water from the Lower Niagara River and Lake Ontario.

6.0 ASSESSMENT OF HUMAN ENDANGERMENT

This section assesses the endangerment, if any, to human health presented by the migration of the APL plume that results from the presence of the NAPL plume in the bedrock under the Niagara River.

This assessment evaluates the potential increased risk to human health from estimated exposure via the pathways summarized in Section 5.5. In addition, this section compares the impact of this chemical flux with applicable government standards and criteria and with the NYSDEC Niagara River Waste Assimilation/Waste Load Allocation.

6.1 HUMAN HEALTH RISK ASSESSMENT

For the health risk assessment, the chemical flux estimates for Study Chemicals, as determined per Section 4.0, were used to estimate exposure point concentrations. The applicable physical-chemical and toxicological constants, exposure scenarios and the related assumptions applied have been adopted from the Affidavit of Joseph V. Rodricks, Ph.D., dated December 11, 1985 (Rodricks Affidavit), which was presented in support of the Stipulation on Requisite Remedial Technology Program for the Hyde Park Landfill. Physical-chemical properties of chemicals examined are presented in Appendix E (Appendix I of the Rodricks Affidavit). The scenario descriptions used for exposure assessment are presented in Appendix F (taken from Appendix IV of the Rodricks Affidavit). The UCR and BCF values were updated with more current values presented in the EPA's Integrated Risk Information System (IRIS, 1989) (Appendix G).

For the various isomers of Polychlorinated Dibenzofurans (PCDF), the UCRs and BCFs necessary to evaluate their impact are not presented in the Rodricks Affidavit and are not available. For carcinogenic risk assessment of various PCDF isomers, the UCR for 2,3,7,8-TCDD was modified by appropriate adjustment factors. The adjustment factors which are noted in the following list were selected from Table III, Chlorinated Dioxins Work Group Position Paper - April 1985 - updated "Interim Risk Assessment Procedure for Mixture of Chlorinated Dibenzodioxins and Dibenzofurans (CDD and CDF)".

Chemical	Adjustment Factor
Total PCDF	0.001
Total HxCDF	0.0001
1,2,3,4,6,7,8-HpCDF	0.0001
Total HpCDF	0.00001
OCDF	0.0

The EPA 2,3,7,8-TCDD UCR of $1.56 \times 10^{+5}$ is probably conservative because the Center for Disease Control (CDC) and Food and Drug Administration have used a lower potency factor for 2,3,7,8-TCDD and EPA is considering adopting a UCR which is 16 times smaller.

With respect to the BCF, the BCF of 67,000 for 2,3,7,8-TCDD presented in the Rodricks Affidavit, Appendix II, was used for this assessment for all the PCDF isomers. This BCF is conservative, since it is much greater than EPA and the State have used for regulatory purposes.

6.1.1 Chemicals Evaluated

Flux values were calculated for the following Study Chemicals detected in the APL plume (Tables 4.5 through 4.8):

- 1,2,3-Trichlorobenzene (1,2,3-TCB)
- 1,2,4-Trichlorobenzene (1,2,4-TCB)
- Phenol
- PCB-1248
- alpha-Hexachlorocyclohexane (a-HCCH)
- Pentachlorodibenzofuran (PCDF)
- Hexachlorodibenzofuran (HxCDF)
- 1,2,3,4,6,7,8-Heptachlorodibenzofuran (1,2,3,4,6,7,8-HpCDF)
- Heptachlorodibenzofuran (HpCDF)
- Octachlorodibenzofuran (OCDF)

6.1.2 Potential Exposure Concentrations and Risk Quantifications

To calculate Study Chemical concentrations in the NYSPA Conduits, the lowest average monthly flow for the NYSPA Conduits was used. This flow was calculated by averaging the flows presented in the July 1987 NYSPA document entitled "Draft Amendment to Application for Amendment of License, FERC Project No. 2216", and selecting the lowest combination of night and day flow rates during any one month. This NYSPA

Conduits flow is calculated to be 63,000 cfs and is the diluting water volume used in this risk assessment.

For this assessment, the concentrations in the NYSPA Conduits and Reservoir were assumed to be the same. The estimated Study Chemical concentrations in the NYSPA Reservoir are presented in Table 6.1.

Human exposure at the NYSPA Reservoir is limited to potential consumption of fish from the NYSPA Reservoir and recreational use of the NYSPA Reservoir for swimming. Applying the scenario for fish ingestion as presented in Appendix E and summarized in Table 6.2, exposures and risk quantification were calculated and are presented in Table 6.3. Table 6.3 shows the predicted fish ingestion to be several orders of magnitude below acceptable daily intake levels and to present an increased cancer risk of 2.62×10^{-7}.

The swimming scenario is presented in Table 6.4. The associated exposure and ADI comparisons and risk characterization are presented in Table 6.5. Table 6.5 shows the predicted exposure levels to be several orders of magnitude below acceptable daily intake levels and to present an increased lifetime cancer risk of 8.87×10^{-12} for an adult.

Exposures via fish ingestion and swimming could occur due to the final discharge of NYSPA Conduits water to the Lower Niagara River and, finally, to Lake Ontario. This would involve an additional dilution of the conduit flow of 3.24 times based on the total flow (204,000 cfs) in the Lower Niagara River. Thus, in the Lower Niagara River and Lake

TABLE 6.1

RESERVOIR CONCENTRATIONS OF STUDY CHEMICALS

Study Chemical	*Study Chemical Flux lbs/day*	*Reservoir Water Conc. ug/L*	*Bio Concentration Factor*	*Concentration Fish ug/kg*
1,2,3-TCB	1.41 E-01	4.17 E-04	1.90 E+03	7.92 E-01
1,2,4-TCB	7.90 E-01	2.33 E-03	2.80 E+03	6.53 E+00
Phenol	4.72 E-02	1.39 E-04	1.40 E+00	1.95 E-04
a- HCCH	1.71 E-02	5.05 E-05	1.30 E+02	6.57 E-03
PCB -1248	1.32 E-03	3.90 E-06	7.30 E+04	2.85 E-01
Total PCDF	6.86 E-07	2.03 E-09	6.7 E+04	1.36 E-04
Total HxCDF	7.36 E-07	2.17 E-09	6.7 E+04	1.46 E-04
1,2,3,4,6,7,8-HpCDF	2.50 E-06	7.38 E-09	6.7 E+04	4.95 E-04
Total HpCDF	3.07 E-06	9.07 E-09	6.7 E+04	6.08 E-04
OCDF	1.26 E-05	3.74 E-08	6.7 E+04	2.51 E-03

TABLE 6.2

ASSUMPTIONS FOR SCENARIO: INGESTION OF FISH*

Quantity of fish consumed per day:	
Average intake (chronic)	14 grams
Maximum intake	42 grams**
Bioconcentration Factors:	See Appendix E
Lifetime	70 years
Average Body Weight	70 kg
Acceptable Daily Intakes (ADI)	See Appendix E
Unit Cancer Risk (UCR)	See Appendix E

* as reported in Rodericks Affidavit unless otherwise noted.

** Proposed in State/Federal comments as a more appropriate maximum daily intake of fish.

TABLE 6.3

ADULT INGESTION OF FISH

EXPOSURE LEVELS AND EXPOSURE/ADI AND RISK QUANTITATION

Study Chemical	*Study Chemical Exposure via Fish ug/d*		*Exposure/ADI (1)*		*Additional Lifetime Cancer Risk Average*
	Average	*Maximum*	*Average*	*Maximum*	
1,2,3-TCB	1.11 E-02	3.33 E-02	7.92 E-06	2.38 E-05	NA
1,2,4-TCB	9.14 E-02	2.74 E-01	6.53 E-05	1.96 E-04	NA
Phenol	2.73 E-06	8.19 E-06	9.75 E-10	2.92 E-09	NA
a-HCCH	9.19 E-05	2.76 E-04	NA	NA	8.27 E-09
PCB-1248	3.99 E-03	1.20 E-02	NA	NA	2.47 E-07
Total PCDF	1.90 E-06	5.71 E-06	NA	NA	4.24 E-09
Total HxCDF	2.04 E-06	6.11 E-06	NA	NA	4.54 E-10
1,2,3,4,6,7,8-HpCDF	6.93 E-06	2.08 E-05	NA	NA	1.54 E-09
Total HpCDF	8.51 E-06	2.55 E-05	NA	NA	1.90 E-10
OCDF	3.51 E-05	1.05 E-04	NA	NA	0.00
Total			7.32 E-05	2.20 E-04	2.62 E-07

(1) Exposure divided by ADI
ADI = Acceptable Daily Intake as reported in Rodricks Affidavit, Appendix I.

NA = Not Applicable

TABLE 6.4

ASSUMPTIONS FOR SCENARIO: RECREATIONAL SWIMMING*

		ADULT	CHILD
Body surface area (cm^2)		18,000	6,950
Body Exposure to Water (mg of H_2O/cm^2)		2	2
Absorption (%)			
PCDFs, HCCH, PCBs		50	50
All other chemicals		1	1
Swimming habit	(times per day)	5	5
	(times per month)	30	30**
	(months per year)	2.5	2.5**
	(years)	35	12**
Body weight (kg)		70	17.5

* as reported in Rodricks Affidavit unless otherwise noted.

** Rodericks Affidavit did not present cancer risk scenario for child, therefore, these assumptions are not included in the Rodericks affidavit.

TABLE 6.5

INTAKE AND POTENTIAL RISK FROM STUDY CHEMICALS FROM NAPL PLUME UNDER THE NIAGARA RIVER VIA SWIMMING EXPOSURE IN NYSPA RESERVOIR

Study Chemical	*Reservoir Water Conc. ug/L*	*Daily Intake ug/kg/d*		*Exposure/ADI (1)*		*Additional Lifetime Cancer Risk*	
		Adult	*Child*	*Adult*	*Child*	*Adult*	*Child*
1,2,3-TCB	4.17 E-04	1.07 E-08	1.66 E-08	5.36 E-10	8.28 E-10	NA	NA
1,2,4-TCB	2.33 E-03	6.00 E-08	9.26 E-08	3.00 E-09	4.63 E-09	NA	NA
Phenol	1.39 E-04	3.58 E-09	5.53 E-09	8.95 E-11	1.38 E-10	NA	NA
a-HCCH	5.05 E-05	1.33 E-09	7.06 E-10	NA	NA	8.41 E-12	4.45 E-12
PCB-1248	3.90 E-06	1.03 E-10	5.46 E-11	NA	NA	4.47 E-13	2.37 E-13
Total PCDF	2.03 E-09	5.36 E-14	2.84 E-14	NA	NA	8.36 E-15	4.43 E-15
Total HxCDF	2.17 E-09	5.74 E-14	3.04 E-14	NA	NA	8.95 E-16	4.74 E-16
1,2,3,4,6,7,8-HpCDF	7.38 E-09	1.95 E-13	1.03 E-13	NA	NA	3.04 E-15	1.61 E-15
Total HpCDF	9.07 E-09	2.40 E-13	1.27 E-13	NA	NA	3.74 E-16	1.98 E-16
OCDF	3.74 E-08	9.89 E-13	5.23 E-13	NA	NA	0.00	0.00
Total				3.62 E-09	5.60 E-09	8.87 E-12	4.69 E-12

(1) Exposure divided by ADI
ADI = Acceptable Daily Intake as reported in Rodricks Affidavit, Appendix I.

NA = Not Applicable

Ontario, the daily intake and risks related to Study Chemicals via fish ingestion and swimming as listed in Tables 6.3 and 6.5 would be lowered by the dilution factor of 3.24.

It is apparent from these evaluations that the intakes and health risks from exposure to Study Chemicals via the ingestion of fish and swimming is very small and does not present a significant endangerment to human health.

An additional exposure could occur due to the use of Lake Ontario and Lower Niagara River water for drinking water supply. The ingestion of drinking water scenario is presented in Appendix F. The exposure and risk quantification information is presented in Table 6.6. Table 6.6 shows the predicated chemical intake to be several orders of magnitude below acceptable daily intake levels and to present on increased lifetime cancer risk of 2.96×10^{-9}.

Again, it is apparent from these evaluations that the intakes and health risks from exposure to Study Chemicals via drinking water supply is very small and does not present a significant endangerment to human health.

Assuming that some individuals might be exposed to a combination of all the exposures determined to be present from the migration of Study Chemicals in the APL plume from the NAPL in the bedrock under the Upper Niagara River, the potential risks estimated from each exposure have been added and are presented on Table 6.7. Table 6.7

TABLE 6.6

INTAKE AND POTENTIAL RISK FROM STUDY CHEMICALS FROM NAPL PLUME UNDER THE NIAGARA RIVER VIA DRINKING WATER FROM LOWER NIAGARA RIVER AND LAKE ONTARIO

Chemicals	*(1) Water Conc. ug/L*	*Daily Intake ug/kg/d*	*Exposure/(2) ADI*	*Lifetime Risk*
1,2,3-TCB	1.29 E-04	3.68 E-06	1.84 E-07	NA
1,2,4-TCB	7.19 E-04	2.06 E-05	1.03 E-06	NA
Phenol	4.29 E-05	1.23 E-06	3.07 E-08	NA
a-HCCH	1.56 E-05	4.45 E-07	NA	2.81 E-09
PCB-1248	1.20 E-06	3.44 E-08	NA	1.49 E-10
Total PCDF	6.27 E-10	1.79 E-11	NA	2.79 E-12
Total HxCDF	6.70 E-10	1.92 E-11	NA	2.99 E-13
1,2,3,4,6,7,8-HpCDF	2.28 E-09	6.51 E-11	NA	1.02 E-12
Total HpCDF	2.80 E-09	8.00 E-11	NA	1.25 E-13
OCDF	1.15 E-08	3.30 E-10	NA	0.00
Total			1.24 E-06	2.96 E-09

(1) Water concentration in Lower Niagara River below Power plant. Lake Ontario concentration assumed to equal Lower Niagara River.

(2) Exposure divided by ADI.
ADI = Acceptable Daily Intake as reported in Rodericks Affidafit, Appendix I.

NA = Not Applicable

TABLE 6.7

SUMMATION OF DAILY INTAKES AND CANCER RISKS RELATED TO STUDY CHEMICALS FROM NAPL PLUME UNDER THE NIAGARA RIVER AT THE LOWER NIAGARA RIVER, NYSPA RESERVOIR AND LAKE ONTARIO

	Exposure/ADI		*Increased Lifetime*
Exposure	*Avg. Exposure*	*Max. Exposure*	*Risk of Cancer (Average Exposure)*
Fish Ingestion from Reservoir	7.32E-05	2.20E-04	2.62E-07
Water Consumption from Lower River or Lake	1.24E-06	1.24E-06	2.96E-09
Swimming NYSPA Reservoir			
Adult	3.62E-09	3.62E-09	8.87E-12
Child	5.60E-09	5.60E-09	4.69E-12
TOTALS - ALL EXPOSURES	7.45E-05	2.21E-04	2.65E-07

shows the predicted total intake from the several pathways to be several orders of magnitude below acceptable daily intake levels and to present an increased lifetime cancer risk of 2.65×10^{-7}. Again it is apparent that the intakes and health risks from exposure to Study Chemicals from a combination of all exposures is very small and does not present a significant endangerment to human health.

6.2 COMPARISON WITH GOVERNMENT STANDARDS AND CRITERIA

In Table 6.8, the estimated concentrations of Study Chemicals in the NYSPA Reservoir , Lower Niagara River and Lake Ontario which result from APL migration from the NAPL plume under the Niagara River are compared to applicable drinking water standards and criteria. The Table shows that the estimated concentrations of Study Chemicals in these water bodies meet the EPA Maximum Concentration Limits (MCL) and Water Quality Criteria (WQC) as well as the New York State Division of Water (TOGS) standards and guidance limits.

6.3 WATER ASSIMILATION CAPACITY/ WASTE LOAD ALLOCATION (WAC/WLA)

Table 6.9 presents pertinent information related to New York State Department of Environmental Conservation's assimilative capacity/waste load allocations designated for the Lower River segment of the Niagara River. For those Study Chemicals listed and for which allocations

TABLE 6.8

COMPARISON OF LOWER NIAGARA RIVER AND LAKE ONTARIO WATER CONCENTRATIONS OF STUDY CHEMICALS WITH AMBIENT WATER STANDARDS AND CRITERIA

Chemicals	*Reservoir Conc. ug/L*	*River/Lake (1) Conc. ug/L*	*MCL (2) ug/L*	*WQC (3) ug/L*	*TOGS (4) STD*	*GUID*
1,2,3-TCB	4.17 E-04	1.29 E-04	NV	NV	NV	NV
1,2,4-TCB	2.33 E-03	7.19 E-04	NV	NV	NV	NV
Total TCB	2.75 E-03	8.48 E-04	NV	NV	1.00 E+01	1.00 E+01
Phenol	1.39 E-04	4.29 E-05	NV	3.50 E+03	5.00 E+00	NA
a-HCCH	5.05 E-05	1.56 E-05	NV	9.20 E-03	1.00 E-02	2.00 E-02
PCB-1248	3.90 E-06	1.20 E-06	NV	7.90 E-02	1.00 E+00	1.00 E+00
Total PCDF	2.03 E-09	6.27 E-10	NV	1.30 E-05*	1.00 E-03*	NV
Total HxCDF	2.17 E-09	6.70 E-10	NV	1.30 E-04*	1.00 E-02*	NV
1,2,3,4,6,7,8-HpCDF	7.38 E-09	2.28 E-09	NV	1.30 E-04*	1.00 E-02*	NV
Total HpCDF	9.07 E-09	2.80 E-09	NV	1.30 E-03*	1.00 E-01*	NV
OCDF	3.74 E-08	1.15 E-08	NV	NA	NA	NV

NV = Not Available
(1) = Dilution of 3.24 is assumed from conduit to Niagara River at NYSPA power plant. No dilution factor assumed from River to Lake.
(2) MCL = EPA Maximum Concentration Limits.
(3) WQC = EPA Water Quality Criteria for the protection of human health for the consumption of drinking and aquatic organisms.
(4)TOGS = Division of Water Technical and Operational Guidance Series.
STD = New York State Ambient Water Quality Standards.
GUID = New York Sate Ambient Water Guidance Values.
* = Values based on Criteria and Standards for 2,3,7,8 TCDD and adjusted by cancer potency conversion factors noted in text.
NA = Not applicable because chemical does not have carcinogenic potential.

TABLE 6.9

ASSIMILATIVE CAPACITY/LOAD ALLOCATION IN THE LOWER NIAGARA RIVER SEGMENT

	S-Area (1) *Study Chemical Flux lbs/d*	*WAC/WLA* (2)		
Chemicals		*Alloc. lbs/d*	*Balance lbs/d*	*% of Balance* (3)
1,2,3 TCB	0.141	N V	N V	
1,2,4 TCB	0.79	19.5	19.5	4.1
Total TCB	0.931	19.5	19.5	4.8
Total HCCH	0.0171	2.7	2.7	0.63
PCBs	0.00132	--	-0.008	16.5

(1) Chemcial Flux estimated from NAPL bedrock plume under the Upper Niagara River to NYSPA Conduits and ultimately to lower segment of the Niagara River. No WAC/WLA allocations available for polychlorodibenzofurans.

(2) WAC/WLA - Water Assimilation Capacity/Waste Load Allocation
Alloc. = Allocation to lower segment of the Niagara River (NYSPA Power Plant to Lake Ontario)
Balance = Balance of above allocation after subtracting existing allocation to industry discharging to the lower segment.
Source: NYSDEC, "Rationale for Waste Load Allocations for SPDES Permitted Discharges to the Niagara River, Attachment A: Procedure for Allocating SPDES Permit Effluent Limit Loadings for Discharges to the Niagara River Basin; Niagara River Load Allocation Printout", 1982.

(3) Study Chemical Flux/Balance x 100

NV = Not Available

have been designated in the WAC/WLA document, none of the estimated fluxes from the NAPL plume under the Upper Niagara River approach the quantity allocated for these chemicals in the lower river segment of the Niagara River. In the case of total TCB, the chemical flux accounts for approximately 4.8% of the balance of the allocation in the lower segment. For a-HCCH and PCBs, the percent of the balance values are 0.63% and 16.5%, respectively. These low percentages indicate that the chemical flux from the NAPL plume in the bedrock under the Upper Niagara River has a very small impact on surface water quality in the Lower River segment of the Niagara River.

6.4 CONCLUSIONS

The chemical flux from the NAPL in the bedrock under the Upper Niagara River which reaches the NYSPA Reservoir, Lower Niagara River and Lake Ontario:

(1) results in exposure to non-carcinogens which are well below Acceptable Daily Intakes,

(2) results in a total exposure to carcinogens which represents an additional lifetime cancer risk of approximately three in ten million,

(3) do not exceed Federal or New York State water quality standards and criteria, and

(4) do not significantly impact the applicable allocation balance for those chemicals in the Niagara River to which allocations have been assigned under the Waste Assimilation Capacity/Waste Load Allocation process of the New York State Department of Environmental Conservation.

Therefore, it is concluded that the NAPL plume under the Upper Niagara River does not present an endangerment to human health.

7.0 REFERENCES

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APPENDIX A

REGIONAL HYDROGEOLOGY OF THE SILURIAN AND ORDOVICIAN SEDIMENTARY ROCK UNDERLYING NIAGARA FALLS, ONTARIO, CANADA

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REGIONAL HYDROGEOLOGY OF THE SILURIAN AND ORDOVICIAN SEDIMENTARY ROCK UNDERLYING NIAGARA FALLS, ONTARIO, CANADA

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ABSTRACT

Due to concern over the potential for widespread groundwater contamination in the sedimentary rock underlying the Niagara Falls area, this study was done to investigate the hydrogeology of the Silurian and Ordovician stratigraphy underlying the Upper Niagara River and the Eastern Niagara Peninsula. Seven boreholes (up to 150 m deep) were drilled, instrumented with multiple packer casing, tested for permeability, sampled for inorganic and organic solutes and monitored for hydraulic head to provide data for a conceptual model of regional groundwater flow. Results show that there are at least three distinct groundwater flow regimes in the bedrock. The uppermost regime consists of fracture zones in the Guelph and Lockport Formations, within which hydraulic conductivity, hydraulic head measurements and geochemical analyses indicate active groundwater circulation primarily discharging towards the Niagara Gorge and Escarpment. Underlying the Lockport Formation are an overpressured (high hydraulic head) regime in the Clinton-Upper Cataract-Lower Queenston Formation and an underpressured (low hydraulic head) regime in the Lower Cataract-Upper Queenston Formation. In both regimes, geochemical analyses and permeability measurements indicate very old and saline groundwater which probably has undergone minimal migration since pre-Pleistocene time. The implication based on the study so far, is that potential groundwater contamination below the bottom of the Lockport Formation is probably not significant in the Niagara Falls area except adjacent to the Niagara Gorge where vertical permeability in the lower flow regimes may be enhanced.

INTRODUCTION

During the late 1970's and early 1980's, considerable international attention focused on the Niagara Frontier when it was determined that numerous toxic waste disposal sites, particularly on the U.S. side of the Niagara River, were contaminating groundwater in the area. In 1982, the U.S. Geological Survey conducted a hydrogeological reconnaissance of 138 known toxic waste disposal sites in a three mile wide band along the Niagara River in New York State (Koszalka et al., 1985). In the Niagara Falls area alone, one half of the 63 sites investigated showed a potential for contaminant migration. A few of these sites such as Love Canal, S-area and Hyde Park have garnered considerable media attention because of their dangerous nature.

Most of the early work on groundwater migration in the Niagara River region was conducted as part of broad water resources surveys (Reck and Simmons, 1952; Lasala, 1967; Haefeli, 1972) or as specific drainage basin and groundwater resource studies (Johnston, 1964; Ostry, 1971). Johnston (1964), in particular, presented a very detailed study of the groundwater in both the overburden and in the Silurian and Ordovician sedimentary rock immediately underlying Niagara Falls, New York. Both Johnston (1964) and Ostry (1971) recognized the importance of the influence of the Niagara Escarpment on regional groundwater flow in the lower stratigraphy. The Niagara

Falls themselves were the focus of a detailed international geological study (International Joint Commission, 1974) in which a large component of the work pertained to the flow of groundwater in the fractured caprock and underlying stratigraphy at the Falls.

More recently, contaminant migration has been studied at specific waste disposal sites. Kozalka et al. (1985) provides a review and compilation of the existing hydrogeological information for most of the waste sites identified in the U.S. side of the region. In addition, a number of numerical simulations of the hydrogeological conditions in the overburden and shallow bedrock have been conducted to aid in the interpretation of contaminant migration at several of these sites (Maslia and Johnston, 1984; Mercer et al., 1984; Wong et al., 1985; Osborne and Sykes, 1986). In almost all of these studies, no consideration is given to groundwater flow beneath the shallow bedrock. Therefore, as a means of qualifying this potential, this study of regional groundwater flow in the Silurian and Ordovician sedimentary rock underlying the Canadian side of Niagara Falls was initiated.

The objective of this study is to synthesize information on geology, hydrostratigraphy and geochemistry to develop a conceptual model for regional groundwater flow in the Niagara Falls area. More specifically, we wish to identify the geological structure that may influence groundwater flow, quantify the three-dimensional distribution of hydraulic head, determine hydraulic conductivity in both the horizontal and in particular the vertical direction and estimate deep groundwater flow rates and velocity. The results of this study can be used to help assess the potential for deep groundwater contamination at particular waste sites where contamination has reached the upper bedrock.

The study area is loosely bounded by the Niagara Escarpment to the north, the Welland Ship Canal to the east (eastern edge of the map as shown in Fig. 1), the Niagara River to the west and the edge of the Silurian gas field to the south, about 12 km south of Niagara Falls (Fig. 1). The boreholes utilized for this study lie for the most part in the center of this area and penetrate to below Lake Ontario water levels.

GEOLOGICAL SETTING

Regional Geologic Setting and Stratigraphy

The Niagara Falls Region is located on the southeastern flank of the northeast-southwest trending Algonquin-Findlay arch system in a thickening sequence of Silurian and Ordovician sediments (Clark and Stern, 1979). The most significant physiographic feature in the Niagara Peninsula is the east-west trending Niagara Escarpment. The Niagara Escarpment is capped by the resistant Middle-Silurian Lockport

Dolostone (Liberty, 1981) and forms the eastern rim of the Michigan Basin to the north of the Algonquin-Findlay arch system (Telford, 1978). The Escarpment continues into western New York State and becomes discontinuous towards Rochester.

The stratigraphy, generally flat between Niagara Falls, Ontario and the Niagara Escarpment, steepens to a southwestward dip of 4 m per km between Niagara Falls and Lake Erie (Liberty, 1981). The City of Niagara Falls is situated in a bedrock low, lying between the Niagara Escarpment and the Onandaga Cuesta to the south (Flint and Lolcama, 1985). The Onandaga Cuesta forms part of the north shore of Lake Erie.

The bedrock in the Niagara Region is covered by a thin veneer of Quaternary deposits ranging from a minimum of less than 5 m deep near the Niagara Escarpment to greater than 30 m deep to the south of Niagara Falls (Feenstra, 1981). The unconsolidated material generally consists of approximately equal amounts of till and glaciolacustrine deposits, Wisconsinian in age (Calkin and Brett, 1978; Feenstra, 1981). Some sands and gravels were deposited as part of the Niagara Falls Moraine which trends approximately east-west, just south of the City of Niagara Falls (Calkin and Feenstra, 1985). The basal till immediately overlying the bedrock is coarse textured and the lower part is pervaded by gravel and boulders, possibly ancestral river channel deposits (Calkin and Brett, 1978).

The bedrock surface is generally characterized by a highly fractured weathered zone (Johnston, 1964). The nature of the weathered zone is largely independent of bedrock lithology and pervasive throughout the study area.

Table 1 shows the Paleozoic stratigraphy compiled from Bolton (1957), Telford (1975) and Kilgour and Liberty (1981). In general, Canadian nomenclature has been adopted, although U.S. and other nomenclature is referenced. The uppermost formation underlying the unconsolidated material in the southern part of the study area is the Salina Formation, a sequence of Upper-Silurian salts, anhydrite, shales and dolostones ranging from 0 to 90 m thick. The Salina Formation is transitionally underlain by the Guelph Dolostone, a brown, finely crystalline dolomite with interbedded grey shale about 37 m thick. The Guelph Formation conformably overlies the Lockport Group, which consists of three dolostone and limestone members about 30 m thick. The Clinton Group disconformably underlies the Lockport Formation, although it is of the same age (Middle-Silurian). The Clinton Group is about 32 m thick and mostly consists of the Rochester Shale occurring between thin (2-3 m thick) dolostone and shale units. The contact between the lowermost formation in the Clinton Group and the uppermost formation in the Cataract Group (Lower-Silurian) is transitional and defined by textural change. The Cataract Group consists of three shale and sandstone formations and is approximately 32 m thick at the Niagara Gorge. The lowermost formation which outcrops in the most northerly part of the Niagara Gorge is the Upper Ordovician Queenston Formation which is about 520 m thick at Niagara Falls (well no. 6669 K, Kreidler et al., 1972). The strata underlying the Queenston are Ordovician in age and consist predominantly of shale and shale-limestone formations (Telford, 1978). Pre-Cambrian basement is encountered at 925 m depth (well no. 6669 K, Kreidler et al., 1972).

Structural Geology

Successive periods of tectonic activity during the Paleozoic, particularly the Taconic and Appalachian Orogens were responsible for changes in compressive stress that generated movement along pre-existing planes of weakness in the basement rocks of southwestern Ontario (Sanford et al., 1985). During periods of fracture rejuvenation, fault bounded blocks were tilted and rotated to form oil and gas traps in the Cambrian, Ordovician and Silurian sediments. A structural map of the base of the Rochester Formation (Koepke and Sanford, 1965) shows evidence of a vertical displacement fault trending in the northeast quadrant and a shorter lineament oriented orthogonally both within the study area on the Canadian side. Recent surface geophysical studies conducted along a line of high-yielding wells in Niagara Falls, N.Y. suggests that the northeast trending fault and associated fractures may be traced across the Niagara River

(Yager and Kappel, 1987). The only other major structural features identified in the Niagara Region are a fault with about 30 m throw near Batavia, New York, about 80 km east of Niagara Falls (International Joint Commission, 1974), and a lineament recognized on LANDSAT which suggests that a fault or small syncline may provide control for the current position of the Niagara River (Liberty, 1981). Some localized up and downwarping due to the presence of bioherms is evident along the Niagara Gorge (Liberty, 1981).

Contemporary regional stress in the Michigan and Allegheny Basins is compressive near the bedrock surface and oriented in the northeast quadrant (Haimson, 1978; Zoback and Zoback, 1980; Plumb and Cox, 1987). In the Niagara Falls locale, maximum principal stress is oriented ranging from 050° to 060° (International Joint Commission, 1974; Lo, 1978; Williams et al., 1985) as determined from direct measurement and pop-ups. As a result of high compressive stress oriented horizontally, joint orientations can be expected to coincide with the general direction of the principal stress (Engelder, 1982). Fig. 3 shows the joint orientations obtained from outcrops of the Silurian and Devonian strata exposed in the Niagara Peninsula (Williams et al., 1985). Of the four joint sets evident, the set oriented in the same direction as the contemporary stress is weakest. The other three sets are probably related to paleotectonic events and the influence of local geologic structure. Joint orientations in the Lower Devonian rocks of New York State just southeast of Niagara Falls are predominated by a set trending in the southeast quadrant and show little influence from the contemporary stress field (Engelder and Gleser, 1980).

Fig. 2 illustrates the major geological features important in controlling the regional groundwater flows in the Niagara Falls area. A zone of tensile stress along the Niagara Escarpment and adjacent to the Niagara Gorge has created enhanced vertical and horizontal permeability particularly within the limestone and dolostone units in the stratigraphy (International Joint Commission, 1974). The St. Davids Buried Gorge is infilled with high permeability glacial outwash material (Hobson and Terasmae, 1968) and acts as a sink for groundwater flowing towards the escarpment to the north. Other bedrock surface features which might influence groundwater flow include the Crystal Beach buried channel system and a buried valley on the U.S. side of the Upper Great Gorge. The linears identified from the structure of the base of the Rochester Shale (Koepke and Sanford, 1965) are shown on Fig. 2, although other more direct evidence of their presence is unavailable. Fig. 2 also shows the subcrop of the east-west striking and southward dipping Paleozoic strata. Depending on the hydraulic head in the formation, groundwater may prefer to flow along bedding planes toward Lake Erie (Liberty, 1981).

Joint orientations and patterns are considered unimportant in terms of the directional flow properties of the rock in the Niagara area. This is because measurements of fracture spacing at undisturbed outcrops of the Lockport Formation, for example, show vertical to sub-vertical fractures to be infrequent with average spacing as large as 20 m. Consequently, the anisotropy of the hydraulic conductivity field will more likely depend on the heterogeneity of individual bedding plane fractures which are far more closely spaced. Because of the infrequency of vertical fractures, vertical hydraulic conductivity between bedding plane fracture zones is expected to be minimal. The southern boundary of the study site is marked as the edge of the Silurian natural gas field in the Clinton-Cataract Groups according to maps compiled by Koepke and Sanford (1965). The presence of natural gas in commercial quantity indicates that most of the strata here has very low vertical permeability.

METHODS

Core Drilling and Borehole Geophysics

Seven boreholes were diamond-core drilled either in direct support of this study or for alternate purposes and were adopted for this study (Fig. 1). Boreholes NF-2 to NF-4 were drilled as part of a geotechnical investigation (Semec and Huang, 1984) and the casing in these holes was subsequently installed as part of this study. The NI series holes and CH-1 were drilled and instrumented specifically for this study. The boreholes are all 76 mm in diameter and were drilled using triple-tube techniques (45.0 mm diameter core). Two of the boreholes, NI-1 and NI-3, are inclined at 64° and 65°, respectively;

the remainder are vertical. Borehole CH-1 and the NI-series boreholes were drilled with an organic dye tracer (Flouroscien LT) in the drill water so that it could be detected during subsequent geochemical sampling. The boreholes range in length from 100 to 150 m (Table 2).

The precise location of the NF series boreholes was dictated by the objectives of the geotechnical study; however, the spatial distribution of NF-2,3 and 4 proved to be suitable to determine groundwater flow directions beneath the City of Niagara Falls and were selected for instrumentation for this reason. Borehole CH-1 was located to triangulate with the NF and NI series boreholes and was drilled adjacent to the northeast trending linear identified in the geological model. The NI series boreholes were drilled to conduct vertical and horizontal cross-hole hydraulic tests and to obtain hydraulic head measurements beneath the Niagara River.

In addition to the geologic information obtained from core samples, each borehole was logged with a standard suite of downhole geophysical sondes including at least electric (40 cm, 160 cm resistivity and single point resistance) and nuclear (natural gamma, density and porosity) logs. Caliper, fluid temperature, fluid resistivity and sonic (for fracture identification) logs were also obtained for the NF and NI series boreholes. The borehole geophysics were used in conjunction with the core logs to identify lithologic boundaries and to locate structural features, such as bioherms, cross-bedding, fractures and vugs.

Multiple-Packer Casing Strings

After conducting the borehole logging, hydraulic testing and development (by pumping), the boreholes were completed with commercially available multiple-packer casing strings. For boreholes CH-1 and the NI series, hydraulic testing was completed after the casing strings were installed. The casing strings prevent vertical groundwater flow between fracture zones and provide access through valved ports for sampling, testing and monitoring the isolated intervals. Black et al. (1986) present a complete description of the casing string and associated equipment. The casing strings were installed usually within two weeks to a month after the borehole was drilled so that the hydraulic head and groundwater geochemistry in individual hydraulic regimes were not significantly perturbed.

Table 2 shows a summary of the isolated intervals for each borehole. There are a total of 94 intervals distributed amongst the seven boreholes with average interval lengths ranging from 5.0 m to 12.3 m. Table 2 also shows the percentage of the borehole length sealed by packer inflation. The greater the percent seal, the greater the confidence in the measured hydraulic head in each borehole. The location of each packer in an individual borehole was determined based on the core logs, geophysical logs and hydraulic conductivity (where available).

Hydraulic Testing

Hydraulic testing to measure hydraulic conductivity in single boreholes was conducted using constant head injection and slug testing techniques. The constant head tests were generally conducted in all accessable intervals, except for those in which natural gas exsolution prevented stable shut-in pressure (about 25-30% of all intervals). Slug tests were conducted only in the medium to higher permeability (10^{-8} m/s to 10^{-5} m/s) intervals except for a few shut-in slug tests conducted in lower permeability intervals in borehole NI-2.

Constant head injection tests were conducted by pumping or injecting water at a constant injection pressure until a steady flow rate of water was achieved. This method can be used either within the multiple-packer casing string or using a double-packer arrangement with a spacing or interval length of 1 to 5 m which can be moved incrementally up or down the borehole. The flow rate, Q, and the injection head, ΔH, is related to the transmissivity, T, of the test interval by the expression (Bear, 1979):

$$\frac{Q}{\Delta H} = \frac{2\pi T}{\ln(r_e/r_w)} \tag{1}$$

where r_e is the radius of influence of the test, which according to Bliss and Rushton (1984) can usually be approximated at 10 m, and r_w is the radius of the borehole. With equipment available for this study, the range of testing capability using the constant head injection method was between 10^{-6} m/s and 10^{-11} m/s for horizontal hydraulic conductivity, K_h (T=Kb, where b is the test interval length). Doe and Remer (1980) provide a more complete discussion on conducting constant head tests in fractured rock.

Slug tests are commonly employed in overburden materials where hydraulic conductivity is high, and less frequently in fractured rock. These tests, however, can be a valuable check on the results from constant head tests and can also provide information on borehole skin effects (Hawkins, 1956; Sageev, 1986). Slug tests were conducted in an open-wellbore format by adding or removing a known volume of water and recording the rise or fall in hydraulic head in the borehole with time using a pressure transducer. Alternatively, for measuring lower permeabilities, slug tests were also conducted in a shut-in format where the water column in the isolated interval was, in turn, isolated from the free surface and a small slug of water was added by means of injection to generate a pressure rise. The subsequent response to the change in pressure depends on the compressibility of the water, test equipment and formation as well as the permeability. Slug tests completed following the open-wellbore format also depend on the volume of water in the open standpipe. The overall range of detection for horizontal hydraulic conductivity is from 10^{-4} m/s to less than 10^{-12} m/s with the appropriate equipment. Open-wellbore tests have a practical range of about 10^{-4} m/s to 10^{-8} m/s for 76 mm boreholes in fractured rock. Slug test results were analysed using both steady state (Hvorslev, 1951) and transient (Cooper et al., 1967; Sageev, 1986) solutions.

Hydraulic Head Distribution

Hydraulic head measurements were obtained mostly on a quarterly basis after casing installation using a monitoring device equipped with a pressure transducer. The observed pressures were converted to hydraulic head, h, using (Freeze and Cherry, 1979):

$$h = z + \frac{p}{\rho g} \qquad (2)$$

where z is the elevation above datum (sea level - IGLD), p is the gage pressure as measured by the pressure transducer, ρ is the density of the water and g is gravitational acceleration. The density of the water measured with depth was used. Where density measurements were not made, density was estimated.

Groundwater Chemistry

Groundwater samples were obtained through the multiple-packer casing strings using standard procedures and protocols (Barcelona et al., 1985). Where permeability was greater than 10^{-7} m/s and hydraulic head elevations near ground surface, water was purged from a given sampling interval by continual pumping and the sample was taken when Eh and pH flow-cell measurements showed that stable conditions were achieved. For lower permeabilities and in low-hydraulic-head features, groundwater was purged from the intervals by evacuating the casing water and allowing recovery over long periods of time (up to a month). Samples were obtained using a bailer when at least two interval volumes (the volume of water in the interval isolated by the casing packers) had been purged. Eh and pH measurements were not obtained for the bailed samples. In most cases the samples were fluoresced to determine if any drilling water was present. Groundwater sampling was not done until at least one year after the installation of the multiple-packer casing. Groundwater samples for inorganic and organic solutes were collected at the same time for each sampling period.

RESULTS

Core Drilling and Borehole Geophysics

Identification and correlation of the lithology based on core logs and the results of the borehole geophysics show general agreement with descriptions given in Table 1. A weathered zone about 4-5 m thick was observed at the top of the bedrock in each borehole. This zone is characterized by frequent bedding plane partings (fractures) 2-3 cm apart that have been subjected to considerable dissolution. Vertical fracturing interconnects most of these partings, especially at the top of the zone. The separation of the partings increases to about 0.2 m near the bottom of the zone. Fracture and rubble zones 0.1 m to 0.5 m thick were also observed at a variety of depths in the Guelph Formation and Lockport Group but did not correlate well from borehole to borehole even between the closely spaced NI series holes.

Only a marker horizon in the Goat Island Formation characterized by increased porosity and gypsum filled vugs and fractures, does correlate well between all boreholes. Below the top of the Rochester Formation very few open bedding plane partings are observed in any of the core.

During the core logging, particular attention was paid to identification of vertical fractures in the core from the two inclined boreholes. Although numerous short (a few cm in length) and healed vertical and sub-vertical fractures were identified in both boreholes, no through-going open vertical fractures were observed. The healed vertical fractures show no evidence of displacement and are oriented randomly.

Of the geophysical logs conducted, the electric logs and the natural gamma log were found to be most useful in terms of lithologic identification. The caliper log was most useful in identifying larger fractures and fracture zones which appeared as wash-outs. The sonic logs proved to be unsatisfactory in identifying smaller fractures, the bulk of which provide the permeability in each formation. The porosity and neutron logs were also valuable tools for lithologic identification and were helpful to identify larger fracture zones. Fluid resistivity logs show water of very high conductivity in the boreholes, in the order of 6000 to 10,000 μ S.cm^{-1}. Significant resistivity anomolies with depth that might indicate flux of water in or out of the borehole are not apparent. Fluid temperature and especially differential temperature show that some groundwater is entering the boreholes through fracture zones near the bedrock surface.

Hydrostratigraphy

Table 3 shows the results of the hydraulic testing expressed as a range of hydraulic conductivities for each major lithologic unit and for each borehole. The negative log of the geometric mean of each range is also given. The overall range of hydraulic conductivity is between 10^{-4} m/s to $<10^{-11}$ m/s. The values expressed here are reliably representative of the formation properties in the higher hydraulic conductivity range but less so for reported K_h of 10^{-10} to 10^{-11} m/s. The lower K values were determined largely from constant head tests of relatively short duration (200 min or less). Preliminary long term slug tests show K_h of the formations for these intervals are much lower in the order of 10^{-12} to 10^{-13} m/s. This suggests that there are significant skin effects caused by permeability enhancement generated during drilling. However, intervals that have K_h greater than 10^{-9} m/s, show a permeability reduction near the borehole by up to several orders of magnitude. The reason for this transition from enhanced to reduced near-borehole permeability is not immediately evident but may be the result of reduced rock flour penetration at lower permeabilities. The high permeability intervals near the bedrock surface show no skin effects whatsoever.

The general range of hydraulic conductivity shows decline in permeability with depth with the shale formations having the lowest permeability. In the boreholes nearest to the Niagara Gorge (the NF series boreholes) permeability is greater in the Lockport and Clinton Groups probably because of increased vertical and horizontal fractures.

Table 4 shows the hydraulic head distribution with respect to the major lithologic units in each borehole. The head measurements are reliable to no better than ±0.5 m (estimated) due to uncertainty in the accuracy of the density measurements used to convert field pressure readings. Accuracy of the measurements obtained from the intervals in the Guelph Formation and Lockport Group is probably much better, however for the purpose of this presentation, this accuracy is not shown. The hydraulic head measurements presented in Table 4 were obtained after at least one year of equilibration and subsequent monitoring has shown little or no fluctuation in these values.

Several general trends are evident in the data in Table 4. Hydraulic head in the Guelph Formation shows very little variation across the study area. A broad range of hydraulic head from 141 masl to as high as 202 masl is observed in the Lockport Group measurements where values in the higher end of the range are from the boreholes farthest from the Niagara Gorge. Hydraulic head in the Clinton Group is largely overpressured (pressures above ground surface) except for the boreholes adjacent to the Gorge. Measurements obtained from the Cataract Group and Queenston Formation range from overpressured to a low of about 123 which is about 50 m below the average ground surface elevation.

Figs. 4 and 5 show the stratigraphy, hydraulic conductivity and hydraulic head distribution for boreholes NI-2 and NF-2 respectively, and are used to illustrate the difference between boreholes close to the Niagara Gorge (i.e. NF-2) and those away from the Gorge (i.e. NI-2).

The hydraulic conductivity near the top of borehole NI-2 (Fig. 4) is highest in the Guelph Formation and decreases uniformly to 10^{-11} m/s and lower in the Clinton and Cataract Groups. Moderate permeability is evident at the top of the Queenston Formation perhaps at the Queenston-Whirlpool contact.

Hydraulic head in the Guelph Formation and top of the Lockport Dolostone in NI-2 are fairly uniform and in hydraulic communication with water in the Upper Niagara River. The uniformity of the hydraulic head suggests vertical hydraulic communication between the major fracture zones. In the middle of the Lockport, where permeability begins to decline, the hydraulic head increases to almost 60 m above ground surface in the Rochester Shale. Except for the high heads in the Rochester Formation, the bulk of the measurements in the Clinton and Cataract Groups are about 35 m above ground level. The lower Cataract Group shows a significant decline in hydraulic head from about 200 m to a low between 125 and 130 m at the top of the Queenston Formation. This low-head feature is probably associated with higher permeability and suggests strong hydraulic connection to the the water level in the plunge pool below the Niagara Falls, at an elevation of about 125 m.

The permeability in borehole NF-2 (Fig. 5) is generally somewhat higher than in borehole NI-2, probably because of more vertical and horizontal fracturing near to the Gorge. Other permeability measurements in the Lockport Formation and upper Rochester Formation (Maslia and Johnston, 1984) obtained near to the Gorge are in agreement if not somewhat higher than at borehole NF-2. Several distinct high permeability zones, some in the Lockport Formation, are evident in this borehole. However, below the Upper Clinton Group, the permeability declines to about 10^{-11} m/s or perhaps less, again except for a slightly higher permeability zone at the top of the Queenston Formation.

The hydraulic head measurements in the Guelph Formation in NF-2, like in borehole NI-2, are uniform and close to the elevation of the Niagara River. In borehole NF-2, however, the high permeability zone at the top of the Lockport has hydraulic heads about 10 to 15 m below river level suggesting good connection to the Niagara Gorge. The Clinton Group has a head of about 10 m above river level, 50 m less than that observed in borehole NI-2. The Cataract Group shows declining heads toward the low-head feature at the top of the Queenston Formation, similar to that seen in NI-2. Borehole NF-2 penetrates the Queenston Formation deeper than any other of the boreholes and has a hydraulic head 20 m above river level. High hydraulic heads at this depth also occur in borehole NI-1, which also deeply penetrates the Queenston Formation.

Groundwater Chemistry

Fig. 6 shows the results of the inorganic chemical analysis for samples obtained from the Guelph and Lockport Formations, the Clinton and Upper Cataract Group and the Lower Cataract Group (or the Upper Queenston Formation). These samples were mostly obtained from boreholes NF-2, NI-1 and NI-2. The presence of drill water contamination was not found in any of the samples presented in Fig. 6.

Samples obtained from the Guelph and Lockport Formations are predominantly Ca-SO_4 type near the top of the Guelph Formation and trend towards a more saline NaCl type near the bottom of the Lockport Group. This is a typical evolutionary trend for downward migrating groundwater in sedimentary basins (Freeze and Cherry, 1979, p. 242). However, because the hydraulic gradients are predominantly upwards at the top of the Clinton Group for the boreholes from which the samples were obtained and because the number of samples are few, it is also possible to suggest that the trend is simply a mixing line between meteoric and more saline water.

The total dissolved solid (TDS) content ranges from a low of 0.5 g/L for samples at the top of the Guelph Formation to about 6 to 7 g/L at the top of the Lockport and 38 g/L at the base of the Lockport. The pH generally ranges from values of 7.0 to 8.0 where the higher values were obtained from the shallower intervals in the Guelph and Lockport Formations. Eh measurements (by platinum electrode) average less than -300 mV indicating a pervasively reducing environment.

The composition of the water obtained from the Clinton and Cataract Groups is of NaCl type varying in TDS between 22 to 38 g/L. This composition is similar to other highly saline connate water found in sedimentary basins in Europe (Andrews et al., 1987). However, the TDS content is considerably less than those seen elsewhere in the Niagara Peninsula (Barker et al., 1987) and may reflect deep mixing or dilution of brines in the Niagara Falls area. Eh and pH measurements are similar to those obtained from the overlying Guelph and Lockport Formations.

Groundwater samples obtained from the Upper Guelph, Lockport and Rochester Formations were analysed by gas chromatography for volatile organic compounds. Benzene, toluene and xylenes (BTX) were found at or below the detection limit in the Guelph and Lockport samples. Benzene was detected at concentrations of about 20 ppb in the Rochester shale sample. Volatile organo-sulphide compounds were found at ppm levels in all samples. The Rochester Formation and Clinton Group is well known as one of the principal source beds for hydrocarbons in southwestern Ontario (Sanford et al., 1985). Therefore the high benzene concentrations in the Rochester Formation are very probably natural constituents evolved from the sedimentary matter. The concentration of hydrocarbons in saline water or brines can vary widely and benzene concentrations as high as 10 mg/L have been observed in source rocks (McAuliffe, 1969).

DISCUSSION

Based on the hydrostratigraphy, geology and geochemistry, groundwater flow in the stratigraphy underlying Niagara Falls can be divided into three flow regimes: the upper weathered zone and fracture zones in the Guelph and Lockport Formations; the low permeability-high hydraulic head Clinton-Upper Cataract Group and Lower Queenston Formation and the moderate permeability-low hydraulic head feature in the Lower Cataract Group - Upper Queenston Formation. Fig. 7 depicts, in an simplistic way, an example of the conceptual groundwater flow regime beneath the Upper Niagara River between Navy Island

and the Niagara Falls. The more traditional cross-sectional diagram showing lines of equipotential is not appropriate here due to the substantial differences in hydraulic head between the flow regimes.

Guelph-Lockport Flow Regime

At least two and more often three or four high permeability zones (usually fracture zones) occur in the Guelph and Lockport Formations in each borehole. The location of the high K zones with respect to the stratigraphy varies from borehole to borehole except for the weathered zone and the fracture zone in the Goat Island Member. This suggests that some of the fracture zones are probably discontinuous across the study area and may have little influence on the regional flow regime in the Guelph-Lockport. In general, regional groundwater flow in the Guelph and Lockport Formations is towards the Niagara Gorge (Fig. 7) and controlled by those fracture zones that are interconnected laterally. Hydraulic gradients toward the Gorge between NI-2 and NF-2 range from about $4x10^{-4}$ in the weathered zone to about $3x10^{-3}$ in the fracture zone in the Goat Island Formation (see Fig. 4 and 5).

The rate of groundwater flow in the unfractured bulk rock of the Lockport Formation is probably much less than that in the fracture zones. Although the unfractured bulk rock is influenced by the same lateral hydraulic gradient as in the weathered zone, the K_h is considerably smaller, as low as 10^{-11} m/s (data from the Lockport Formation, borehole NI-1).

Vertical fracturing that might interconnect horizontal fracture zones was not directly observed in the inclined boreholes, NI-1 and NI-3. However, on the basis of the mixing trend observed in geochemical samples and the uniformity of hydraulic head with respect to depth, some vertical connection probably exists. The rate of flux in the vertical direction is likely very small in consideration of the low permeability of the rocks in the Clinton Group. In general, upward mixing of Clinton Group water with Guelph-Lockport Formation water is observed only in boreholes well away from the proximity of the Gorge such as borehole NI-2, other NI series boreholes and CH-1. However, where vertical fracturing is known to be enhanced, directly adjacent to the Gorge such as at borehole NF-2, the hydraulic gradient is reversed (vertically downward) and Clinton Group water no longer mixes with Guelph-Lockport water except at the base of the Lockport Formation. The transition between upward and downward gradients in the Guelph-Lockport occurs at considerable distance from the Gorge; somewhere between NF-2 and NI-2 for example.

Geochemical samples obtained from the weathered zone at the overburden-bedrock contact uniformly show Ca-SO_4 type water with little or no bicarbonate present. This suggests that present-day recharge through the overburden is very slow, probably as a result of the low-permeability glacial deposits. Elsewhere on the Niagara Peninsula, groundwater obtained from the same glacial deposits has been dated at the age of the formation of these deposits (Desaulniers et al., 1981). Therefore, recharge to the Guelph-Lockport flow regime is probably localized along the Niagara River, Welland River, Niagara Falls Moraine and possibly through man-made water diversions and sewers.

The groundwater flow regime in this hydrostratigraphic unit likely formed from topographic changes caused by erosion and from stress release caused by isostatic rebound and erosional unloading during the Cenozoic

Clinton-Upper Cataract and Lower Queenston Formation Flow Regime

Groundwater migration in the Clinton-Upper Cataract Groups and the Lower Queenston Formation is minimal relative to the that in Guelph-Lockport flow regime. Hydraulic head measurements from those boreholes farthest from the Niagara Gorge are uniformly above ground surface. Flow directions are primarily vertical except near the Gorge (Fig. 7) where some horizontal discharge may occur. The vertical flow likely takes place only near the upper part of the Clinton Group and lower towards the base of the Cataract Group, solely a result of the very large vertical gradients in these strata.

The influence of active vertical faults or through-going fractures would probably act to dissipate the high heads near to the feature. However, hydraulic head measurements in borehole CH-1, near to a suspected vertical fault, are equally as high as observed in other boreholes suggesting that the fault is inactive and may be unimportant with regard to regional groundwater flow.

Anomolously high hydraulic head as observed in the Clinton Group and Lower Queenston Formation are common to sedimentary basins and hydrocarbon bearing rock throughout North America (Hanshaw and Hill, 1969; Toth and Corbet, 1986; Neuzil, 1986). In this case, however, the anomolous heads occur in low-permeability formations that are relatively shallow within the stratigraphic section. There are numerous potentially viable explanations as to the source of these pressures including sedimentary burial and denudation (Toth and Millar, 1983; Neuzil, 1986), lateral tectonic compression (Graf, 1982) and physiochemical effects (Neuzil, 1986). Alternatively, the pressures may be generated by a current basin-wide regional flow system in which the Niagara Falls region acts as a discharge area. The latter is unlikely, however, because the source beds of the high hydraulic head are low-permeability shale formations. Regional flow systems within such rock would require considerable periods of geologic time to establish, during which numerous other geological events (tectonic events for example) would act to modify the regional recharge and discharge areas (Toth and Corbet, 1986 as an example). Determination of the geopressuring process will require further field investigation and is beyond the scope of this paper.

Lower Cataract-Upper Queenston Flow Regime

The Lower Cataract Group-Upper Queenston Formation has a moderately low permeability of about 10^{-8} to 10^{-9} m/s and a pervasively low hydraulic head. Groundwater flows in this regime are slow and in a lateral direction. Hydraulic gradients between boreholes NI-2 and NF-2 are in the order of $1x10^{-4}$ (Figs. 4 and 5). In general, the lateral flow direction is likely northward and towards the Niagara Gorge. In consideration of the vertical hydraulic gradients in the Upper Cataract Group and Lower Queenston Formation, the groundwater in this feature is probably derived from both the overlying and the underlying formations and therefore reflects the chemical character of the water in these units. There is probably no influence on the magnitude and direction of groundwater flow at this depth by man-made surface drainage or the Upper Niagara River. Again, evidence of the influence of a large scale fault is not observed in the measured hydraulic heads.

The anomolously low hydraulic heads in the Lower Cataract-Upper Queenston flow regime are observed in all the study boreholes and have been observed elsewhere along the Niagara Escarpment (Nadon, 1981). Two explanations can be offered as to the source of the underpressured zone. First and most obvious is that the presence of the Gorge and Escarpment have provided a source for low hydraulic heads which are accessed along the moderate permeability feature. This means that the low heads observed in the Niagara Falls area and immediately south are likely Holocene-aged phenomenon generated by the advance of the Niagara Gorge since the last glaciation. Alternatively, erosional unloading may have enlarged the pore structure and enhanced the permeability (Neuzil and Pollock, 1983) in the Whirlpool sandstone. Surrounded by very low-permeability material, the decline in pore pressure has yet to readjust through the influx of water. This would probably be a longer term geologic process directly related to the periods of erosional unloading. If the former hypothesis is accepted then the level of the hydraulic head in this feature should be observed to rise towards the levels of the over and underlying formations with distance from the Gorge. This is, in fact, noted in hydraulic head measurements from borehole CH-1 which indicate slight underpressure (a few metres below ground surface) but are much closer in value to heads in the Clinton Group and Queenston Formation than observed in other boreholes closer to the Gorge.

CONCLUSIONS

Measurement of hydraulic conductivity, hydraulic head and groundwater geochemistry were used to formulate a conceptual model of groundwater flow in the Niagara Falls Region, Ontario, Canada. The results show that there are at least three major and distinct groundwater flow regimes in the Silurian and Ordovician stratigraphy underlying the study area. The uppermost flow regime is in the Guelph Formation and Lockport Group and is characterized by high-permeability zones some of which are probably continuous across the study area. The high-permeability zones are separated by low-permeability dolostone that although not pervaded with vertical fractures does have some hydraulic interconnectivity. Groundwater flux in the upper flow regime is primarily lateral towards the Niagara Gorge and is probably not large except near the Gorge and Escarpment. The groundwater in this regime is primarily of Ca-SO_4 type with TDS contents well above drinking water guidelines and moderate to high background concentrations of natural volatile organic compounds.

Underlying the upper flow regime is an overpressured zone in the Clinton-Upper Cataract Groups and Lower Queenston Formation and an underpressured zone in the Lower-Cataract Group Upper-Queenston Formation. Groundwater migration in these flow regimes is very slow relative to the upper flow regime and occurs primarily in the vertical direction within the study area. Groundwater from these zones is of NaCl type and has TDS contents ranging from about 18 to 38 g/L. Vertical and horizontal permeability is very low except in the proximity of the Niagara Gorge. The influence of through-going vertical structural features are not recognized in any of these data.

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Table 1. The Silurian and Ordovician stratigraphy underlying Niagara Falls, Ontario.

Age	Group	Formation	Description	Lower Contact	Thickness
Upper Silurian — Cayugan		Salina	brown dolomite and grey calcareous shale, abundant gypsum, anhydrite sparse fossils.	transitional	up to 90 m
Middle Silurian — Niagaran	Lockport Group*	Guelph Oak Orchard*	tan or brown, uniformly textured, sugary, finely crystalline dolostone. Thick bedded, sparse fossils, stylolites, carbonaceous partings and vugs common.	sharp, conformable	37 m
		Eramosa Member — Lockport Formation	dark grey to brown or black, very finely crystalline, dense and laminated dolostone, gypsum filled vugs, carbonaceous partings, black chert throughout.	arbitrary at lowest occurrence of very finely crystalline dolostone	range from 3 m to 10 m
		Goat Island Member — Lockport Formation	brownish-grey, locally grey, medium to fine grained, sugary dolostone. medium to thick bedded, white chert with stylolites and carbonaceous partings.	sharp conformable; determined by change in crystallinity	range from 5 m to 8 m
		Gasport Member — Lockport Formation	grey or blue grey, locally pink, fine to locally coarse grained limestone and dolostone. medium to massive bedded, fossilferous, shale partings, stylolites common, vuggy.	sharp, disconformable	13.5 m at Niagara Gorge
	Clinton	Decew	medium to dark grey, very finely crystalline, thin to medium bedded dolostone, conchoidal fracture in upper part, cross-bedded in lower part, some solution cavities.	transitional	3.5 m at Niagara Gorge
		Rochester	dark bluish to brownish grey, calcareous fossilferous, some argillaceous limestone layers. upper half grey shale, lower half brownish grey.	sharp, conformable	16.75 m
		Irondequoit	white to tan weathered, light to dark grey fresh, fine to medium crystalline limestone, massive to thin bedded, porous, fossiliferous locally, basal conglomerate.	sharp, possible disconformity	3 m
		Rockway Member* Reynales Merritton Member*	upper member-grey blue lithographic to sublithographic, thin to massive bedded, dolostone. lower member-blue, thin bedded, fine grained, dolostone.	sharp, conformable	4.2 m at Niagara Gorge
		Neagha	green to olive green shale, minor very finely crystalline limestone. shale weathers to a light grey colour.	sharp, conformable	2.1 m at Niagara Gorge
		Thorold	greenish, thinly bedded, very fine grained sandstone. thin, green shale partings.	transitional defined by textural change	range from 2.0 to 3.0 m
Lower Silurian — Alexandrian	Cataract Medina*	Grimsby	red with pale green and yellow mottling, massive, fine grained, red sandstone. red shale interbedded in lower part; some red shale in upper part.	transitional	12.8 m to 15.8 m
		Cabot Head Power Glen*	grey and greenish-grey, finely laminated shales with sandstone interbeds, fine grained with occasional limestone interbeds.	transitional	11 m at Niagara Gorge
		Whirlpool	light grey to white-brown, weathered sandstone, medium to thick bedded with fine to very fine grained sub-rounded, sub-sorted grains, shale partings.	sharp, disconformity	up to 7.6 m
Upper Ordovician — Cincinnatian		Queenston	purplish-red, with thin greenish beds and streaks, hematitic calcareous shale, fissile and micaceous.	unknown	> 250 m Niagara Gorge

* denotes alternate nomenclature.

Table 2. Summary of intervals isolated in each borehole using the multiple-packer casing string.

	NF-2	NF-3	NF-4	NI-1	NI-2	NI-3	CH-1
Total Length of Borehole (m)	147.4	130.2	117.4	152.9	135.4	101.2	154.0
Number of Intervals	10	9	8	23	14	15	15
Average Length of Intervals (m)	12.3	12.2	11.9	5.3	7.9	5.0	8.4
Percent Seal (%)	6.1	6.2	6.1	13.5	9.3	13.3	8.8

Table 3. Range of hydraulic conductivities, K (m/s), for each major lithologic unit in each borehole. Also shown is the negative log of the geometric mean for each range. Some values were indeterminant as a result of high gas exsolution.

	NF-2#	NF-3*#	NF-4#	NI-1	NI-2	NI-3	CH-1
Guelph Formation	$2.8x10^{-4}$ -$2.2x10^{-8}$ 6.0	$1.0x10^{-6}$ 6.0	-	$9.2x10^{-5}$ -$2.7x10^{-8}$ 6.0	$2.4x10^{-5}$ -$1.4x10^{-8}$ 6.6	$4.0x10^{-5}$ -$2.0x10^{-8}$ 6.2	$4.5x10^{-5}$ -$2.0x10^{-5}$ 4.5
Lockport Group	$5.5x10^{-4}$ -$4.5x10^{-10}$ 6.1	$1.0x10^{-5}$ -$7.0x10^{-7}$ 5.6	$2.3x10^{-5}$ -$3.7x10^{-9}$ 6.6	$4.9x10^{-5}$ -$4.1x10^{-9}$ 6.8	$1.4x10^{-8}$ -$7.8x10^{-11}$ 8.8	$2.7x10^{-8}$ -$1.7x10^{-9}$ 8.2	$3.5x10^{-6}$ -$6.1x10^{-8}$ 6.6
Clinton Group	$1.7x10^{-6}$ -$3.6x10^{-11}$ 8.3	$2.0x10^{-6}$ -$2.0x10^{-8}$ 6.9	$1.4x10^{-7}$ -$1.1x10^{-11}$ 8.6	$3.1x10^{-8}$ -$1.2x10^{-9}$ 8.1	$3.2x10^{-9}$ -$7.8x10^{-11}$ 9.3	$5.4x10^{-11}$ -$3.5x10^{-11}$ 10.4	$2.3x10^{-9}$ gas 8.6
Cataract Group	$2.7x10^{-8}$ -$3.0x10^{-11}$ 9.5	$2.0x10^{-8}$ -$2.0x10^{-9}$ 8.2	$2.0x10^{-7}$ -$<1.0x10^{-11}$ 9.6	$5.7x10^{-10}$ -$4.8x10^{-11}$ 9.9	$2.2x10^{-8}$ -$7.7x10^{-9}$ 7.9	-	$3.5x10^{-9}$ -$5.8x10^{-10}$ 8.8
Queenston Formation	$2.7x10^{-10}$ -$1.2x10^{-11}$ 10.4	$1.0x10^{-8}$ -$8.0x10^{-9}$ 8.0	$5.6x10^{-10}$ -$<1.0x10^{-11}$ 10.4	$1.1x10^{-9}$ -$5.3x10^{-11}$ 9.6	gas	-	$1.8x10^{-10}$ 9.7

* Drill stem tests: poor reliability

\# From Semec and Huang (1984)

Table 4. Range of hydraulic head (masl) for each major lithologic unit in each borehole. Hydraulic head measurements from intervals that straddle lithologic boundaries are included in the entries for both lithologic units.

	NF-2	NF-3	NF-4	NI-1	NI-2	NI-3	CH-1
Guelph Formation	170*	-	-	170*	171*	171*	173-174
Lockport Group	161*	141-152	167-169	170-174	172-202	171-175	172-175
Clinton Group	164-174	125-175	160-175	172-209	200-234	179-201	194-196
Cataract Group	128-155	122-162	113-157	123-200	149-198	-	169-203
Queenston Formation	182	123	126	171	123	-	166-180
Elevation of Ground Surface	175(169[+])	182	181	174(171[+])	175(171[+])	174(171[+])	178

* All measurements within ±0.5 m.

[+] Elevation of average Upper Niagara River level

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Figure 2 The geological model showing the structural and stratigraphic features important to regional groundwater flow.

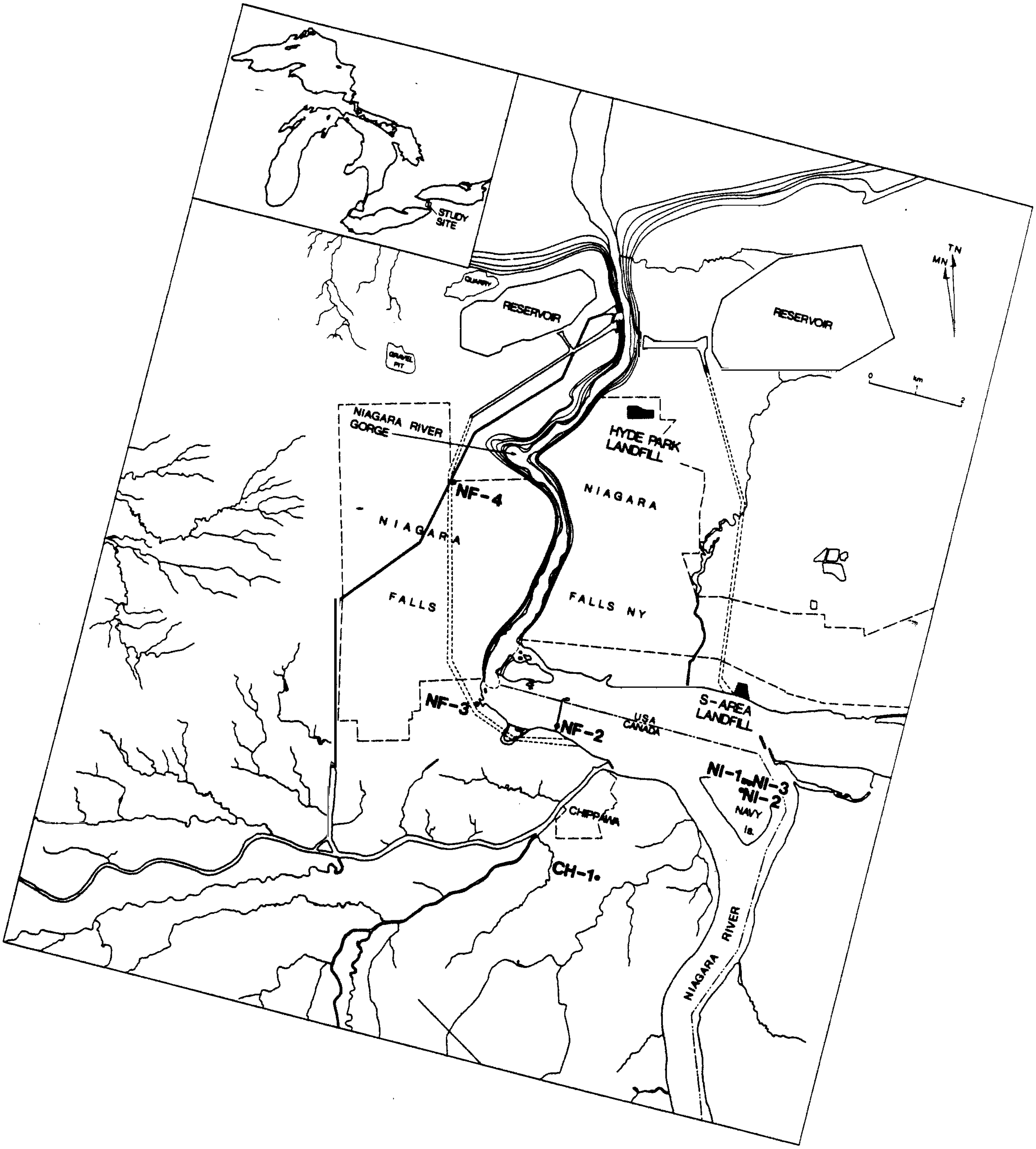
Figure 3 Joint orientations determined from both Silurian and Devonian rocks in the Niagara Peninsula (after Williams et al., 1985).

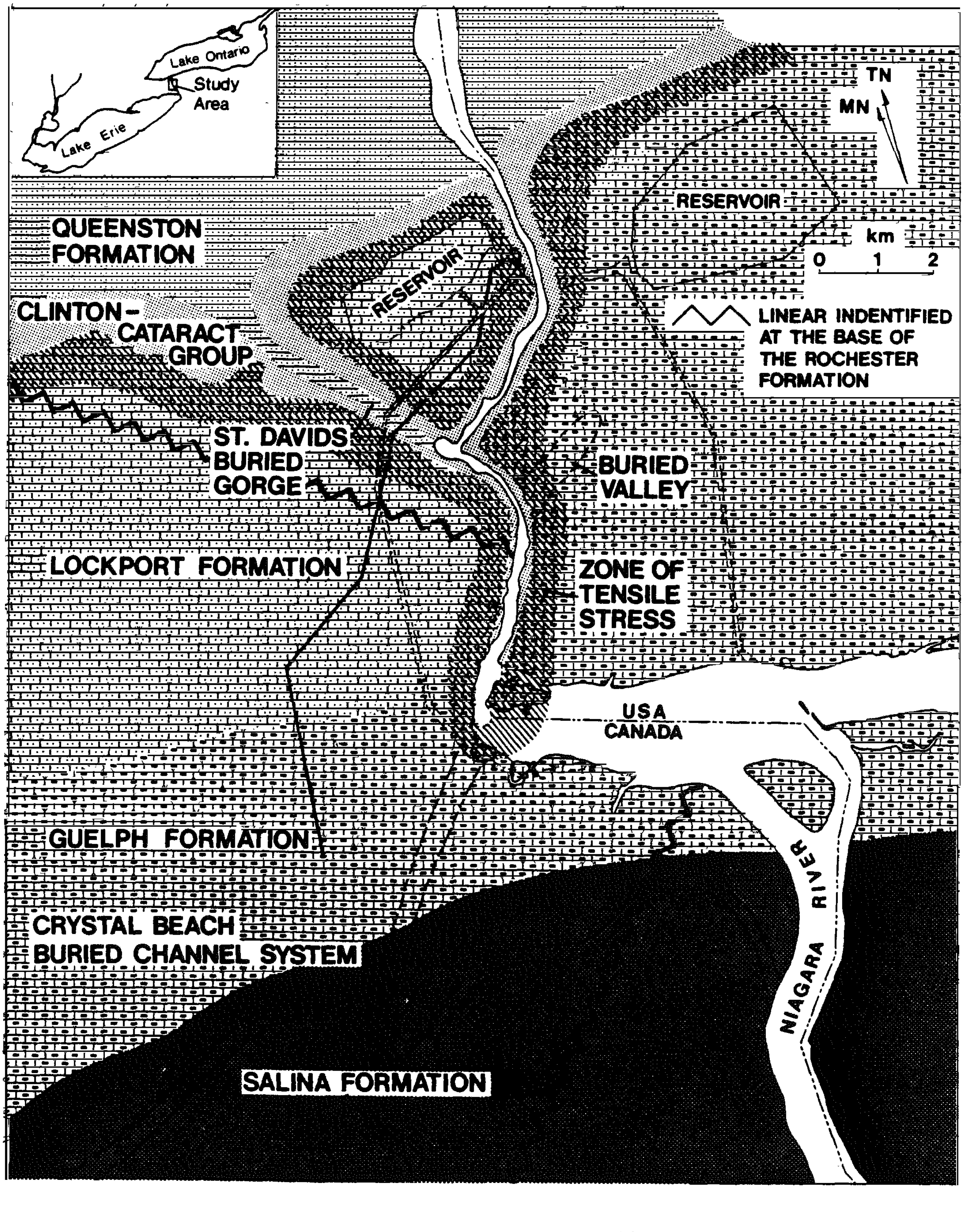
Figure 4 The hydraulic conductivity (negative logarithm), hydraulic head and lithology as determined from borehole NF-2.

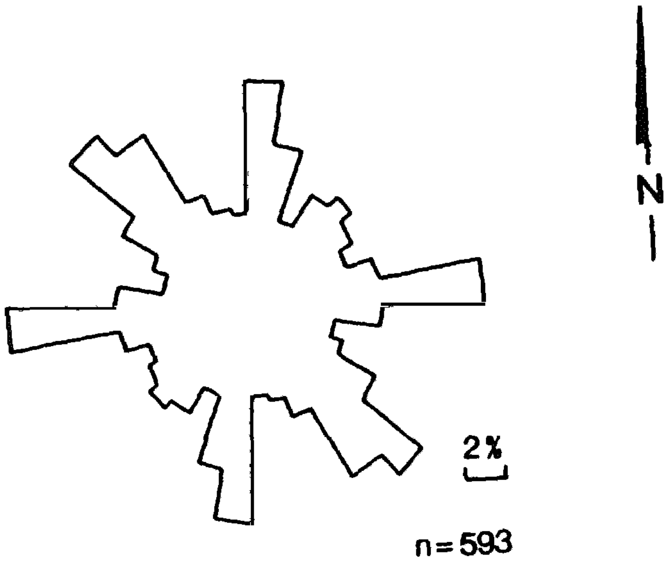
Figure 5 The hydraulic conductivity (negative logarithm), hydraulic head and lithology as determined from borehole NI-2.

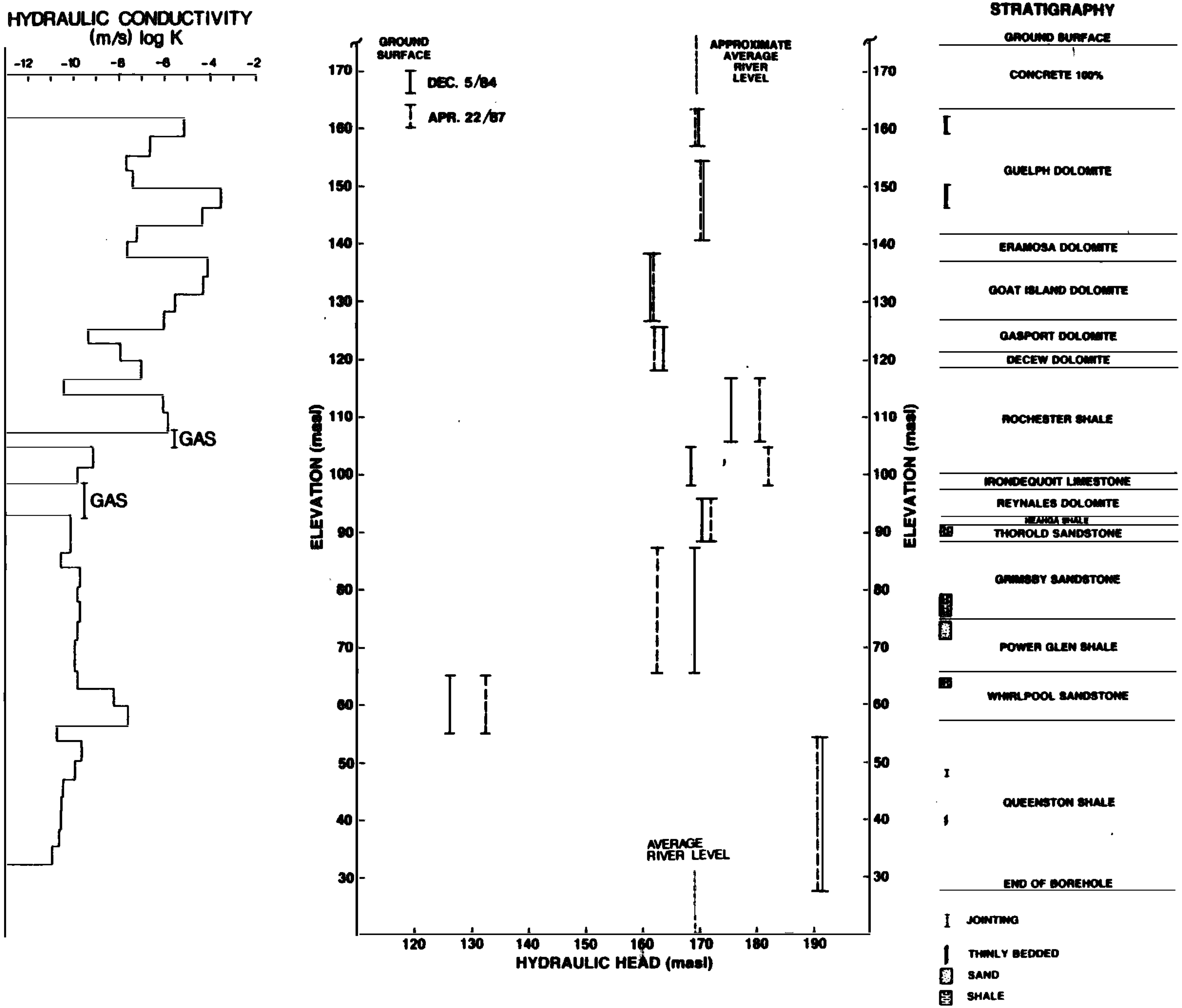
Figure 6 Tri-linear diagram showing the inorganic chemistry of groundwater samples obtained from the study boreholes. Classified according to hydrostratigraphic unit.

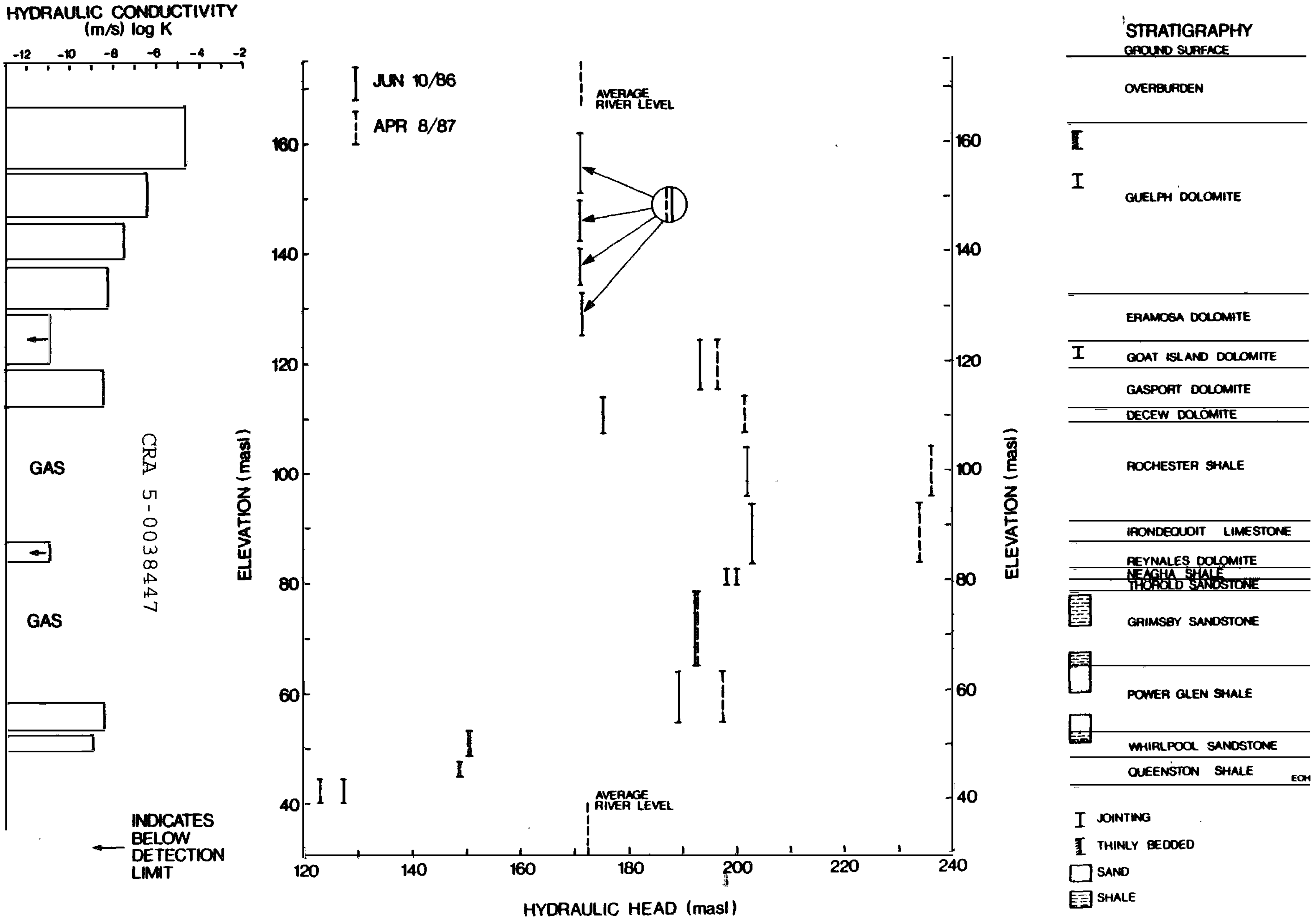
Figure 7 Simplified cross section of the groundwater flow regimes between Navy Island and Niagara Falls.

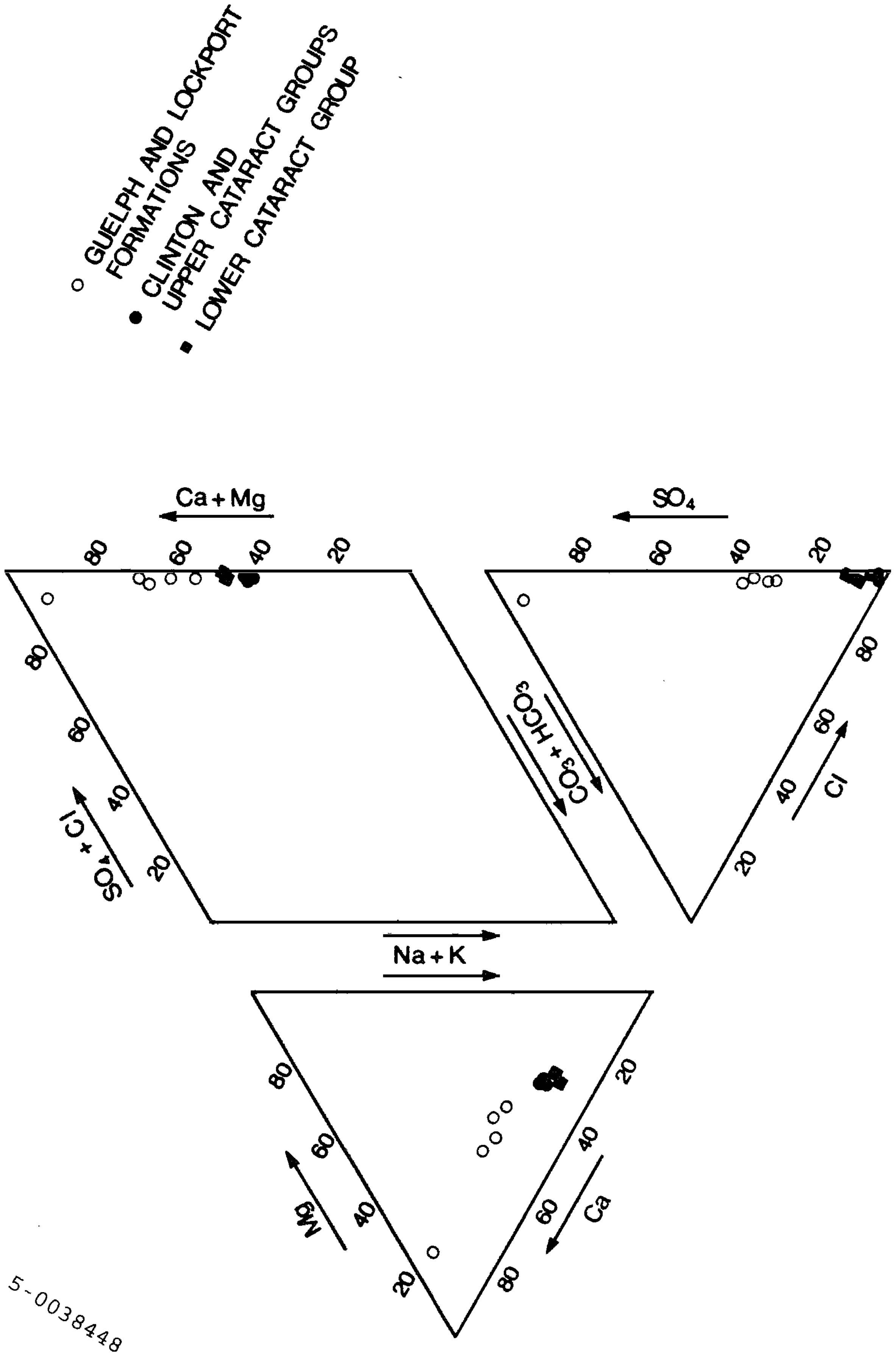

STUDY SITE
QUARRY
RESERVOIR
GRAVEL PIT
RESERVOIR
TN
MN
0 km 1 2
NIAGARA RIVER GORGE
HYDE PARK LANDFILL
NF-4
NIAGARA FALLS
NIAGARA FALLS NY
NF-3
NF-2
USA
CANADA
S-AREA LANDFILL
NI-1
NI-3
NI-2
NAVY Is.
CHIPPAWA
CH-1
NIAGARA RIVER

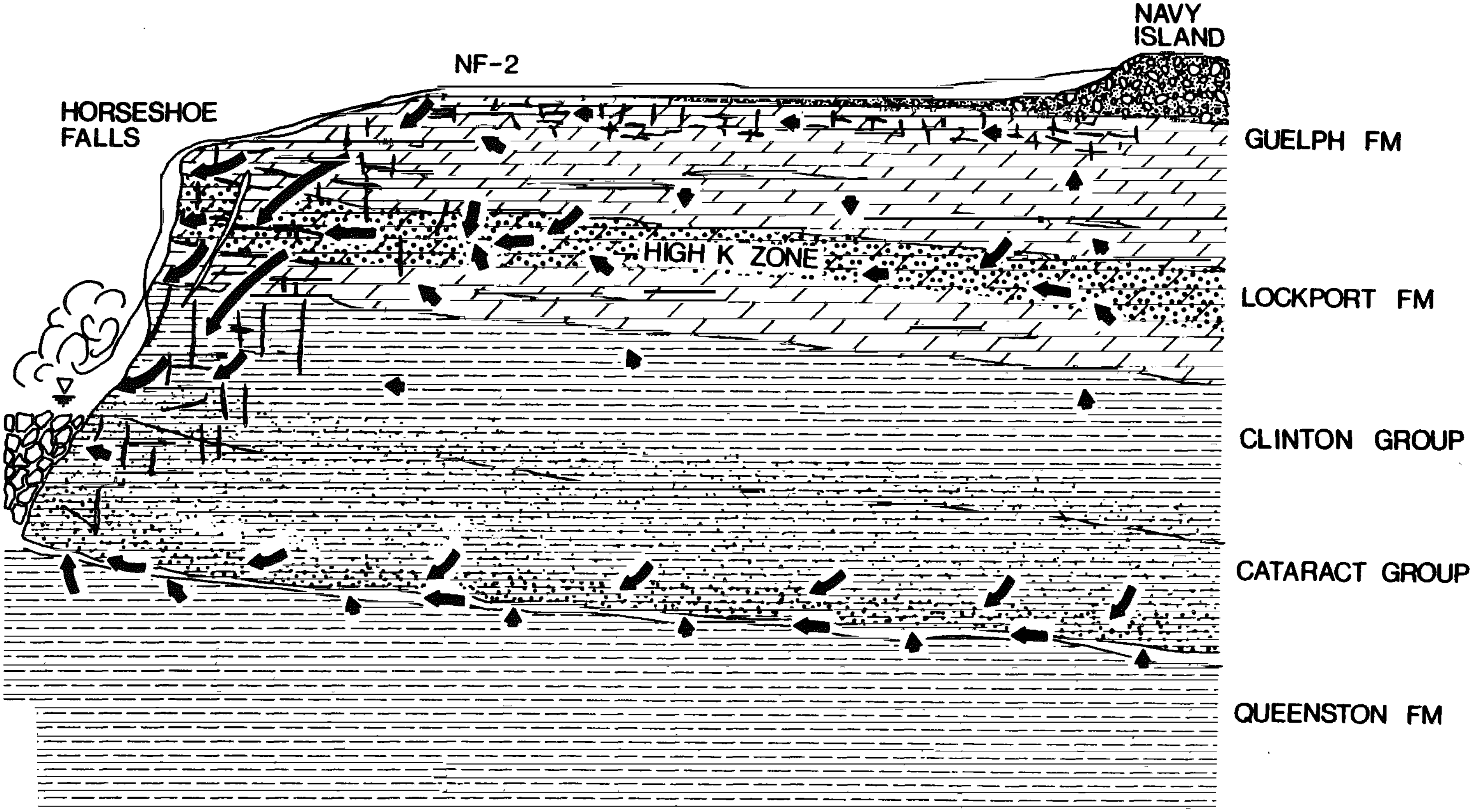

Lake Ontario
Study Area
Lake Erie
TN
MN
RESERVOIR
km
0 1 2
LINEAR INDENTIFIED AT THE BASE OF THE ROCHESTER FORMATION
QUEENSTON FORMATION
CLINTON-CATARACT GROUP
RESERVOIR
ST. DAVIDS BURIED GORGE
BURIED VALLEY
LOCKPORT FORMATION
ZONE OF TENSILE STRESS
USA
CANADA
GUELPH FORMATION
CRYSTAL BEACH BURIED CHANNEL SYSTEM
NIAGARA RIVER
SALINA FORMATION

N
2%
n=593


HYDRAULIC CONDUCTIVITY
(m/s) log K
-12
-10
-8
-6
-4
-2
GAS
GAS
GROUND SURFACE
DEC. 5/84
APR. 22/87
APPROXIMATE AVERAGE RIVER LEVEL
AVERAGE RIVER LEVEL
ELEVATION (masl)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
120
130
140
150
160
170
180
190
HYDRAULIC HEAD (masl)
STRATIGRAPHY
GROUND SURFACE
CONCRETE 100%
GUELPH DOLOMITE
ERAMOSA DOLOMITE
GOAT ISLAND DOLOMITE
GASPORT DOLOMITE
DECEW DOLOMITE
ROCHESTER SHALE
IRONDEQUOIT LIMESTONE
REYNALES DOLOMITE
NEAHGA SHALE
THOROLD SANDSTONE
GRIMSBY SANDSTONE
POWER GLEN SHALE
WHIRLPOOL SANDSTONE
QUEENSTON SHALE
END OF BOREHOLE
JOINTING
THINLY BEDDED
SAND
SHALE


HYDRAULIC CONDUCTIVITY (m/s) log K
-12
-10
-8
-6
-4
-2
GAS
GAS
INDICATES BELOW DETECTION LIMIT
ELEVATION (masl)
160
140
120
100
80
60
40
JUN 10/86
APR 8/87
AVERAGE RIVER LEVEL
AVERAGE RIVER LEVEL
120
140
160
180
200
220
240
HYDRAULIC HEAD (masl)
STRATIGRAPHY
GROUND SURFACE
OVERBURDEN
GUELPH DOLOMITE
ERAMOSA DOLOMITE
GOAT ISLAND DOLOMITE
GASPORT DOLOMITE
DECEW DOLOMITE
ROCHESTER SHALE
IRONDEQUOIT LIMESTONE
REYNALES DOLOMITE
NEAGHA SHALE
THOROLD SANDSTONE
GRIMSBY SANDSTONE
POWER GLEN SHALE
WHIRLPOOL SANDSTONE
QUEENSTON SHALE
EOH
JOINTING
THINLY BEDDED
SAND
SHALE


○ GUELPH AND LOCKPORT FORMATIONS
● CLINTON AND UPPER CATARACT GROUPS
■ LOWER CATARACT GROUP
Ca + Mg
80
60
40
20
SO_4 + Cl
20
40
60
80
SO_4
80
60
40
20
CO_3 + HCO_3
Cl
20
40
60
80
Na + K
Mg
20
40
60
80
Ca
20
40
60
80


NAVY ISLAND
NF-2
HORSESHOE FALLS
HIGH K ZONE
GUELPH FM
LOCKPORT FM
CLINTON GROUP
CATARACT GROUP
QUEENSTON FM

APPENDIX B

SIMULATION OF THREE-DIMENSIONAL FLOW OF IMMISCIBLE FLUIDS WITHIN AND BELOW THE UNSATURATED ZONE

C.R. FAUST, J.H. GUSWA AND J.W. MERCER

SIMULATION OF THREE-DIMENSIONAL FLOW OF IMMISCIBLE FLUIDS WITHIN AND BELOW THE UNSATURATED ZONE

Prepared by:

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GeoTrans, Inc.

Submitted to:

Water Resources Research

ABSTRACT

A three-dimensional, finite-difference model is introduced and used to analyze immiscible fluid transport at two chemical waste landfills near Niagara Falls, New York. At both sites, denser than water, non-aqueous phase liquids (NAPLs) are present in the groundwater regimes in relatively large quantities. The model is an extension of Faust's model (1985) and accounts for three-dimensional flow as well as a flow system defined by two-dimensional, cylindrical coordinates. It uses an iterative matrix solution technique designed to take advantage of parallel computer processing. The two-phase model is posed in terms of water saturations and NAPL pressure. It uses three-phase capillary pressure and relative permeability relationships to permit simulation within and/or below the unsaturated zone. The model applications address several technical concerns at the two sites, including the effectiveness of clay as a capillary barrier, the three-dimensional aspects of dense NAPL flow, and the sensitivity of NAPL recovery in pumping wells due to various hydrogeologic and fluid properties. The results of the applications show that (1) even under a downward hydraulic gradient, natural differences in capillary pressure relationships for different lithologies can prevent downward migration of NAPL; (2) in the absence of any lithologic-capillary barrier, an upward hydraulic gradient induced by a dewatering system can prevent downward migration of NAPL; (3) NAPL recovery at wells is sensitive to relative permeability, a relationship that requires field calibration in many settings; and (4) the three-dimensional aspects of two-phase flow and hydrogeologic stratification require explicit treatment in many settings.

INTRODUCTION

Nonaqueous phase liquids (NAPL) have been discovered at numerous hazardous waste sites (e.g., Mercer et al., 1985; Faust, 1985; Cohen et al., 1987). In addition, NAPL is often identified with contamination problems associated with underground storage tanks. Typical wastes and waste-producing processes that may involve NAPL include transformer oil containing polychlorinated biphenyls (Robert et al., 1982; Schwartz et al., 1982), trichloroethylene and related chlorinated hydrocarbons (Palombo and Jacobs, 1982; Carpenter, 1984), coal tars from illuminating gas production (Wilson and Stevens, 1981; Yazicigil and Sendlein, 1981; Lafornara et al., 1982; Anastos et al., 1983; Thompson et al., 1983; Unites and Houseman, 1982; Villaume, 1982; Adams and Atwell, 1983; Villaume et al., 1983a; Villaume et al., 1983b; Villaume, 1984), steel industry coking operations (Coates et al., 1982), and wood treating operations (Hult and Schoenberg, 1981; Ramsey et al., 1981; Ehrlich et al., 1982; Hickok et al., 1982; Pereira et al., 1983).

Although the chemical properties and site-specific conditions vary from site to site, the basic principals that govern the fate and transport of these NAPLs are the same; they may be used at each site to understand better the contamination problem and as a means to evaluate remediation of the problem. Unfortunately, development of state-of-the-art technology for dealing with NAPL problems lags behind the technology developed for many other groundwater contamination problems. Although several models are available to simulate the flow of NAPL and water, obtaining chemical-specific and site-specific data is difficult. Consequently, for most sites, these models may only be used in a conceptualization mode.

Petroleum reservoir codes for simulating the flow of immiscible fluids have existed for more than 20 years (see, for example, Peaceman, 1977 or Chichlow, 1977) but, with few exceptions, it has only been in the last few years that these same techniques have been used to examine oil spill problems. These codes, used to examine NAPL flow, are reviewed in Pinder and Abriola (1986).

Early recognition of NAPL movement in groundwater as a two-phase flow phenomenon is attributed to Van Dam (1967). Several models were subsequently developed to describe mathematically the immiscible flow of lighter than water NAPL in the subsurface (Mull, 1969, 1971, 1978; Dracos, 1978; Schiegg, 1977, Holzer, 1976; Hochmuth and Sunada, 1985). Common to each of these is the assumption of negligible capillarity (pistonlike flow).

An early code used to examine multiphase well flow that accounts for capillarity is presented by Brutsaert (1973). The model is radial and based on a finite-difference approximation. A one-dimensional (vertical) finite-difference, two-phase flow simulator was subsequently developed by Arthur D. Little, Inc. (1983). This work was extended by Faust (1985) to accommodate two dimensions and a third, static, air phase, a necessary step to simulate NAPL flow in the unsaturated zone.

A model similar to Faust's model (1985), but without the air phase, was applied to the Hyde Park landfill, Niagara Falls, New York by Osborne and Sykes (1986). Abriola and Pinder (1985a,b) developed a model that also considers volatization and dissolution. A similar model is presented in Corapcioglu and Baehr (1987) and Baehr and Corapcioglu (1987). A subsequent extension was to incorporate hysteretic constitutive relations, which is done in Parker and Lenhard (1987) and Lenhard and Parker (1987).

The existing models are capable of simulating in fewer than three dimensions. As pointed out by Abriola and Pinder (1986), "The extension of existing two-dimensional models to this third dimension, and the solution of such three-dimensional problems presents a formidable task." One purpose of this paper is to extend the model described in Faust (1985) to three dimensions. Also described is the solution technique, which takes advantage of parallel computer processing. Finally, to demonstrate the capabilities and limitations of the model, three applications at two hazardous waste sites in New York are presented. The applications were originally conducted to evaluate NAPL migration and remedial alternatives. Recent investigations at one of the two sites has confirmed some of the significant conclusions drawn from the results of the model simulations.

NUMERICAL MODEL

The mathematical models developed for multiphase simulation are nonlinear and are not amenable to convenient analytical solution. Additionally, the highly nonlinear saturation-capillary pressure-relative permeability relationships in the model render even numerical solution a difficult task. The techniques used to solve these complex equations have been used successfully in the petroleum and geothermal industries (see, for example, Faust and Mercer, 1979). These techniques consist of a finite-difference approximation of the differential equations, the Newton-Raphson method to treat the nonlinearities, and the Slice Successive Over-Relaxation (SSOR) method for matrix solution. For SSOR, both the conventional SSOR and a modified SSOR are used, where the modified SSOR takes advantage of parallel-vector architecture. All of these techniques and the governing equations are discussed in this section.

GOVERNING EQUATIONS

The basis of the mathematical description of multiphase fluid flow in porous media is the conservation equation for mass and momentum for each phase. The mathematical model presented here is based on a simplification of the conventional three-phase flow equations used in petroleum reservoir simulation. The conventional equations (Peaceman, 1977) for three-phase fluid flow in terms of water (w), nonaqueous phase (n), and air (a) are:

$$\nabla \cdot \left[\frac{k\rho_w k_{rw}}{\mu_w} (\nabla p_w - \rho_w g \nabla D) \right] + q'_w = \frac{\partial(\phi \rho_w S_w)}{\partial t} , \qquad (1)$$

$$\nabla \cdot \left[\frac{k\rho_n k_{rn}}{\mu_n} (\nabla p_n - p_n g \nabla D) \right] + q'_n = \frac{\partial(\phi \rho_n S_n)}{\partial t} , \qquad (2)$$

and

$$\nabla \cdot \left[\frac{k\rho_a k_{ra}}{\mu_a} (\nabla p_a - \rho_a g \nabla D \right] + q'_a = \frac{\partial(\phi \rho_a S_a)}{\partial t} , \qquad (3)$$

In the above equations, k is the intrinsic permeability (L^2), ρ is the density (M/L^3), k_r is the dimensionless relative permeability, μ is the dynamic viscosity (M/LT), p is the fluid pressure (M/L^2), g is the gravitational acceleration (L/T^2), D is depth (L), q′ is the mass source/sink (M/L^3T), ϕ is the dimensionless porosity, S is the dimensionless volumetric saturation, ∇ is the differential operator (L), and t is time (T). The above equations include 16 dependent variables in the general case. Therefore, an additional 13 independent relationships are necessary to obtain a solution to the system. The most general relationships include:

1. Sum of volumetric saturations (1 relation)

$$S_n + S_w + S_a = 1 \, , \tag{4}$$

2. Densities and viscosities as functions of phase pressures (6 relations),

3. Relative permeabilities as functions of saturations (3 relations),

4. Capillary pressures (p_a-p_n) and (p_n-p_w) as functions of saturations (2 relations), and

5. Porosity as a function of pressure (1 relation).

These relationships are discussed in Faust (1985) and are not elaborated here.

The governing equations are simplified by assuming that pressure gradients in the air phase are negligible. This eliminates the need for equation (3) and permits reformulation of (1) and (2) in terms of NAPL pressure, p_n, and water saturation, S_w, as:

$$\nabla \cdot \left[\frac{k\rho_w k_{rw}}{\mu_w} (\nabla p_n - \rho_w g \nabla D)\right] - \nabla \cdot \left[\frac{k\rho_w k_{rw}}{\mu_w} \nabla pc_{nw}\right]$$

$$+ q'_w = \frac{\partial(\phi\rho_w S_w)}{\partial t} \, , \tag{5}$$

and

$$\nabla \cdot \left[\frac{k\rho_n k_{rn}}{\mu_n} (\nabla p_n - \rho_n g \nabla D)\right] + q'_n = \frac{\partial[\phi\rho_n(1-S_w-S_a)]}{\partial t} \, , \tag{6}$$

where pc_{nw} is the difference between the pressures in the nonaqueous phase and water. If it is also assumed that phase densities and viscosities are constant, then the mathematical description may be completed by expressions for source terms, boundary conditions, initial conditions, two relative permeability relationships, two capillary relationships, and one porosity relationship (see Faust, 1985).

NUMERICAL APPROACH

The three-dimensional model includes capabilities for one-, two-, or three-dimensional simulations in Cartesian coordinates and two-dimensional simulations in cylindrical coordinates. The final governing equations (5) and (6) are highly nonlinear due to the relative permeability and capillary pressure relationships involving the independent variables. The numerical methods used in this model are well adapted to the solution of nonlinear problems. The methods include finite-difference approximations, Newton-Raphson iteration, direct matrix solutions for two- or one-dimensional problems, and Slice Successive Over-Relaxation (SSOR) for matrix solution of three-dimensional problems.

Cylindrical geometry (r-z) is included in the numerical model as an option. The procedure used in the model to treat terms in the radial direction is outlined by Settari and Aziz (1974). This procedure involves transforming the radial terms into r^2. The radial space-derivative terms in the final equations presented earlier have the following form:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(\lambda_r r \frac{\partial p}{\partial r}\right) \tag{7}$$

With $r^* = r^2$, this term is equivalent to the following:

$$4\frac{\partial}{\partial r^*}\left(\lambda_r r^* \frac{\partial p}{\partial r^*}\right) \tag{8}$$

Having made this transformation, the grid is discretized in r^*. This is accomplished by specifying the positions of the node point (r_i) and then calculating the position of the grid block boundaries by the following:

$$r^*_{i+\frac{1}{2}} = \frac{r^*_{i+1} - r^*_i}{\ln\left(\frac{r^*_{i+1}}{r^*_i}\right)} \tag{9}$$

Hence, the block boundaries represent a logarithmic mean radius in r^2.

The application of finite-difference approximations and the Newton-Raphson method produce a system of linear equations that require a solution for each iteration (see Faust, 1985). The coefficient matrix of the linearized equations is banded but nonsymmetric. For two-dimensional problems, the nonsymmetric matrix equation is solved by Gauss-Doolittle decomposition, a direct method.

An iterative method, SSOR, is used for three-dimensional problems. This method is imbedded in the Newton-Raphson iteration. For a description of SSOR, see Wattenbarger and Thurnau (1976); for a more general case of block successive over-relaxation, see Woo and Emanual (1976). SSOR is similar to line successive over-relaxation in two dimensions for coupled equations, except that instead of solving each row implicitly, each vertical cross-section of the grid is solved implicitly. The three-dimensional equations have 14 unknowns per equation because pressure and saturation are solved simultaneously. For SSOR, the matrix is divided into blocks so that each slice has ten unknowns per equation. Hence, in this iterative scheme, ten coefficients are treated implicitly, and only four are treated explicitly. The bandwidth of the slice matrix equation for each slice is approximately four times the number of horizontal layers. Each of these matrix equations is solved using a banded Gauss-Doolittle method with normal ordering. Because SSOR is imbedded in the Newton-Raphson iteration, only linearized equations are solved. Therefore, the matrix decomposition for each slice is required only on the first iteration of each Newton-Raphson iteration. On subsequent SSOR iterations, only back substitution is necessary. In addition, because the SSOR is embedded in the Newton-Raphson iteration, the convergence criterion need not be small. The convergence is checked by calculating the following:

$$\delta p^* = \max \left| \frac{p_{ijk}^{m} - p_{ijk}^{m-1}}{p_{ijk}^{1} - p_{ijk}^{0}} \right| \quad \forall\ ijk \;, \tag{10}$$

and

$$\delta S^* = \max \left| \frac{S_{ijk}^{m} - S_{ijk}^{m-1}}{S_{ijk}^{1} - S_{ijk}^{0}} \right| \quad \forall\ ijk \;, \tag{11}$$

where the superscripts m, m-1, 1, and 0 refer to SSOR iteration levels and the subscripts i, j, and k refer to the grid block. A typical convergence criteria for δp^* and δS^* is 0.001 or less, which is usually reached in only six to 20 iterations. Although this tolerance may seem somewhat large, subsequent Newton-Raphson iterations usually provide continued convergence. Newton-Raphson iteration convergence is checked through the use of a mass balance on the NAPL. Convergence is considered acceptable when this mass balance is less than 0.01%.

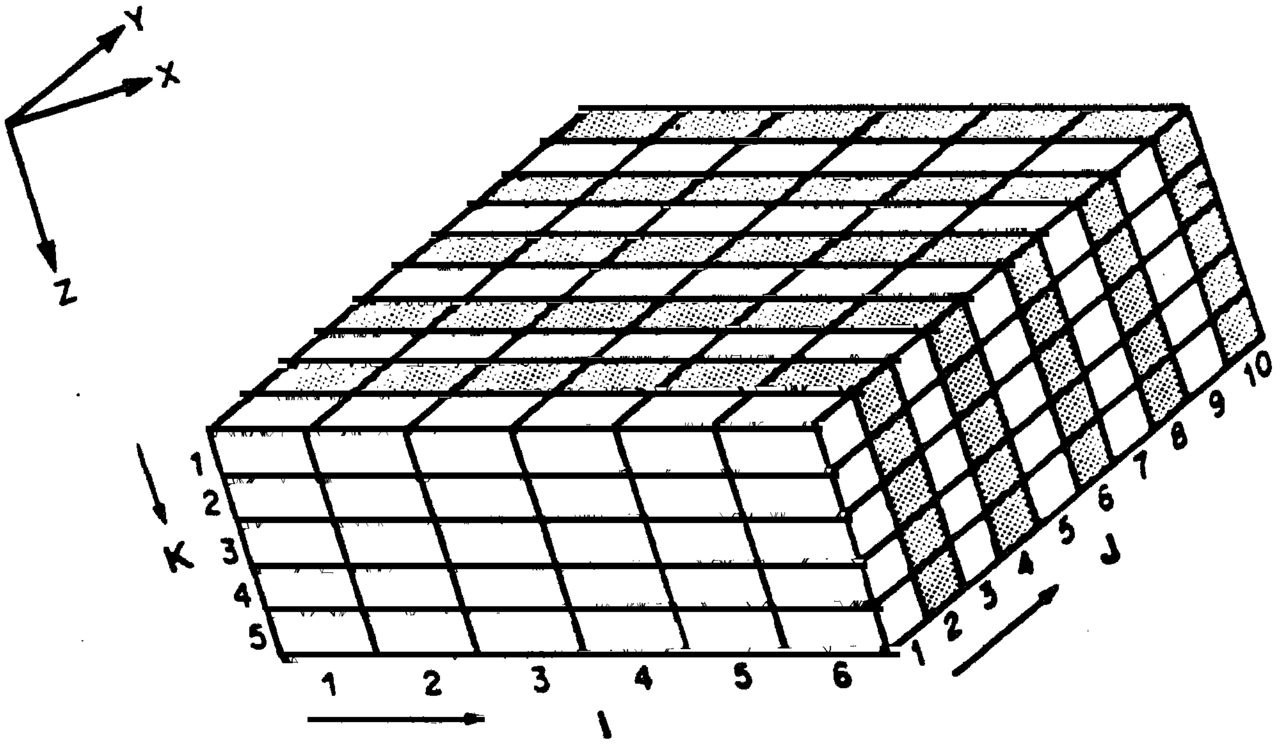
PARALLEL PROCESSING CAPABILITY

Typical three-dimensional applications require a large, fast computer. Most of the faster computers (super computers) achieve part of their speed from vectorized and/or parallel architecture. To take full advantage of super computer capabilities, the key element is structuring the numerical solution to match the architectural features of the computer design. Some increase in speed can be achieved by optimizing compilers but modifications to programming techniques and the numerical solution can provide further increases in efficiency. Peters (1988) discusses many of the features desirable in programming techniques for modeling of groundwater flow on vectorized computers.

The present computer model has been designed to run efficiently on both scaler computers and an inexpensive computer with a parallel-vector architecture. As described by Bethke et al. (1988), this latter computer contains six vector processors that share a common memory. Fast simulations are achieved by vector computations and concurrent processing among the six vector processors.

The bulk of the computational effort in solving a three-dimensional immiscible flow problem occurs in the solution of the nonsymmetric matrix equations arising from the SSOR method. To take advantage of parallel architecture, a modification to the conventional SSOR procedure was made. This modification is referred to as SSOR (ODD-EVEN). In conventional SSOR, the solution for each slice proceeds sequentially. After solution for slice (j), the right-hand side for slice (j+1) is updated based on new values of the unknown variables. On the other hand, the SSOR (ODD-EVEN) method permits concurrent solution of several slices. The slice matrix solution occurs in two steps. In the first step, the equations for the odd numbered slices are solved; in the second step, the equations for the even numbered slices are solved. This is shown schematically in Figure 1. Updating the right-hand side vectors is done at the end of each iterative sweep. In test problems and applications, we have observed little difference in the convergence rates between the conventional SSOR method and the modified method. Yet, for parallel architecture, the SSOR (ODD-EVEN) method produces a savings in computation time.

Figure 1. Schematic representation showing typical three-dimensional, finite-difference grid with alternate slices shaded for SSOR (ODD-EVEN).



APPLICATIONS

The model described in this paper has been verified and benchmarked using the same set of problems given in Faust (1985), with identical results. Therefore, the emphasis here is on illustrative applications of the model. These applications include (1) capillary and hydrodynamic barriers, (2) recovery of immiscible fluids at wells, and (3) three-dimensional flow of a dense immiscible fluid in groundwater. Applications one and three are based on the S-Area landfill, whereas the second application is based on the Hyde Park landfill. They are presented in the order of dimensions considered: (1) one-dimensional, Cartesian, (2) two-dimensional, cylindrical, and (3) three-dimensional, Cartesian.

CAPILLARY AND HYDRODYNAMIC BARRIERS

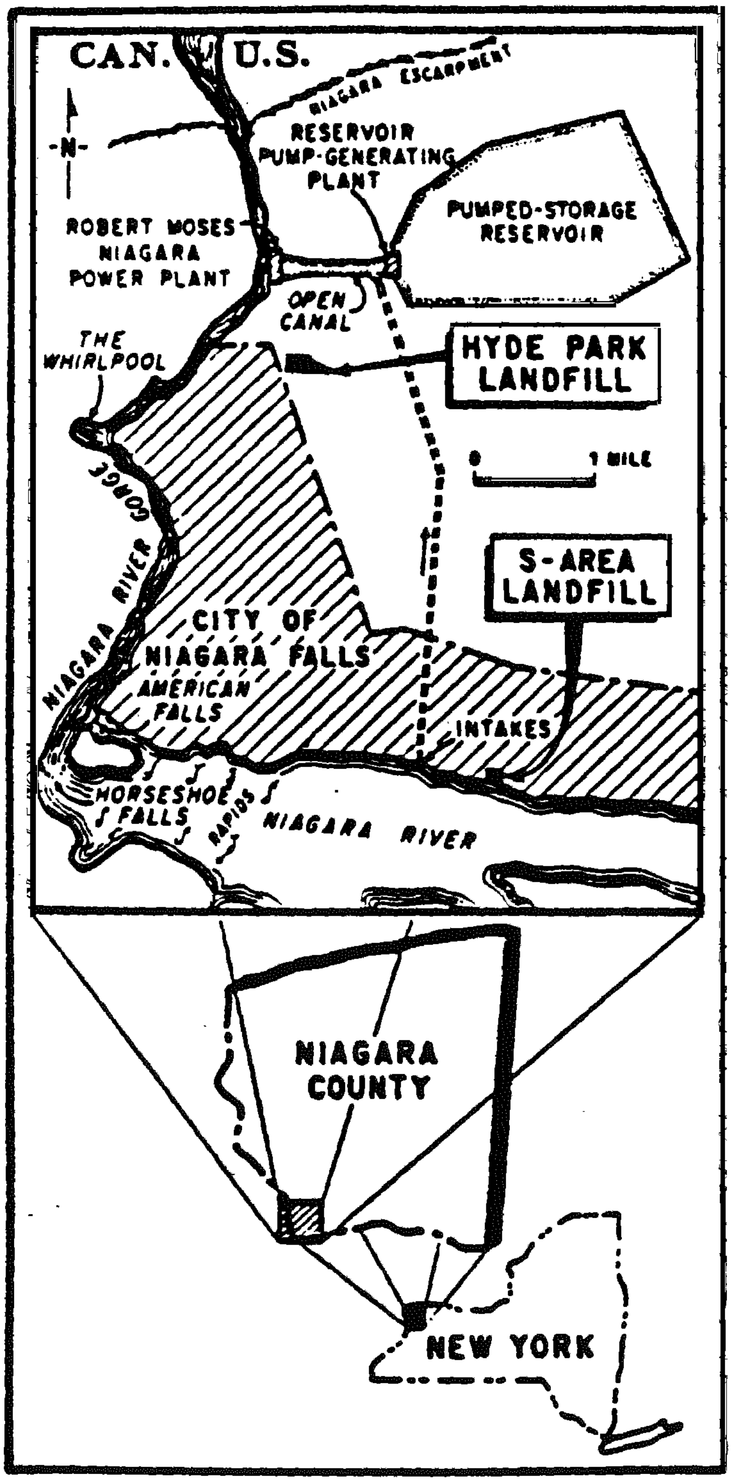
A one-dimensional, two-phase flow model was developed by Arthur D. Little (1983) (also see Guswa, 1985) to evaluate the effects of lithology-dependent capillary pressure functions, hydraulic gradients, and permeability variations on the migration of NAPL. The model was applied in a conceptual manner to the hydrogeologic setting of the S-Area landfill, Niagara Falls, New York (Figure 2).

The ADL model used the IMPES (IMplicit Pressure-Explicit Saturation) method to solve the two coupled equations of flow for an immiscible nonaqueous phase and water. The air phase is neglected. The ADL model also used a mesh-centered grid, whereas the model presented in this paper, referred to as SWANFLOW (Simultaneous Water And NAPL FLOW), uses a block-centered approach.

The NAPL found at S-Area has a specific gravity of approximately 1.5 and consists primarily of tri-, tetra-, and pentachlorobenzene, tetrachloroethylene, hexachlorocyclopentadiene, and octachlorocyclopentene (Guswa, 1985). These liquids have been observed in discrete discontinuous zones in the landfill. Geologic logs indicate a lithologic contact between unconsolidated glacial deposits and bedrock (Lockport Dolomite) at an elevation of about 541 feet. The base of the unconsolidated glacial deposits is a clay ranging in thickness from about 0.25 feet to 15 feet. The clay is overlain by a relatively thick (up to 16 feet) fine sand layer containing scattered zones of silt and fine gravel. This is overlain by about 14 feet of artificial fill. Bedrock water-level measurements indicate a potentiometric elevation of about 561 feet. Water levels measured in the overlying unconsolidated deposits indicate a positive head difference between the overburden and the underlying bedrock of between two and 5.5 feet. Under these conditions, therefore, a vertical downward flow component exists.

The objectives of the original simulations made by ADL (1983) were to assess the potential for downward migration of NAPL and to evaluate

Figure 2. Locations of the Hyde Park and S-Area landfills, Niagara Falls, New York.



remedial measures. The important results of the previous analysis and a comparison of the present model with the one-dimensional ADL (1983) model are summarized here.

To evaluate the potential for downward NAPL flow, a vertical column 23 ft long is divided into 24 blocks (nodes). The model was constructed with a two-foot negative head difference (downward flow) between the water table and bedrock potentiometric level. The domain contains three different porous materials. The upper twenty feet consists of a fine sand with a hydraulic conductivity of 10^{-5} cm/s ($k = 1.02 \times 10^{-14}$ m^2). The fine sand is underlain by one foot of clay ($K = 10^{-7}$ cm/s; $k = 1.02 \times 10^{-16}$ m^2). The clay is underlain by the Lockport Dolomite bedrock ($K = 10^{-3}$ cm/s; $k = 1.02 \times 10^{-12}$ m^2). The residual saturation values for water and NAPL were assumed to be 20 and 10 percent, respectively. Other simulation data are given in Tables 1 and 2.

The results show that a barrier to downward migration of NAPL is provided by capillary pressure differences between the sand and clay (Figure 3). This condition has been confirmed in recent field investigations at the S-Area site.

Figure 3 also provides a comparison between the results of the two numerical models. The saturations calculated by SWANFLOW and the ADL code at approximately 1350 d are shown. The results from the two models compare favorably; however, there are some differences, especially just above the clay layer. The differences are probably caused by some combination of instability in the IMPES technique, alternative gridding and time steps used in the two codes, and slight differences in the relative permeability relationships (the ADL [1983 model] provided for hysteresis in capillary pressure).

The effects of a water-phase hydraulic gradient on NAPL migration was also examined via these simulations, where the clay layer was assumed to be missing. As shown in Figure 4, the results of this series of simulations indicted that a minimum upward head difference of nine feet between the water-table elevation and bedrock potentiometric level in the vicinity of a clay layer discontinuity could be sufficient to prevent downward migration of NAPL into the bedrock (Guswa, 1985). This figure shows NAPL saturations at about 250 d. As shown, there is a noticeable upward movement of NAPL. Data are currently being collected as part of a remedy designed to lower the hydraulic head in the overburden sand. This data will be used to confirm the remedy as well as modeling results.

RECOVERY OF IMMISCIBLE FLUIDS AT WELLS

In this section, an analysis of two-dimensional radial flow of NAPL to a recovery well is presented. A discrete sensitivity analysis is used to determine the effectiveness of a single, low-rate recovery well. The significance of effective porosity, permeability, relative permeability, NAPL viscosity, and location of the pumping interval were

Table 1. Capillary pressure and relative permeability data for ADL simulation 1 (Arthur D. Little, Inc., 1983).

Capillary Pressure (N/m^2)	Water Saturation	Relative Permeabilities Water	NAPL
		Fine sand and bedrock	
103425.0	0.00	0.00000	1.00000
103425.0	0.10	0.00000	0.82000
103425.0	0.20	0.00000	0.68000
27580.0	0.30	0.04000	0.55000
10343.0	0.40	0.10000	0.43000
7585.0	0.50	0.18000	0.31000
7447.0	0.60	0.30000	0.20000
7309.0	0.70	0.44000	0.12000
7171.0	0.80	0.60000	0.05000
7033.0	0.90	0.80000	0.00000
6895.0	1.00	1.00000	0.00000
		Clay	
206850.0	0.00	0.00000	1.00000
206850.0	0.10	0.00000	0.82000
206850.0	0.20	0.00000	0.68000
165480.0	0.30	0.04000	0.55000
134453.0	0.40	0.10000	0.43000
110320.0	0.50	0.18000	0.31000
93082.0	0.60	0.30000	0.20000
82740.0	0.70	0.44000	0.12000
75845.0	0.80	0.60000	0.05000
72398.0	0.90	0.80000	0.00000
68950.0	1.00	1.00000	0.00000

Table 2. Data used in ADL simulation 1.

Parameter	Value
Porosity	0.2
Permeability:	
Fine sand	1.02×10^{-14} m^2
Clay	1.02×10^{-16} m^2
Bedrock	1.02×10^{-12} m^2
Density of water	1000 kg/m^3
Density of NAPL	1500 kg/m^3
Water viscosity	0.001 kg/m-s
NAPL viscosity	0.001 kg/m-s
Δz	0.3048 m

Figure 3. NAPL saturation profiles at one time for the three-layer simulation.

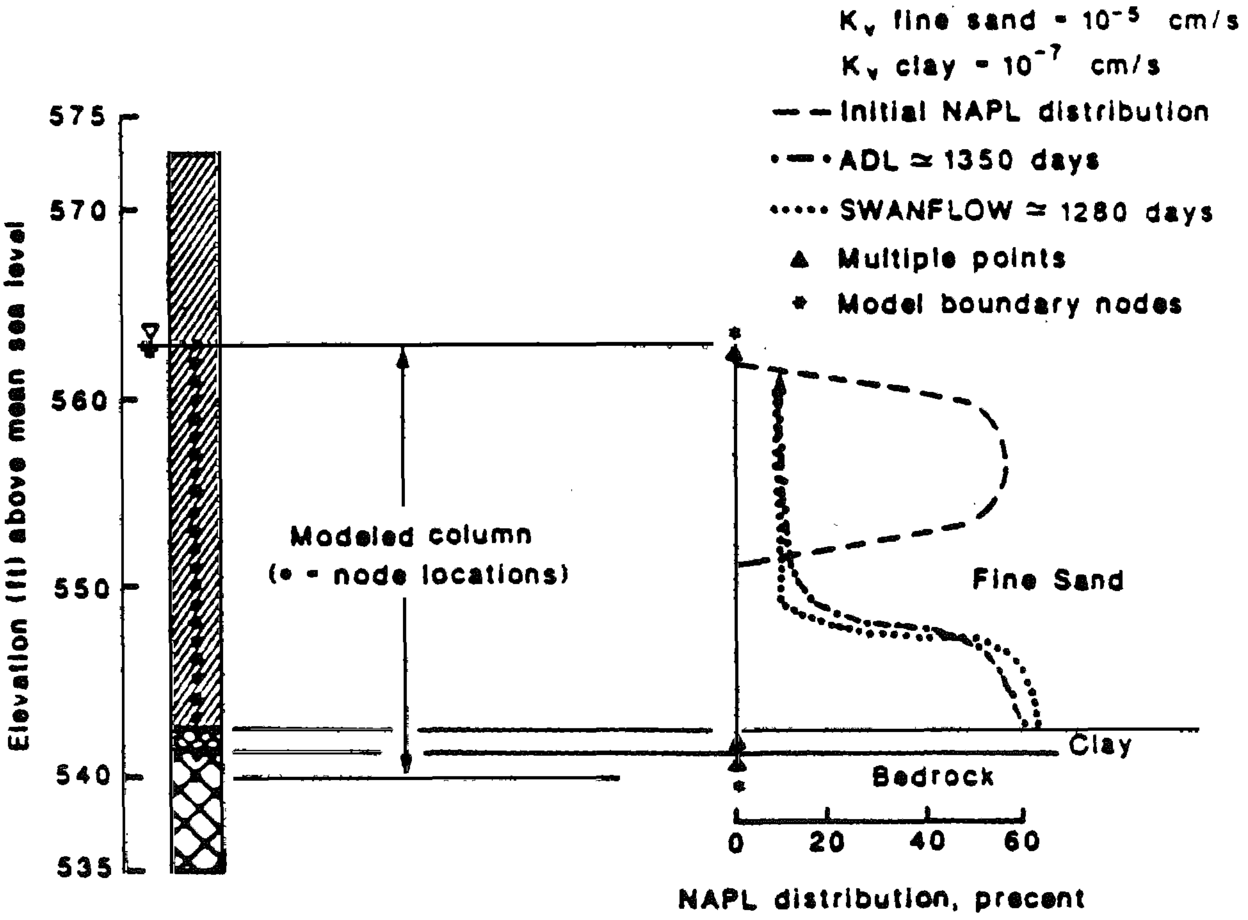
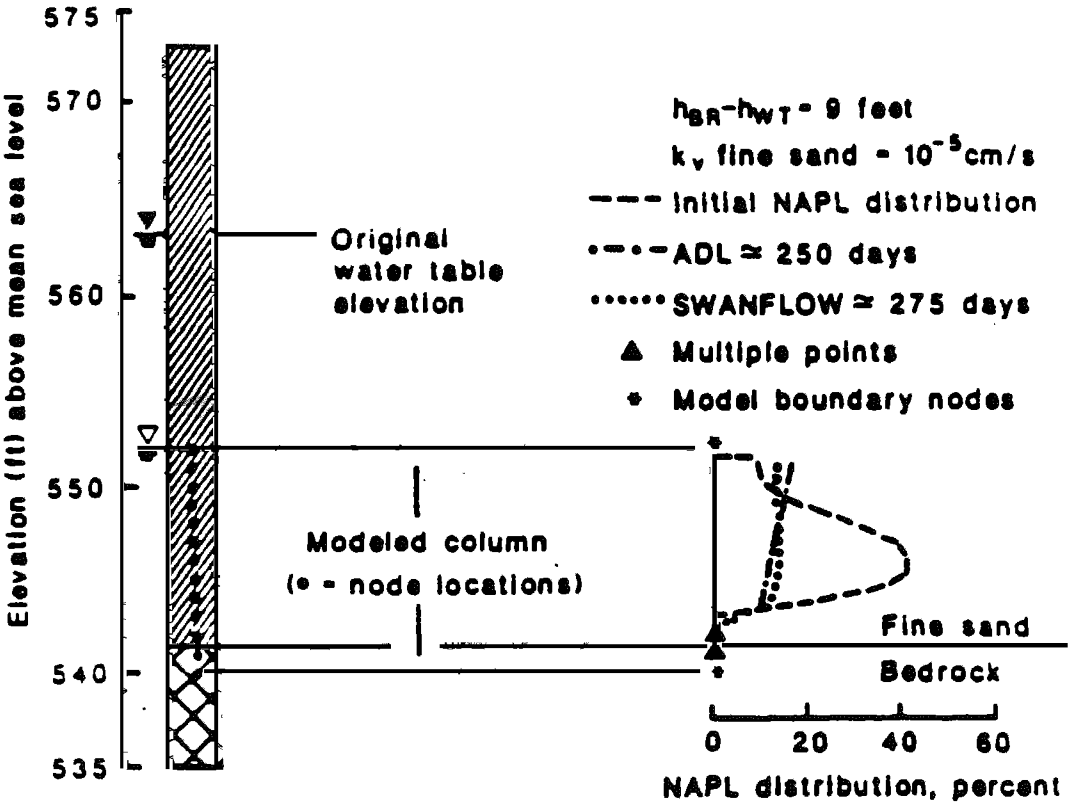


Figure 4. NAPL saturation profiles at one time for the two-layer simulation.



considered in the sensitivity analysis. The results of the study (GeoTrans, 1984) were applied in a conceptual manner to conditions existing at the Hyde Park Landfill, Niagara Falls, New York (Figure 2). The conceptual framework for this analysis includes: (1) description of the geometry of the system; (2) hydrologic conditions (fluid pressures and fluid saturations); (3) hydrologic boundary conditions; (4) fluid properties; and (5) hydrologic properties of the media.

Sufficient data are not available to quantify each of the above elements. Field observations indicate that both the properties of NAPL and the properties of the Lockport Dolomite (the bedrock formation underlying the Hyde Park landfill) have wide spatial variability. Table 3 summarizes the major assumptions used in the simulations and knowledge of the corresponding conditions. As can be seen from this table, the conceptual framework is an idealized description of the site. The simplifications are reasonable given the lack of data and the limited goal of the analysis (to address the sensitivity of various assumptions and parameters on NAPL recovery).

The idealized stratigraphy used in the simulations is shown in Figure 5. The Lockport Dolomite is subdivided into four hydraulic zones. The uppermost layer (9.36 m thick) is the upper permeable zone of the Lockport Dolomite. A less permeable zone (15.6 m thick) underlies the upper zone. Next are the Gasport Member (2.19 m thick) and the Decew Member (3.50 m thick). The Gasport Member acts as an aquitard with low permeability. The Decew Member has similar hydraulic properties to those in the 15.6-m thick zone of the Lockport Dolomite. In the vicinity of Hyde Park, the Lockport Dolomite is overlain by 10 to 30 feet of low permeability glacial deposits and underlain by the low-permeability Rochester Shale.

The finite-difference grid has 20 columns and 10 layers. The upper three layers correspond to the upper zone, layers 4 through 8 correspond to the lower zone, layer 9 is the Gasport Member, and layer 10 is the Decrew Member. The spacing between adjacent columns increases in size by a factor of 1.76 from the column adjacent to the well. The center of the first column is 0.305 m from the center of the well and the well radius is 0.153 m.

The fluid properties include the density and viscosity of water and NAPL. The density and viscosity of water are the same for all simulations (density = 1000 kg/m^3 and viscosity = 0.001 kg/m-s). The density of NAPL is 1216 kg/m^3 for all simulations, but a range of viscosities from 0.01 to 1.0 kg/m-s is tested in the sensitivity analysis.

The saturation-dependent properties are capillary pressure and relative permeability. Data for both water-NAPL and air-NAPL are required. Three alternative sets are used (Table 4). Data set 1 corresponds to the water-NAPL data used by Occidental Chemical Corporation (1984). The second data set is similar to the first except the residual saturation of the NAPL is 0.2 rather than 0.1. The third

Table 3. Major assumptions, probable conditions, and significance of assumptions in the analysis of pumping well recovery.

Assumption	Probable Conditions	Significance
Horizontal hydrologic units of uniform thickness.	General bedrock dip of about 0.01 in Hyde Park vicinity, units of variable thickness.	Effect should not be significant on near well performances.
Fluid pressures and saturations vary with depth but not horizontally.	Fluid pressures and saturations vary with depth and horizontally.	Effect on near well performance should be small, results will tend to predict higher NAPL recoveries if significant.
Constant pressures and saturations maintained at outer radius of 2,000 m.	Seep boundaries at Gorge Place and constant pressure boundaries at Forbay Canal, Niagara River, and buried conduits.	Effect on near well performance should be small, can be evaluated by examination of results.
No-flow boundaries are maintained at top and base of Lockport.	Recharge at top of Lockport and leakage to underlying Rochester shale are significant.	Horizontal flow to the well will dominate water and NAPL migration near the well.
Fluid properties are uniform for each run.	NAPL viscosity is highly variable, NAPL density is variable but generally greater than water density.	Viscosity variability tested with sensitivity analysis, density effects should be less significant.
Hydrologic properties are uniform in each layer, but variable with depth.	Hydrologic properties vary with depth and horizontally.	Tested with sensitivity analysis.

Figure 5. Idealized stratigraphy used in the radial example problem.

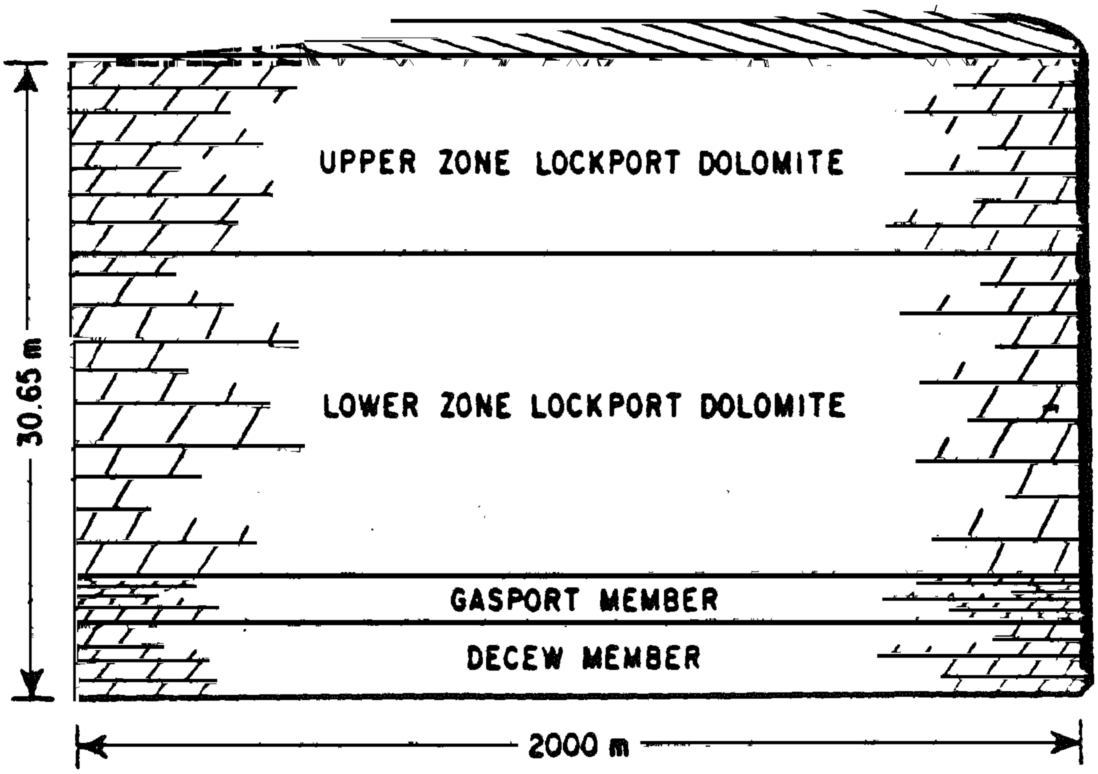


Table 4. Capillary pressure and relative permeability data used in two-phase simulations; capillary pressure in N/m^2; all other terms dimensionless.

Data Set 1

p_c	S_w	k_{rw}	k_{rn}
103425.0	0.00	0.00000	1.00000
103425.0	0.10	0.00000	0.82000
103425.0	0.20	0.00000	0.68000
27580.0	0.30	0.04000	0.55000
10343.0	0.40	0.10000	0.43000
7585.0	0.50	0.18000	0.31000
7447.0	0.60	0.30000	0.20000
7309.0	0.70	0.44000	0.12000
7171.0	0.80	0.60000	0.05000
7033.0	0.90	0.80000	0.00000
6895.0	1.00	1.00000	0.00000

$k_{rnw} = 0.680$

$p_{c_{an}}$	S_a	k_{rn}	k_{ra}
-98000.0	1.00	-0.3200	1.000
0.0	0.00	0.6800	0.000

(Continued)

(Table 4 continued)

Data Set 2

P_c	S_w	k_{rw}	k_{rn}
103425.0	0.00	0.00000	1.00000
103425.0	0.10	0.00000	0.80000
103425.0	0.20	0.00000	0.60000
27580.0	0.30	0.04000	0.44000
10343.0	0.40	0.10000	0.30000
7585.0	0.50	0.18000	0.18000
7447.0	0.60	0.30000	0.10000
7309.0	0.70	0.44000	0.04000
7171.0	0.80	0.60000	0.00000
7033.0	0.90	0.80000	0.00000
6895.0	1.00	1.00000	0.00000

$k_{rnw} = 0.600$

$P_{c_{an}}$	S_a	k_{rn}	k_{ra}
-98000.0	1.00	0.0000	1.000
-88200.0	0.90	0.0000	0.900
-78400.0	0.80	0.0000	0.800
-68600.0	0.70	0.0000	0.700
-58800.0	0.60	0.0000	0.600
-49000.0	0.50	0.1000	0.500
-39200.0	0.40	0.2000	0.400
-29400.0	0.30	0.3000	0.300
-19600.0	0.20	0.4000	0.200
-9800.0	0.10	0.5000	0.100
0.0	0.00	0.6000	0.000

(Continued)

(Table 4 continued)

Data Set 3

p_c	S_w	k_{rw}	k_{rn}
103425.0	0.00	0.00000	1.00000
103425.0	0.10	0.00000	0.62430
103425.0	0.20	0.00000	0.36600
27580.0	0.30	0.00024	0.19750
10343.0	0.40	0.00390	0.09530
7585.0	0.50	0.19800	0.03900
7447.0	0.60	0.06250	0.01230
7309.0	0.70	0.15230	0.00240
7171.0	0.80	0.31640	0.00015
7033.0	0.90	0.58620	0.00000
6895.0	1.00	1.00000	0.00000

$k_{rnw} = 0.366$

$p_{c_{an}}$	S_a	k_{rn}	k_{ra}
-98000.0	1.00	0.0000	1.000
-88200.0	0.90	0.0000	0.900
-78400.0	0.80	0.0000	0.800
-68600.0	0.70	0.0000	0.700
-58800.0	0.60	0.0520	0.600
-49000.0	0.50	0.1050	0.500
-39200.0	0.40	0.1570	0.400
-29400.0	0.30	0.2040	0.300
-19600.0	0.20	0.2620	0.200
-9800.0	0.10	0.3140	0.100
0.0	0.00	0.3660	0.000

data set is based on a fourth-order relationship between relative permeability and saturation, whereas the first two sets correspond to parabolic relationships. Also shown in Table 4 are the relative permeability and capillary pressure relationships for the air-NAPL system. These data are required under conditions where pumping causes the aquifer to become unconfined.

The hydraulic properties include permeabilities in the radial and vertical directions and effective porosities. Radial (horizontal) permeabilities were varied between 3.6 and 8.85 x 10^{-12} m^2, except that 3.6×10^{-14} m^2 was used for the Gasport Member in some simulations. The vertical permeability is either 0.01 or 0.001 times that of the horizontal permeability. The effective porosity of the fractured dolomite was varied over a range of 0.001 to 0.1.

The initial pressures and saturation used in all simulations are given in Table 5. The pressures are specified for the middle of each grid block and are based on a static water level in the bedrock of 4.5 ft above the top of the Lockport Dolomite. Hydrostatic increases with depth are assumed in computing pressures with depth. The pressures are uniform in each horizontal layer. The hydrostatic pressure assumption neglects the downward component of flow in the Lockport Dolomite, but under pumping conditions, horizontal flow of water will dominate.

The boundary conditions are no-flow at the top and base of the Lockport Dolomite, constant pressures and saturations at the outer radius (2,000 m from the well), and specified flow rate for the well. The specified flow rate applies to the total flow to the well. The total flow rate is allocated among layers on the basis of layer mobilities. The mobility of a layer is given by the following:

$$f = k \left[\frac{k_{rw}\rho_w}{\mu_w} + \frac{k_{rn}\rho_n}{\mu_n}\right] \Delta z \qquad (12)$$

in which f is the mobility, Δz is the layer thickness, and other terms have been defined previously. If the well is not open to a particular layer, its mobility is assumed to be zero.

The results of 39 simulations are given in Table 6. Also shown in Table 6 are the values of fluid properties, hydraulic properties, and pumping rates specified. The first 24 runs considered the variation in viscosity, relative permeability and capillary pressures, permeability, degree of anisotropy, and effective porosity using the most simplified geometry, i.e., the same properties for all four hydraulic layers. The well was assumed open throughout the Lockport Dolomite and pumped at a rate of 1.2680 kg/s, which is equivalent to 20 gal/min for water. Two performance measures are of interest: the total amount of NAPL recovered and the ratio of NAPL to total fluid recovered. The duration

Table 5. Initial conditions used in two-phase simulations.

Row	Depth (m)	NAPL pressure (N/m^2)	Water saturation (dimensionless)
1	1.562	27193.0	0.7838
2	4.686	57976.0	0.6769
3	7.810	88253.0	0.6012
4	10.934	119530.0	0.5564
5	14.058	159370.0	0.5092
6	17.182	182310.0	0.4598
7	20.306	216330.0	0.3911
8	23.430	251740.0	0.3644
9	26.090	282490.0	0.3379
10	28.940	315870.0	0.3020

Table 6. Results of two-phase flow simulations for a single pumping well.

Run Number	Time Steps	Time (days)	Viscosity (kg/m-s)	K_r-P_c Table Number	k (10^{-12} xm^2)	Ratio K_x:k_z	Porosity	Pumping Rate (kb/s)	NAPL Extracted (kg)	Water Extracted (kg)	Ratio NAPL (NAPL water)
1	28	180.0	0.50	1	8.850	100:1	0.030	1.2680	0.7151E 05	0.1965E 08	0.3627E
2	28	180.0	0.50	2	8.850	100:1	0.030	1.2680	0.4791E 05	0.1967E 08	0.2430E
3	--	-----	0.50	3	8.850	100:1	0.030	1.2680	-----	-----	-----
4	28	180.0	0.05	1	8.850	100:1	0.030	1.2680	0.6778E 06	0.1904E 08	0.3435E
5	28	180.0	0.05	2	8.850	100:1	0.030	1.2680	0.4657E 06	0.1925E 08	0.2862E
6	--	-----	0.05	3	8.850	100:1	0.030	1.2680	-----	-----	-----
7	28	180.0	0.10	1	8.850	100:1	0.030	1.2680	0.3487E 06	0.1937E 08	0.1769E
8	28	180.0	1.00	1	8.850	100:1	0.030	1.2680	0.3587E 05	0.1968E 08	0.1819E
9	28	180.0	0.10	1	8.850	100:1	0.030	1.2680	0.2859E 07	0.1686E 08	0.1450E
10	28	180.0	0.50	1	8.850	1000:1	0.030	1.2680	0.7165E 05	0.1965E 08	0.3634E
11	28	180.0	0.50	1	8.850	100:1	0.100	1.2680	0.7164E 05	0.1965E 08	0.3633E
12	28	180.0	0.50	1	8.850	1000:1	0.100	1.2680	0.7166E 05	0.1965E 08	0.3635E
13	28	180.0	0.50	1	8.850	100:1	0.010	1.2680	0.7116E 05	0.1965E 08	0.3609E
14	28	180.0	0.50	1	8.850	1000:1	0.010	1.2680	0.7161E 05	0.1965E 08	0.3632E
15	28	180.0	0.50	1	8.850	100:1	0.001	1.2680	0.6778E 05	0.1965E 08	0.3438E
16	28	180.0	0.50	1	8.850	1000:1	0.001	1.2680	0.7115E 05	0.1965E 08	0.3609E
17	47	180.0	0.50	1	3.605	100:1	0.100	1.2680	0.8817E 05	0.1963E 08	0.4472E
18	60	25.97	0.50	1	3.605	1000:1	0.100	1.2680	0.1185E 05	0.2833E 07	0.4164E-
19	--	-----	0.50	1	3.605	100:1	0.030	1.2680	-----	-----	-----
20	60	1.875	0.50	1	3.605	1000:1	0.030	1.2680	0.8384E 03	0.2046E 06	0.4082E
21	--	-----	0.50	1	3.605	100:1	0.010	1.2680	-----	-----	-----
22	--	-----	0.50	1	3.605	1000:1	0.010	1.2680	-----	-----	-----
23	60	0.1245	0.50	1	3.605	100:1	0.001	1.2680	0.4482E 02	0.1962E 05	0.3286E-
24	60	0.06944	0.50	1	3.605	1000:1	0.001	1.2680	0.2121E 02	0.7598E 04	0.2788E-
25	28	180.0	0.50	1	3.605	100:1	0.030	0.2536	0.1421E 05	0.3929E 07	0.3608E-
26	28	180.0	0.50	1	3.605	100:1	0.030	0.5072	0.1857E 05	0.8758E 07	0.3628E-
27	29	180.0	0.50	1	3.605	100:1	0.030	0.7608	0.4594E 05	0.1187E 08	0.3883E-
28	29	180.0	0.50	1	3.605	100:1	0.030	1.0144	0.6513E 05	0.1571E 08	0.4129E-
29	--	-----	0.50	1	3.605	100:1	0.030	1.2680	-----	-----	-----

Table 6 (cont'd) Results of two-phase flow simulations for a single pumping well.

Run Number	Time Steps	Time (days)	Viscosity (kg/m-s)	K_r-P_c Table Number	k (10^{-12}xm^2)	Ratio K_x:k_z	Porosity	Pumping Rate (kb/s)	NAPL Extracted (kg)	Water Extracted (kg)	Ratio NAPL (NAPL water
30	28	180.0	0.50	1	8.850	100:1	0.030	0.3170	0.1137E 06	0.4816E 07	0.2307
31	28	180.0	0.50	2	8.850	100:1	0.030	0.3170	0.8009E 05	0.4840E 07	0.1807
32	28	180.0	1.00	1	8.850	100:1	0.030	0.3170	0.5822E 05	0.4871E 07	0.1181
33	28	180.0	0.01	1	8.850	100:1	0.030	0.3170	0.3071E 07	0.1858E 07	0.6230
34	28	180.0	0.50	1	8.850	100:1	0.100	0.3170	0.1162E 06	0.4813E 07	0.2357
35	28	180.0	0.50	1	8.850	100:1	0.001	0.3170	0.1337E 06	0.4796E 07	0.2718
36	29	180.0	0.50	1	(u) 8.850	100:1	0.030	1.2680	0.4438E 05	0.1967E 08	0.2251
				1	(l) 3.605	100:1	0.010				
				1	(g) 0.03605	1:1	0.010				
				1	(d) 3.605	100:1	0.010				
37	28	180.0	0.50	1	(u) 8.850	100:1	0.030	0.3170	0.9193E 05	0.4837E 07	0.1865
				1	(l) 3.605	100:1	0.010				
				1	(g) 0.03605	1:1	0.010				
				1	(d) 3.605	100:1	0.010				
38	30	180.0	0.01	1	(u) 8.850	100:1	0.030	0.3170	0.2832E 07	0.2097E 07	0.5746E
				1	(l) 3.605	100:1	0.010				
				1	(g) 0.03605	1:1	0.010				
				1	(d) 3.605	100:1	0.010				
39	28	180.0	0.05	1	(u) 8.850	100:1	0.030	0.3170	0.7846E 06	0.4145E 07	0.1592E
				1	(l) 3.605	100:1	0.010				
				1	(g) 0.03605	1:1	0.010				
				1	(d) 3.605	100:1	0.010				

u - Upper Lockport
l - Lower Lockport
g - Gasport
d - Decew

of pumping was 180 days or about half a year. The amount of NAPL recovered during that period ranged from zero to 2,860,000 kg (3,150 tons). The value of zero corresponded to those conditions in which the specified flow rate caused significant dewatering of the aquifer near the well. This occurred for the lower permeability estimates and the relative permeability data based on the fourth-order expression (data set 3). The high value corresponded to the case of low NAPL viscosity (0.01 kg/m-s). The total recovery of NAPL for a viscosity of (0.5 kg/m-s) was 71,500 kg (78.7 tons). The ratios of NAPL recovered to total fluid recovered ranged from 0.0018 to 0.145. Again, the high ratio corresponded to the low viscosity case.

In the first set of 24 runs, it was found that a 20 gpm (1.268 kg/s) pumping rate could not be maintained for the lower permeability cases. The next five runs (25 through 29) correspond to run #19 except that lower pumping rates were assumed corresponding to 4, 8, 12, 16, and 20 gpm. The results showed that for the lower permeability (3.6×10^{-12} m^2), a flow rate of 16 gpm (1.01 kg/s) could be sustained without causing adverse drawdowns near the wells.

The next series of simulations (30 through 35) investigated the effect of pumping from zones that contain the highest amount of NAPL. It was assumed that the pumping well was cased down to 3.5 m above the base of the Lockport Dolomite and only open to the bottom 3.5 m. The NAPL saturation at that level is initially about 0.70. Runs 30, 31, 32, 33, 34, and 35 correspond to runs 1, 2, 8, 9, 11, and 13 except for the interval of the producing zone. In each case, the amount of NAPL recovered was significantly greater for the well open only to the lowest 3.5 m of the Lockport Dolomite. This occurred even though the pumping rate was reduced to 5 gpm (0.317 kg/s).

The final four runs were similar to previous runs except that the properties of the four hydraulic layers varied. Higher values of permeability and effective porosity were assigned to the upper zone in the Lockport Dolomite. Intermediate values were assigned to the lower zone in Lockport Dolomite and Decrew Member. The Gasport Member was assigned a very low value of horizontal permeability. For run 36, a viscosity of 0.5 kg/m-s was used and pumping occurred from all zones at a total rate of 1.268 kg/s (20 gpm). This run is similar to run 1. With the lower permeability/porosity zones, however, both the amount of NAPL recovered and the ratio of NAPL recovered to total fluid recovered were significantly lower. The final three simulations (37 through 39) assumed that the pumping zone was the bottom 8.81 m of the Lockport Dolomite and that the pumping rate was 0.317 kg/s (5 gpm). Again, optimal placement of the recovery interval leads to greater recovery at reduced pumping rates.

THREE-DIMENSIONAL FLOW OF A DENSE IMMISCIBLE FLUID IN GROUNDWATER

The final problem provides an example of a fully three-dimensional flow field in which both NAPL and water are present. This conceptual application was performed for the S-Area Landfill in Niagara

Falls, New York (Figure 2). One concern at the S-Area site was whether NAPL known to be leaking into the bedrock aquifer could migrate significant distances from the site, particularly down-dip toward the Niagara River and the Canadian border.

The conceptual model (GeoTrans, 1985) of this problem consists of a landfill leaking NAPL into a uniform groundwater flow field. The Lockport Dolomite aquifer underlying S-Area consists of two distinct zones, an upper permeable zone and a lower less permeable zone. The upper zone is 5-m thick and is represented in the model as one layer. The lower zone is discretized into three layers. The layer thicknesses and aquifer properties are given in Table 7. The finite-difference grid is shown in Figure 6, where a vertical exaggeration of ten was used in the perspective diagram. The aquifer dips at an angle of 3.5 degrees (30 ft/mile) counter to the regional hydraulic gradient of 0.0067 m/m. The NAPL has the same viscosity as water; however, the density is 50 percent greater than that of water. The capillary pressure/relative permeability curves are the same as those listed in Table 4. Data set 1 is used for layer 1 and data set 3 is used for the lower layers.

The problem was simulated in two steps. The first step consisted of establishing a steady-state flow field based on the boundary conditions. These steady-state pressures then served as initial conditions (along with water saturations of 1.0) for the transient simulation. The transient simulation consisted of two periods. During the first period (30.8 years), leakage of NAPL into the aquifer is assumed to be 100,000 kg/yr. Because the model takes advantage of symmetry to reduce by half the number of grid blocks, the modeled source rate is 50,000 kg/yr. During the second period, the leakage of NAPL into the aquifer from the landfill is assumed to be negligible (in response to landfill containment examined in the first application of this paper).

The results of the simulations are illustrated in Figure 7, which shows a series of NAPL saturation distributions (vertical sections through the center of the source area and aligned with the direction of bedrock dip). The saturation sections show that the NAPL migrates away from the source in all directions, but has a strong tendency to sink to the base of the aquifer. Highest saturations occur in the lower part of the aquifer because of the differences in the assumed relative permeability functions. In particular, the relative permeability of NAPL is higher at lower saturations in the uppermost modeled layer.

In addition to the three-dimensional simulation just described, three alternative two-dimensional simulations were performed. The purpose of these simulations was to determine whether the three-dimensional problem could reasonably be approximated by a two-dimensional model. The first alternative simulation considered flow only in the uppermost permeable portion of the Lockport Dolomite. The second and third simulations allowed flow to occur through the entire thickness of the Lockport Dolomite. Only the assumed relative

Table 7. Data used in the three-dimensional flow example.

Parameter	Value
Porosity - layer 1	0.1
Porosity - lower layers	0.01
Rock compressibility	1×10^{-7} m^2/N
k_x - layer 1	1.02×10^{-11} m^2
k_y - layer 1	1.02×10^{-11} m^2
k_z - layer 1	1.02×10^{-13} m^2
k_x - lower layers	1.02×10^{-12} m^2
k_y - lower layers	1.02×10^{-12} m^2
k_z - lower layers	1.02×10^{-14} m^2
Density of water	1,000 kg/m^3
Density of NAPL	1,500 kg/m^3
Viscosity of water	0.001 kg/m-s
Viscosity of NAPL	0.001 kg/m-s
Number of columns (x-direction)	23
Number of slices (y-direction)	9
Number of layers (z-direction)	4

Figure 6. Perspective diagram of finite-difference grid used in the three-dimensional example application.

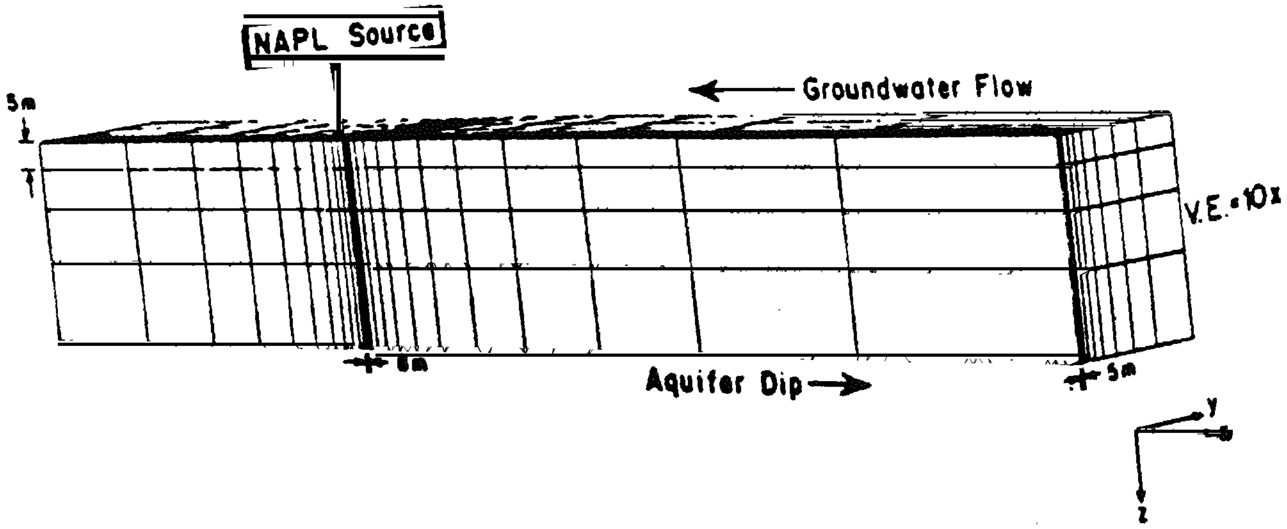
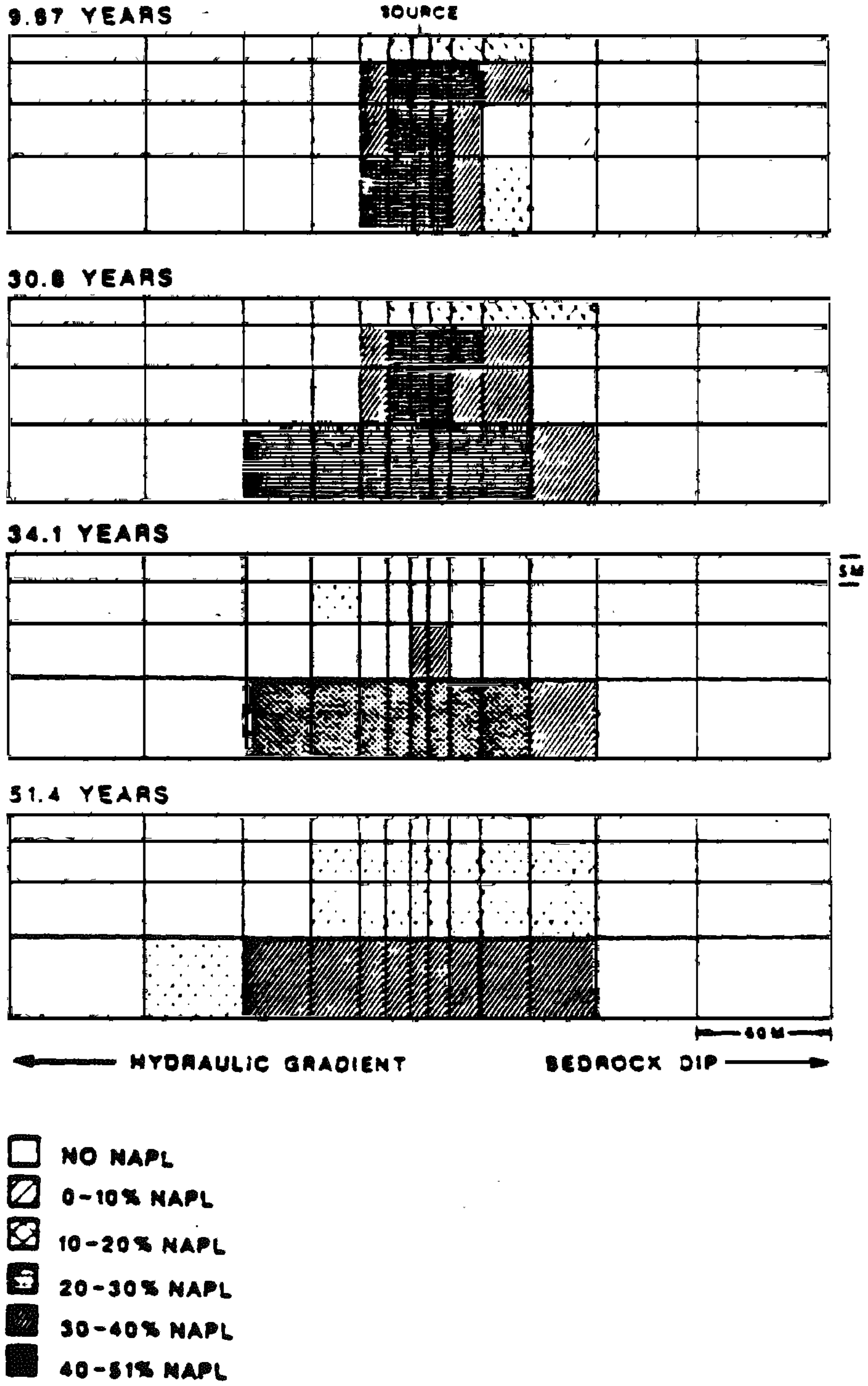


Figure 7. NAPL saturation distribution with time in vertical section through the center of the source area and aligned with the direction of bedrock dip.



permeability functions were different in these latter two simulations (data set 1 and data set 3 in Table 4). For the full thickness simulations, permeability and porosity data were vertically averaged over the thickness of the Lockport Dolomite ($k_x = k_y = 2.24 \times 70^{-12}$ m^2 and $\phi = 0.022$). The results of the two-dimensional simulations are compared with the results of the three-dimensional simulation in Figures 8 and 9. Predicted saturations for each of the simulations are plotted along the center line of landfill and in the direction of bedrock dip. Averaged saturations (on a pore volume basis) from the three-dimensional simulation are used for comparison to computed saturations from the two-dimensional simulations. None of the two-dimensional profiles compare favorably with the three-dimensional profile. For this example, the three-dimensional aspects and heterogeneity must be simulated directly.

PARALLEL PROCESSING BENCHMARK RESULTS

The three-dimensional example discussed above was used as a benchmark problem for evaluating the efficiency gained by vector and parallel processing. The results of the benchmarking are strictly meaningful only for the grid size and numerical criteria (convergence, number of SSOR iterations, and number of nonlinear iterations) specific to this example. However, the results provide a relative sense of the practical range of speed-up that can be achieved by vector and parallel processors. Furthermore, this particular example demonstrates the limitations of relying solely on optimizing compilers to enhance execution speed.

The benchmark results (summarized in Table 8) show computer processing times in seconds (CPU) for four alternately optimized versions of the model. In terms of the total execution time, the scaler version is about 12 times slower than the vector/parallel version (optimized by compiler with solution modifications) and about four times slower than the vectorized (by compiler only) version. The results of the version that included automatic compiler optimization for concurrency (parallel processing) and vectorization were actually slower than the results of the vectorized-only version.

The benchmarking results also indicate the relative amount of time required for major computation tasks (or subroutines) in the model. The major subroutines in the program (in terms of computational effort) include: SOLVE - performs Gauss-Doolittle decomposition, forward elimination, and back substitution on banded nonsymmetric matrix equation for each slice; FORMR - computes righthand side for slice matrix equation for each SSOR iteration; FORMEQ - computes lefthand side matrix for each slice, once for each Newton-Raphson iteration; UPDATE - updates unknown values of the matrix equation after each SSOR iteration; and PRPTY - computes nonlinear coefficients after each Newton-Raphson iteration. In the scaler version, SOLVE used 67.5% of the total CPU time (143.01) seconds. The automatically vectorized version reduced CPU time for SOLVE to 22.52 seconds, a speed-up factor of 6.35. The compiler optimized version for both vectorization and

Figure 8. NAPL saturation profiles for 9.9 years of leakage; through source area and aligned with the direction of bedrock dip: results for four alternative simulations.

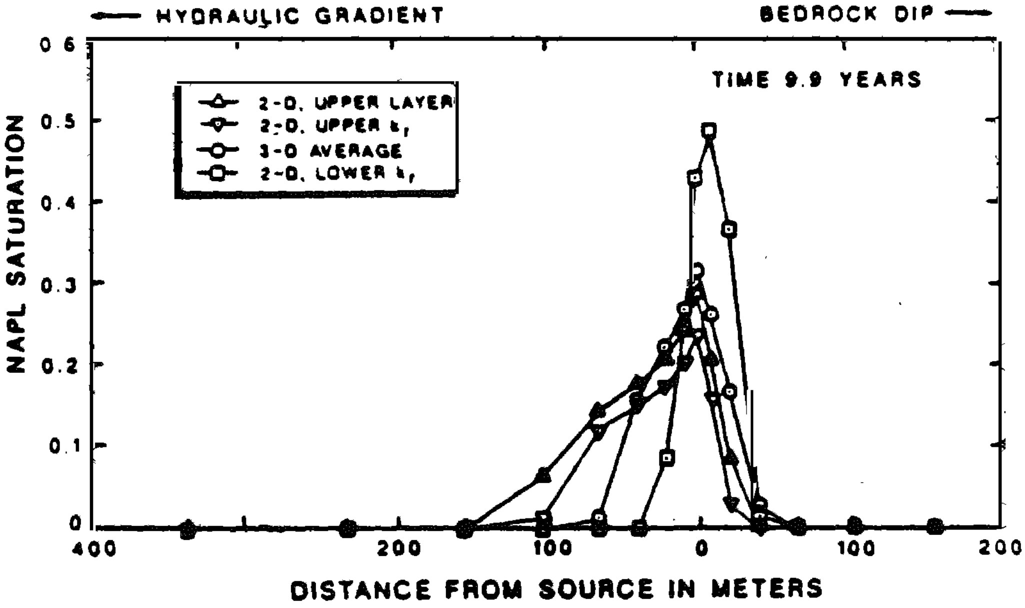


Figure 9. NAPL saturation profiles for 30.8 years of leakage; through source area and aligned with the direction of bedrock dip: results for four alternative simulations.

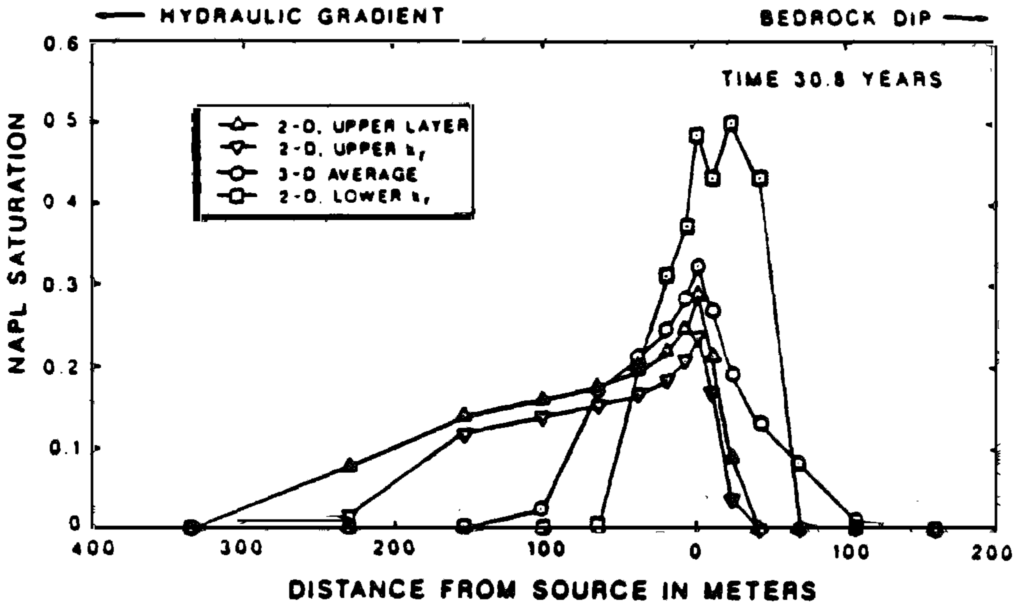


Table 8. Results (CPU time in seconds) of benchmarking four alternately optimized versions of the numerical model.

Version	SOLVE (2232)	FORMR (2160)	FORMEQ (72)	UTDAT (2160)	PRPTY (9)	TOTAL Program*
Scaler	143.01 67.5%	42.44 20.0%	11.54 5.4%	9.54 4.5%	1.12 0.5%	211.76 100%
Compiler Vectorization	22.57 48.1%	13.05 27.9%	3.71 7.9%	3.34 7.1%	0.75 1.6%	46.81 100%
Compiler Vectorization & Concurrency	41.44 75.0%	3.41 6.2%	3.54 6.4%	3.79 6.9%	0.85 1.5%	55.22 100%
Modified Solution and Compiler Vectorization & Concurrency	6.26 36.9%	3.52 20.8%	1.46 8.6%	1.20 7.1%	0.87 5.1%	16.96 100%

*Total program time includes times for other subroutines and main program not included in table.

concurrency was actually much less efficient than the vectorized-only version. However, the version that included the modification, SSOR (ODD-EVEN), for parallel processing described earlier was able to achieve a significant speed-up (3.6) relative to the vectorized version (a 22.8 speed-up factor relative to the scaler version).

DISCUSSION

The immiscible flow model presented here was applied to field-scale problems in a conceptual manner. Some of the predictive results of the applications were confirmed by subsequent field investigations. The conclusion that clay would act as a capillary barrier to dense NAPL appears to be valid. Exploratory drilling to the clay layer showed minimal (less than a few centimeters) penetration. We anticipated that NAPL migration in the Lockport Dolomite below S-Area would be strongly controlled by the bedrock dip. Modeling done before extensive bedrock drilling indicated that significant amounts of NAPL would move with the groundwater (counter to bedrock dip). The distribution of NAPL identified by drilling agrees with the modeled results. NAPL in the Lockport Dolomite is observed in the deeper layers and has migrated in all directions from the site. Although these qualitative comparisons are reassuring, further validation of immiscible flow theory to the field-scale applications is necessary. Current field work at S-Area and Hyde Park, the two sites described, will provide valuable data on NAPL migration and recovery in the next several years.

For many applications, a three-dimensional model may be necessary to account for heterogeneous conditions and lack of symmetry. Because many applications must address downward migration, concepts such as vertical equilibrium may not apply. The concept of vertical equilibrium is used in petroleum reservoir engineering to permit two-dimensional (aerial) simulation (Coats et al., 1969). For the three-dimensional example presented here, no suitable two-dimensional simulation was identified.

Three-dimensional multiphase simulations require powerful computers. Most powerful computers are based on a vector and/or parallel architecture. For this model, we made a modification to the iterative matrix solution technique to take full advantage of parallel processing. As the need for more complex simulations increases, more effort will be directed to development of numerical methods that are efficient on vector and parallel processing computers.

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ACKNOWLEDGMENTS

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APPENDIX C

OW413 INJECTION
TEST RESULTS

OW413A

Interval	Feet Below Ground Surface	Feet Below Top of Rock	Hydraulic[1] Conductivity (cm/sec)	Waterbearing	Depth to Static Water Level (ft. BGS)	Date
A	27.0 - 42.5	0.5 - 16.0	$1.5\times10^{-4} - 4.9\times10^{-4}$	Yes	7.0[2]	04/12/89
B	39.4 - 55.1	12.9 - 28.6	$2.3\times10^{-4} - 6.2\times10^{-4}$	Yes	5.58	04/19/89
C	54.4 - 70.1	27.9 - 43.6	$<1\times10^{-7} - 2.4\times10^{-6}$	No	5.76[3]	04/19/89
D	69.4 - 85.1	42.9 - 58.6	$1.1\times10^{-6} - 1.5\times10^{-6}$	No	5.81[3]	04/18/89
E	84.4 - 100.1	57.9 - 73.6	$<1\times10^{-7} - 9.2\times10^{-7}$	No	4.95[3]	04/18/89
F	99.4 - 115.1	72.9 - 88.6	$<1\times10^{-7} - 7.1\times10^{-7}$	No	3.78[3]	04/18/89
G	114.4 - 130.1	87.9 - 103.6	$<1\times10^{-7}$	No	3.98[3]	04/18/89
H	129.4 - 145.1	102.9 - 118.6	$<1\times10^{-7} - 3.1\times10^{-6}$ (4.7×10^{-5} hydrofracture)	No	4.01[3]	04/18/89
I	144.4 - 160.1	117.9 - 133.6	$1.5\times10^{-3} - 4.9\times10^{-3}$	Yes	4.23	04/17/89
J	159.4 - 178.5	132.9 - 152.0	$7.3\times10^{-4} - 1.1\times10^{-3}$	Yes	16.43	04/17/89

[1] Hydraulic Conductivity calculated assuming R/ro = 10.
[2] Measured Water Level
[3] May not have reached static prior to start of injecting water due to low hydraulic conductivity.

APPENDIX D

STUDY CHEMICAL PROGRAM
ANALYTICAL RESULTS

OCCIDENTAL CHEMICAL CORPORATION
ENVIRONMENTAL DATABASE SYSTEM

ND - Not Detected above quantitation level

S-AREA
RRT STUDY(S) CHEMICAL MONITORING PROGRAM

Special Codes: D - FIELD DUPLICATE
* - Identified using CLP criteria at a concentration below the method specified quantitation limit.

Analytes:	Units:	Quantitation Levels:	Sample Date: 01/10/89 Sample Description: OW 237 Special Code:	01/10/89 OW 238	01/10/89 OW 239	01/10/89 OW 240	01/10/89 OW 240 D
1,1-Dichloroethylene	ug/L	5	ND	ND	ND	ND	ND
2-Chlorophenol	ug/L	10	ND	ND	ND	ND	ND
2,4-Dichlorophenol	ug/L	10	ND	ND	ND	ND	ND
2,4,5-Trichlorophenol	ug/L	50	ND	ND	ND	ND	ND
2,4,6-Trichlorophenol	ug/L	10	ND	ND	ND	ND	ND
4-Chloro-3-Methylphenol	ug/L	10	ND	ND	ND	ND	ND
Pentachlorophenol	ug/L	50	ND	ND	ND	ND	ND
Phenol	ug/L	10	ND	110	ND	ND	ND
Total Phenols	ug/L		ND	110	ND	ND	ND
Endosulfan I	ug/L	10	ND	ND	ND	ND	ND
Endosulfan II	ug/L	10	ND	ND	ND	ND	ND
1,2,3-Trichlorobenzene	ug/L	7	11	190	200	25	20
1,2,4-Trichlorobenzene	ug/L	7	63	1200	930	140	120
Hexachlorobenzene	ug/L	7	ND	ND	ND	ND	ND
a-Hexachlorocyclohexane	ug/L	7	ND	18	19	ND	ND
b-Hexachlorocyclohexane	ug/L	7	ND	ND	ND	ND	ND
g-Hexachlorocyclohexane	ug/L	7	ND	ND	ND	ND	ND
d-Hexachlorocyclohexane	ug/L	7	ND	ND	ND	ND	ND
Perchloropentacyclodecane (Mirex)	ug/L	7	ND	ND	ND	ND	ND
PCB-1248 (AROCHLOR 1248)	ug/L	1	ND	ND	1	ND	
2,3,7,8-Tetrachloro-dibenzo-p-dioxin	ng/L	0.5	ND	ND	ND	ND	ND
Total Tetrachlorodibenzo-p-dioxins	ng/L	0.5	ND	ND	ND	ND	ND
1,2,3,7,8-Pentachlorodibenzodioxin	ng/L	0.5	ND	ND	ND	ND	ND
Total Pentachlorodibenzodioxins	ng/L	0.5	ND	ND	ND	ND	ND
1,2,3,4,7,8-Hexachlorodibenzodioxin	ng/L	0.5	ND	ND	ND	ND	ND
1,2,3,6,7,8-Hexachlorodibenzodioxin	ng/L	0.5	ND	ND	ND	ND	ND
1,2,3,7,8,9-Hexachlorodibenzodioxin	ng/L	0.5	ND	ND	ND	ND	ND
Total Hexachlorodibenzodioxins	ng/L	0.5	ND	ND	ND	ND	ND
1,2,3,4,6,7,8-Heptachlorodibenzodioxin	ng/L	0.5	ND	ND	ND	ND	ND
Total Heptachlorodibenzodioxins	ng/L	0.5	ND	ND	ND	ND	ND
Octachlorodibenzodioxin	ng/L	0.5	ND	ND	ND	ND	ND
2,3,7,8-Tetrachlorodibenzofuran	ng/L	0.5	ND	ND	ND	ND	ND
Total Tetrachlorodibenzofurans	ng/L	0.5	ND	ND	ND	ND	ND
1,2,3,7,8-Pentachlorodibenzofuran	ng/L	0.5	ND	ND	ND	ND	ND
2,3,4,7,8-Pentachlorodibenzofuran	ng/L	0.5	ND	ND	ND	ND	ND
Total Pentachlorodibenzofurans	ng/L	0.5	ND	ND	0.6	ND	ND
1,2,3,4,7,8-Hexachlorodibenzofuran	ng/L	0.5	ND	ND	ND	ND	ND
1,2,3,6,7,8-Hexachlorodibenzofuran	ng/L	0.5	ND	ND	ND	ND	ND
2,3,4,6,7,8-Hexachlorodibenzofuran	ng/L	0.5	ND	ND	ND	ND	ND
1,2,3,7,8,9-Hexachlorodibenzofuran	ng/L	0.5	ND	ND	ND	ND	ND
Total Hexachlorodibenzofurans	ng/L	0.5	ND	ND	0.8	ND	ND
1,2,3,4,6,7,8-Heptachlorodibenzofuran	ng/L	0.5	0.8	ND	5.2	ND	ND
1,2,3,4,7,8,9-Heptachlorodibenzofuran	ng/L	0.5	ND	ND	ND	ND	ND
Total Heptachlorodibenzofurans	ng/L	0.5	1.0	ND	6.5	ND	ND
Octachlorodibenzofuran	ng/L	0.5	4.2	0.5	29	ND	ND
Mercury	ug/L	0.2	ND	ND	ND	ND	ND

APPENDIX E

PHYSICAL AND CHEMICAL CONSTANTS

TABLE 1: TOXICOLOGY AND PHYSICAL-CHEMICAL DATA*

	ADI (mg/kg/day)	SOURCE OF ADI**	UCR 1/(mg/kg/day)	UCR STRENGTH-OF-EVIDENCE***	BIOCONCENTRATION FACTOR	% DERMAL ABSORB FROM SOIL	% DERMAL ABSORB FROM WATER
ACENAPHTHENE						0.1	0.01
ACENAPHTHYLENE							
ALDRIN			1.14E+01	2B		0.1	0.01
ANISOLE (METHYL PHENYL ETHER)	2.71E-03	EN,LD50			6.50E+00	0.1	0.01
ANTHRACENE							
benzo(a)-ANTHRACENE							
dibenzo(a,h)-ANTHRACENE							
ARSENIC			1.50E+01	1		0.1	0.01
BENZENE			2.90E-02	1	1.30E+01	0.1	0.01
BENZIDINE			2.34E+02	1	1.10E+00	0.1	0.01
BENZOCHLORODIFLUORIDE							
2,3-BENZOFURAN							
BENZOIC ACID	5.70E-01	EN,Sub,Ma			3.60E+00	0.1	0.01
BROMOBENZENE							
BROMODICHLOROMETHANE							
p-BROMOFLUOROBENZENE							
BROMOFORM							
BROMOMETHANE							
4-BROMOPHENYL PHENYL ETHER							
n-BUTYLBENZENE							
sec-BUTYLBENZENE							
tert-BUTYLBENZENE							
BUTYL BENZOATE	2.49E-03	EN,Sub			4.30E+02	0.1	0.01
BUTYL BENZYL PHTHALATE							
DI-n-BUTYL PHTHALATE	1.26E+00	EPA			1.60E+04	0.1	0.01
CARBON TETRACHLORIDE			1.30E-01	2B	2.20E+01	0.1	0.01
CHLORENDIC ACID	2.10E-02	EN,Sub	1.69E-02		5.90E+02	0.1	0.01
CHLOROBENZENE	1.43E-02	EPA			2.30E+02	0.1	0.01
o-CHLOROBENZOIC ACID	6.46E-02	EN,LD50			2.30E+01	0.1	0.01
o-CHLOROBENZOIC ACID						0.1	0.01
p-CHLOROBENZOIC ACID						0.1	0.01
o-CHLOROBENZOTRIFLUORIDE						0.1	0.01
o-CHLOROBENZOTRIFLUORIDE							
p-CHLOROBENZOTRIFLUORIDE	1.00E-02	EN,Sub			279	0.1	0.01
1-CHLOROCYCLOHEXENE							
CHLOROETHANE	5.36E-01	EN,Sub			1.00E+00	0.1	0.01
bis(2-CHLOROETHOXY) METHANE							
bis(2-CHLOROETHYL) ETHER			1.14E+00	2B		0.1	0.01
2-CHLOROETHYLVINYL ETHER							
CHLOROFORM			7.00E-02	2B	6.00E+00	0.1	0.01
CHLOROMETHANE	5.43E-01	EPA			1.00E+00	0.1	0.01
4-CHLORO-3-METHYLPHENOL							
2-CHLORONAPHTHALENE							
2-CHLOROPHENOL	[illegible]	[illegible]					

TABLE 1: TOXICOLOGY AND PHYSICAL-CHEMICAL DATA*

	ADI (mg/kg/day)	SOURCE OF ADI**	UCR 1/(mg/kg/day)	UCR STRENGTH-OF-EVIDENCE***	BIOCON-CENTRATION FACTOR	% DERMAL ABSORB FROM SOIL	% DERMAL ABSORB FROM WATER
m-CHLOROTOLUENE	1.50E-01	Anal.			9.10E+01	0.1	0.01
o-CHLOROTOLUENE	1.50E-01	EN,Sub			1.25E+02	0.1	0.01
p-CHLOROTOLUENE	1.50E-01	Anal.			9.60E+01	0.1	0.01
o/p-CHLOROTOLUENE							
CHRYSENE							
CUMENE							
CYCLOPROPYLBENZENE							
p-CYMENE							
p,p-DDD							
p,p-DDE							
p,p-DDT			3.40E-01	2B		0.1	0.01
DIBROMOCHLOROMETHANE							
m-DICHLOROBENZENE	6.90E-02	EN			3.20E+02	0.1	0.01
o-DICHLOROBENZENE	9.00E-02	EPA			2.50E+02	0.1	0.01
p-DICHLOROBENZENE	6.90E-02	EN,Sub			2.73E+02	0.1	0.01
DICHLOROBENZOTRIFLUORIDES	5.00E-03	EN,Sub			1.50E+03	0.1	0.01
DICHLORODIFLUOROMETHANE							
1,1-DICHLOROETHANE	1.16E-01	EPA			3.00E+00	0.1	0.01
1,2-DICHLOROETHANE			9.10E-02	2B	2.00E+00	0.1	0.01
1,1-DICHLOROETHYLENE			1.16E+00	3	3.30E+00	0.1	0.01
trans-1,2-DICHLOROETHYLENE	1.10E-02	EN,Sub			1.00E+00	0.1	0.01
2,4-DICHLOROPHENOL	1.00E-01	EPA			3.30E+01	0.1	0.01
1,2-DICHLOROPROPANE			4.00E-02	*	5.00E+00	0.1	0.01
cis-1,3-DICHLOROPROPYLENE			4.10E-01	*	2.60E+01	0.1	0.01
trans-1,3-DICHLOROPROPYLENE							
DICHLOROTOLUENES	4.90E-03				7.70E+02	0.1	0.01
DIELDRIN			3.04E+01	2B		0.1	0.01
DIETHYLPHTHALATE						0.1	0.01
2,4-DIMETHYLPHENOL						0.1	0.01
DIMETHYLPHTHALATE							
2,4-DINITROPHENOL							
2,4-DINITROTOLUENE			3.10E-01	2B		0.1	0.01
2,6-DINITROTOLUENE	1.00E-04	EN				0.1	0.01
DIOCTYLPHTHALATE							
1,2-DIPHENYLHYDRAZINE			7.70E-01	2B		0.1	0.01
ENDOSULFAN I							
ENDOSULFAN II							
ENDOSULFAN SULFATE							
ENDRIN							
ENDRIN ALDEHYDE							
ETHYL BENZENE	1.14E-01	EN,Sub			6.00E+01	0.1	0.01
bis-(2-ETHYLHEXYL)PHTHALATE			8.51E-03		3.80E+02	0.1	0.01

TABLE 1: TOXICOLOGY AND PHYSICAL-CHEMICAL DATA*

	ADI (mg/kg/day)	SOURCE OF ADI**	UCR 1/(mg/kg/day)	UCR STRENGTH-OF-EVIDENCE***	BIOCON-CENTRATION FACTOR	% DERMAL ABSORB FROM SOIL	% DERMAL ABSORB FROM WATER
FLUORANTHENE							
benzo(b)-FLUORANTHENE							
benzo(k)-FLUORANTHENE							
FLUORENE						0.1	0.01
HEPTACHLOR			3.37E+00	2B		0.1	0.01
HEPTACHLOR EPOXIDE							
HEXACHLOROBENZENE			1.67E+00	2B	1.00E+04	0.01	0.5
HEXACHLOROBUTADIENE (C-46)			7.75E-02	3	1.10E+04	0.1	0.01
alpha-HEXACHLOROCYCLOHEXANE			1.11E+01	2B		0.01	0.5
beta-HEXACHLOROCYCLOHEXANE			1.84E+00	3		0.01	0.5
delta-HEXACHLOROCYCLOHEXANE							
gamma-HEXACHLOROCYCLOHEXANE			1.33E+00	2B	4.00E+02	0.01	0.5
HEXACHLOROCYCLOPENTADIENE (C-56)	5.14E-04	EPA			4.80E+03	0.01	0.5
HEXACHLOROETHANE			1.42E-02	3	1.39E+02	0.1	0.01
ISOPHORONE							
MERCURY	2.85E-04	EPA				0.1	0.01
METHYL BENZOATE	4.25E-01	EH,Sub			6.00E+00	0.1	0.01
METHYL CHLOROBENZOATE					5.30E+01	0.1	0.01
2-METHYL-4,6-DINITROPHENOL							
METHYLENE CHLORIDE			6.30E-04	3	1.00E+00	0.1	0.01
MIREX	2.60E-04	EH,Sub	8.33E-01		1.82E+04	0.01	0.5
NAPTHALENE						0.1	0.01
NITROBENZENE							
2-NITROPHENOL							
4-NITROPHENOL							
n-NITROSODIPHENYLAMINE			4.92E-03	2B		0.1	0.01
n-NITROSODI-n-PROPYLAMINE							
OCTACHLOROCYCLOPENTENE							
PCB, 1016/1242							
PCB, 1221							
PCB, (Aroclor 1248)	3.00E-04	EPA	4.34E+00	2B	7.30E+04	0.01	0.5
PCB, 1254						0.1	0.01
PCB, 1260							
PENTACHLOROBENZENE	1.10E-02	EH,Sub			8.30E+03	0.1	0.01
PENTACHLOROETHANE			4.49E-03		6.70E+01	0.1	0.01
PENTACHLOROPHENOL						0.1	0.01
benzo(ghi)-PERYLENE							
PHENANTHRENE						0.1	0.01
PHENOL	1.00E-02	EH,Sub			1.00E+00	0.1	0.01
PHENYL BENZOATE	1.00E-02	EH,Sub			8.20E+01	0.1	0.01
n-PROPYLBENZENE							
PYRENE							
benzo(a)-PYRENE							
indeno(1,2,3-cd)-PYRENE							

TABLE 1: TOXICOLOGY AND PHYSICAL-CHEMICAL DATA*

	ADI (mg/kg/day)	SOURCE OF ADI**	UCR 1/(mg/kg/day)	UCR STRENGTH-OF-EVIDENCE***	BIOCONCENTRATION FACTOR	% DERMAL ABSORB FROM SOIL	% DERMAL ABSORB FROM WATER
STYRENE							
2,3,7,8-TCDD	1.00E-09	EPA	1.56E+05	2B	6.70E+04	0.01	0.5
1,2,3,4-TETRACHLOROBENZENE	3.00E-03	EN,Sub			8.60E+03	0.1	0.01
1,2,4,5-TETRACHLOROBENZENE	3.00E-04	EN,Sub			6.80E+03	0.1	0.01
1,1,2,2-TETRACHLOROETHANE			2.00E-01	3	8.00E+00	0.1	0.01
TETRACHLOROETHYLENE			5.10E-02	3	4.40E+01	0.1	0.01
TETRACHLOROTOLUENES					2.10E+04	0.1	0.01
TOLUENE	4.21E-01	EPA			1.60E+01	0.1	0.01
1,2,3-TRICHLOROBENZENE	2.00E-02	Anal.			1.90E+03	0.1	0.01
1,2,4-TRICHLOROBENZENE	2.00E-02	EN,Sub			1.60E+03	0.1	0.01
1,3,5-TRICHLOROBENZENE	7.60E-02	EN,Sub			3.00E+03	0.1	0.01
1,1,1-TRICHLOROETHANE	2.86E-02	EPA			9.00E+00	0.1	0.01
1,1,2-TRICHLOROETHANE			5.73E-02	3	5.60E+00	-0.1	0.01
TRICHLOROETHYLENE			1.10E-02	3/2B	1.70E+01	0.1	0.01
TRICHLOROFLUOROMETHANE	3.43E-01	EPA			1.60E+01	0.1	0.01
2,4,5-TRICHLOROPHENOL	1.00E-01	EPA			1.90E+03	0.1	0.01
2,4,6-TRICHLOROPHENOL			1.99E-02	2B	1.60E+02	0.1	0.01
TRICHLOROTOLUENES	4.00E-03				4.00E+03	0.1	0.01
1,2,4-TRIMETHYLBENZENE							
1,3,5-TRIMETHYLBENZENE							
VINYL CHLORIDE			1.75E-02	1		0.1	0.01
m-XYLENE	1.70E-03	EN,Sub			2.40E+01	0.1	0.01
o-XYLENE	1.70E-03	EN,Sub			6.30E+01	0.1	0.01
p-XYLENE	1.70E-03	EN,Sub			6.80E+01	0.1	0.01

*For Explanation of Notation Used in this Table see Affidavit (TABLE 1)

**SOURCE OF ADI: EN - ENVIRON calculated ADI
LD50 - ADI based on LD50 data
Sub - ADI based on subchronic data
Hu - ADI based on human data
EPA - EPA draft ADI (USEPA 1984)
Analogy - ADI based on analogy to other chemical

***STRENGTH-OF-EVIDENCE: Explanatory paragraphs follow

APPENDIX F

EXPLOSURE SCENARIOS

Scenario A: Fish Ingestion - Carcinogens

Ingestion of contaminated fish from the Niagara River and Lake Ontario has been identified as a potential route of exposure for local recreational fishermen and others who might consume the fish. Fishermen have been observed on the banks of the Niagara River and Lake Ontario and commercial fishing takes place in Lake Ontario. ENVIRON has analyzed fish consumption in the upper New York region and this report is incorporated as Attachment C of this Affidavit. This analysis reviewed various sources of information concerning types of fish in the region, studies of fish consumption both locally and nationwide, and surveys of sport fishermen both region specific and nationwide. From this analysis, ENVIRON believes the population most exposed to contaminated Lake Ontario and Niagara River fish are local recreational fishermen, based on local creel census, analysis of national fishing patterns, and commerical fishing data (ENVIRON, 1985). It was assumed that the average daily consumption by area fishermen of Niagara River and Lake Ontario sport fish was 14 g/day, which is approximately the consumption of the 90th percentile of all Great Lakes area consumers of fish (ENVIRON 1985)*.

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*The USEPA in its Ambient Water Quality Criteria Documents use 6.5 g/day of freshwater and estuarine fish and shellfish, per capita consumption. The calculations on lifetime exposure to carcinogens in Column A of Table 6, Appendix II can be adjusted to this exposure level by multiplying the calculated risks by approximately 0.45. New York State uses 32.4 g/day as the average consumption for area fishermen, based on the 90th percentile for fish consumers nationwide. The calculations on lifetime exposure to carcinogens in Column A of Table 6, Appendix II can be adjusted to reflect this exposure by multiplying the calculated risks by approximately 2.3.

Other assumptions include the assumption of 100% absorption of the chemical from the gastro-intestinal tract into the body, which may be an overestimate and therefore also overestimate the risk to human health. A dilution factor is used because the sampling of the amount of the chemical entering the water is being made at or prior to the Gorge Face, before it enters the Niagara River and Lake Ontario. A fish, however, will not come in contact with same concentration of the chemical that is at the Gorge Face because, once the chemical enters the water, it is diluted. Thus, a dilution factor of 2.2×10^6 (approximately 2 million, see Affidavit of Dr. Shifrin) is used. The bioconcentration factor (see Affidavit of Ms. Benavides of Gradient Corporation) is used to determine the uptake of the chemical into the fish from the water. The bioconcentration and bioaccumulation factors for 2,3,7,8-TCDD are difficult to determine (see Affidavit of Ms. Benavides) and are discussed further in paragraphs 223 through 229. Bioconcentration factors for the Hyde Park chemicals are listed in Table 1, Appendix I.

The Report of the Task Group on Reference Man (ICRP 1984) supplied the following information on male physiology parameters that is needed for this risk assessment: the average body weight for an adult male is 70 kg.

The upper-bound, lifetime level of risk that would be presented by a specific concentration is determined by the following equations, using a bioconcentration factor of 22 for carbon tetrachloride:

$$\text{LADD} = \frac{(\text{concentration})\,(\text{bioconcentration factor})\,(\text{absorption coefficient})\,(\text{average daily consumption})}{(\text{dilution factor})\,(\text{adult body weight})}$$

$$\text{LADD} = \frac{(c\ \text{mg/L})\ (22\ \text{L/kg fish})\ (1)\ (0.014\ \text{kg fish/day})}{(2{,}200{,}000)(70\ \text{kg})}$$

$\text{LADD} = (2.0 \times 10^{-9})\ (c)\ \text{mg/kg/day}$ for any concentration c of carbon tetrachloride in mg/kg

and,

$\text{UCR} = 0.13\ (\text{mg/kg/day})^{-1}$ for carbon tetrachloride,

$c = 2.1 \times 10^{-4}\ \text{mg/kg}$ (or 1.03×10^{-4} lbs/day).

Since

$\text{Risk} = \text{LADD} \times \text{UCR}$

$\text{Risk} = (4.2 \times 10^{-13}\ \text{mg/kg/day}) \times [0.13\ (\text{mg/kg/day})^{-1}]$

$\text{Risk} = 5.46 \times 10^{-14}$.

The above calculations can be interpreted in the following manner. If a man eats an average of 14 g of fish per day (which is approximately equal to one-half an ounce of fish each day or one fish meal every 3 weeks) and this fish is contaminated with carbon tetrachloride, and the carbon tetrachloride enters the water at a rate of 1.03×10^{-4} (or 0.000103) pounds per day (this amount is prior to dilution by the river and lake and prior to bioconcentration in the fish, i.e., this is not the level of carbon tetrachloride that would be measured in the fish), then his lifetime risk of developing cancer from this exposure (assuming without proof that carbon tetrachloride is a human carcinogen and that it poses a finite risk at all finite exposures) would not exceed 5.46×10^{-14} (or one in 18 trillion).

The upper-bound, lifetime levels of risk for other chemicals evaluated for Hyde Park using this same procedure are presented in Column A of Table 7, Appendix II. For some chemicals that are very hydrophobic, an additional calculation was made. These chemicals are thought to partition preferentially into soil and sediment at the bottom of rivers or lakes, i.e., once in the river most of the chemical tends to attach or adhere to sediment rather than staying in water (see Affidavit of Ms. Benavides). Furthermore, a bioaccumulation factor, which includes the effects of the environment such as ingestion of soils and smaller organisms in addition to chemicals in the water that are considered in a bioconcentration factor, is considered to be more appropriate for these chemicals (see Affidavit of Ms. Benavides for a complete discussion of these issues). Gradient Corporation concluded that for 2,3,7,8-TCDD, PCBs, mirex and hexachlorobenzene a good approximate of the bioaccumulation factor can be derived by multiplying the bioconcentration factor times 10. For 2,3,7,8-TCDD, PCBs, mirex, and hexachlorobenzene, Gradient also estimated that 22% of the loading will remain in the water phase of the lake or river (Dr. Shifrin, 1985, personal communication). Risk levels for chemicals such as 2,3,7,8-TCDD and PCBs, mirex, and hexachlorobenzene can be calculated using this information. The calculations using either the bioconcentration factor or using the bioaccumulation factor and the appropriate distribution among media are noted on Table 7, e.g., 2,3,7,8-TCDD (BCF) and 2,3,7,8-TCDD (BAF), respectively.

Scenario AA: Fish Ingestion - Noncarcinogens

Ingestion of contaminated fish from the Niagara River and Lake Ontario has been identified as a potential route of exposure for local recreational fishermen and others who might consume the fish. Fishermen have been observed on the banks of the Niagara River and Lake Ontario and commercial fishing takes place in Lake Ontario. ENVIRON has analyzed fish consumption in the upper New York region. This report is incorporated as Attachment C of this Affidavit. This analysis reviewed various sources of information concerning types of fish in the region, studies of fish consumption both locally and nationwide, and surveys of sport fishermen both region specific and nationwide. From this analysis, ENVIRON believes the population most exposed to contaminated Lake Ontario and Niagara River fish are local recreational fishermen, based on local creel census, analysis of national fishing patterns, and commerical fishing data (ENVIRON, 1985).

For the purpose of determining exposures to noncarcinogens that might lead to toxicity from the contaminant in the fish, a maximum fish consumption was used. An assumption of a maximum daily fish consumption (amount of fish eaten each day for one or more days) of 460 grams was used (ENVIRON 1985).

Other assumptions include the assumption of 100% absorption of each chemical from the gastro-intestinal tract into the body, which may be an overestimate and therefore also overestimate the risk to human health. A dilution factor is used because the sampling of the amount of the chemical entering the water is being made at or prior to the Gorge Face, before it

Scenario G: Drinking Water - Carcinogens

Drinking water from the Niagara River or Lake Ontario has been identified as a potential exposure for the community around the Hyde Park Landfill. The assumptions were made that an adult would drink 2 liters of water per day for his lifetime. A dilution factor is used because the sampling of the amount of the chemical entering the water is being made at or prior to the Gorge Face before it enters the Niagara River and Lake Ontario. The source of drinking water, however, is Lake Ontario. Thus, contaminated water from the seeps would be diluted by 2,200,000 (approximately 2 million, see Affidavit of Dr.

Shifrin) before it is consumed. Another assumption is that absorption of each chemical into the body is 100%.

The Report of the Task Group on Reference Man (ICRP 1984) supplied the following information on male physiology parameters that is needed for this risk assessment: the average body weight for an adult male is 70 kg.

The upper-bound, lifetime level of risk that would be presented by a specific concentration is determined by the following equations:

$$\text{LADD} = \frac{(\text{concentration})\ \begin{pmatrix}\text{absorption}\\ \text{coefficient}\end{pmatrix}\ \begin{pmatrix}\text{average daily}\\ \text{consumption}\end{pmatrix}}{(\text{dilution factor})\ (\text{adult body weight})}$$

$$\text{LADD} = \frac{(c\ \text{mg/L})\ (1)\ (2\ \text{L/day})}{(2.2 \times 10^{6})\ (70\ \text{kg})}$$

$\text{LADD} = (1.3 \times 10^{-8})\ (c)$ mg/kg/day for any concentration c in mg/kg.

and,

$\text{UCR} = 0.13\ (\text{mg/kg/day})^{-1}$ for carbon tetrachloride

$c = 2.1 \times 10^{-4}$ mg/kg (or 1.03×10^{-4} lbs/day).

Since

$\text{Risk} = \text{LADD} \times \text{UCR}$

$\text{Risk} = (2.73 \times 10^{-12}\ \text{mg/kg/day}) \times [0.13\ (\text{mg/kg/day})^{-1}]$

$\text{Risk} = 3.55 \times 10^{-13}$.

The above calculations can be interpreted in the following manner. If a man drinks an average of 2 liters of water per day, and this water is contaminated with carbon tetrachloride, and the carbon tetrachloride enters the river at a rate of 1.03×10^{-4} (or 0.000103) pounds per day (this level is prior to dilution by the river and lake, i.e., this is not the level of carbon tetrachloride that would be measured in the drinking water), then his upper-bound, lifetime risk of developing cancer from this exposure (assuming without proof that carbon tetrachloride is a human carcinogen and that it poses a finite risk at all finite exposures) would not exceed 3.55 x 10^{-13} (or one in 3 trillion). The upper-bound, lifetime levels of risk for other chemicals evaluated for Hyde Park using this same procedure are presented in Column G of Table 8, Appendix II.

Scenario GG: Drinking Water - Noncarcinogens

Drinking water from the Niagara River or Lake Ontario has been identified as a potential exposure for the community around the Hyde Park Landfill. For the purpose of determining exposures to noncarcinogens that might lead to toxicity from the contaminant in water, an assumption of a maximum daily ingestion of 2 liters of contaminated water was used. Another assumption used is that absorption of each the chemical into the body is 100%.

The Report of the Task Group on Reference Man (ICRP 1984) supplied the following information on male physiology parameters that is needed for this risk assessment: the average body weight for an adult male is 70 kg.

The resulting MDD to ADI ratio is determined by the following equations:

$$\text{MDD} = \frac{(\text{concentration})\ \begin{pmatrix}\text{absorption}\\ \text{coefficient}\end{pmatrix}\ \begin{pmatrix}\text{maximum daily}\\ \text{consumption}\end{pmatrix}}{(\text{dilution factor})\ (\text{adult body weight})}$$

$$\text{MDD} = \frac{(c\ \text{mg/L})\ (1)\ (2\ \text{L/day})}{(2{,}200{,}000)\ (70\ \text{kg})}$$

$$\text{MDD} = (1.3 \times 10^{-8})\ (c)\ \text{mg/kg/day for concentration } c \text{ in mg/kg.}$$

Solving for the MDD to ADI ratio for phenol at a concentration of 8.77×10^{-1} mg/kg (or 0.43 lbs/day) with an ADI of 0.01 mg/kg/day:

$$\frac{\text{MDD}}{\text{ADI}} = \frac{1.14 \times 10^{-8}\ \text{mg/kg/day}}{0.01\ \text{mg/kg/day}}$$

$$\frac{\text{MDD}}{\text{ADI}} = 1.14 \times 10^{-6}$$

The above calculation can be interpreted in the following manner. If a man drinks a maximum of 2 liters of water on any day and the water is contaminated with phenol, and the phenol enters the river at a rate of 4.3×10^{-1} (or 0.43) pounds per day (which is the level prior to dilution by the river and lake, i.e., this is not the level of phenol that would be measured in the drinking water), the MDD to ADI ratio would be 1.14×10^{-6}. This is less than one; hence he would not be expected to suffer adverse effects from this exposure. MDD to ADIs ratios for other chemicals evaluated for Hyde Park can be found in Column GG of Table 8, Appendix II.

Scenario H: Swimming - Carcinogens

Dermal contact with water from swimming in the Niagara River or Lake Ontario has been identified as a potential exposure for people in the community. The assumptions were made that an adult male would swim once a day, 30 days a month, two and one-half months of the year, for 35 years of his lifetime.

It was further assumed that he would expose his entire body surface (18,000 cm^2: ICRP 1984). Exposure would result in 2 mg water/cm^2 of body surface area (Versar 1984). Absorption was assumed to be 50% for 2,3,7,8-TCDD, PCBs, hexachlorocyclopentadiene, and hexachlorocyclohexane and 1% for all other chemicals. A dilution factor is used because the sampling of the amount of the chemical entering the water is being made at or prior to the Gorge Face, before it enters the Niagara River and Lake Ontario. A swimmer, however, will not come in contact with the chemicals in the water until the chemical is diluted. Thus, a dilution factor of 2,200,000 (approximately 2 million, see Affidavit of Dr. Shifrin) is used.

The Report of the Task Group on Reference Man (ICRP 1984) supplied the following information on male physiology parameters that is needed for this risk assessment: the average lifetime for a male is 70 years; the average body weight for an adult male is 70 kg.

The upper-bound, lifetime level of risk that would be presented by a specific concentration is determined by the following equations:

$$\text{LADD} = \frac{(\text{concentration})\left(\begin{matrix}\text{total body}\\ \text{surface area}\end{matrix}\right)\left(\begin{matrix}\text{water/}\\ \text{area}\end{matrix}\right)\left(\begin{matrix}\text{absorption}\\ \text{coefficient}\end{matrix}\right)\left(\begin{matrix}\text{contact/}\\ \text{lifetime}\end{matrix}\right)}{(\text{dilution factor})\,(\text{days/lifetime})\,(\text{adult body weight})}$$

$$\text{LADD} = \frac{(c\ \text{mg/kg})(18{,}000\ \text{cm}^2)(2\text{x}10^{-6}\ \text{kg/cm}^2)(.01)(30\ \text{d/mo})(2.5\ \text{mo/yr})(35\ \text{yr})}{(2{,}200{,}000)\ (365\ \text{d/yr x } 70\ \text{yr/life})\ (70\ \text{kg})}$$

$\text{LADD} = (2.4 \text{ x } 10^{-13})\ (c)$ mg/kg/day for any concentration c of carbon tetrachloride in mg/kg.

and,

$\text{UCR} = 0.13\ (\text{mg/kg/day})^{-1}$ for carbon tetrachloride

$c = 2.1 \times 10^{-4}$ mg/kg (or 1.03×10^{-4} lbs/day).

Since

Risk = LADD x UCR

Risk = (5.04×10^{-17} mg/kg/day) x [0.13 (mg/kg/day)$^{-1}$]

Risk = 6.56×10^{-18}

The above calculations can be interpreted in the following manner. If a man swims an average of once a day, 30 days a month, 2 and one-half months a year for 35 years, and his entire body surface comes in contact with water, and this water is contaminated with carbon tetrachloride, and the carbon tetrachloride enters the water at a rate of 1.03×10^{-4} (or 0.000103) pounds per day (this level is prior to dilution by the river and lake, i.e., this is not the level of carbon tetrachloride that the person would come in contact with), then his lifetime risk of developing cancer from this exposure (assuming without proof that carbon tetrachloride is a human carcinogen and that it poses a finite risk at all finite exposures) would not exceed 6.56×10^{-18} (or one in 150 quadrillion). The upper-bound, lifetime levels of risk for other chemicals evaluated for Hyde Park using this same procedure are presented in Column H of Table 8, Appendix II.

Scenario HH-1: Swimmer (Adult) - Noncarcinogens

Dermal contact with water from swimming in the Niagara River or Lake Ontario has been identified as a potential exposure for people in the community. For the purpose of determining exposures to noncarcinogens that might lead to toxicity from contact with the contaminant in water during swimming by an adult male, a maximum number of 5 swims per day was used.

It was further assumed that he would expose his entire body surface (18,000 cm^2: ICRP 1984). Exposure would result in 2 mg water/cm^2 of body surface area (Versar 1984). Absorption was assumed to be 50% for 2,3,7,8-TCDD, PCBs, hexachlorocyclopentadiene, and hexachlorocyclohexane and 1% for all other chemicals. A dilution factor is used because the sampling of the amount of the chemical entering the water is being made at or prior to the Gorge Face, before it enters the Niagara River and Lake Ontario. A swimmer, however, will not come in contact with the chemicals in the water until the chemical is diluted. Thus, a dilution factor of 2,200,000 (approximately 2 million, see Affidavit of Dr. Shifrin) is used.

The Report of the Task Group on Reference Man (ICRP 1984) supplied the following information on male physiology parameters that is needed for this risk assessment: the average body weight for an adult male is 70 kg.

The resulting MDD to ADI ratio is determined by the following equations, using an absorption coefficient of 1% for phenol:

$$\text{MDD} = \frac{(\text{concentration})\ \left(\begin{array}{c}\text{total body}\\ \text{surface area}\end{array}\right)\ \left(\begin{array}{c}\text{water/}\\ \text{area}\end{array}\right)\ \left(\begin{array}{c}\text{absorption}\\ \text{coefficient}\end{array}\right)\ \left(\begin{array}{c}\text{max. swims/}\\ \text{day}\end{array}\right)}{(\text{dilution factor})\ (\text{adult body weight})}$$

$$\text{MDD} = \frac{(c\ \text{mg/kg})\ (18{,}000\ \text{cm}^2)\ (2 \times 10^{-6}\ \text{kg/cm}^2)\ (.01)\ (5)}{(2{,}200{,}000)\ (70\ \text{kg})}$$

MDD = (1.2×10^{-11}) (c) mg/kg/day for any concentration of phenol c in mg/kg.

Solving for the MDD to ADI ratio for phenol at a concentration of 8.77×10^{-1} mg/kg (or 0.43 lbs/day) with an ADI of 0.01 mg/kg/day:

$$\frac{MDD}{ADI} = \frac{1.05 \times 10^{-11} \text{ mg/kg/day}}{0.01 \text{ mg/kg/day}}$$

$$\frac{MDD}{ADI} = 1.05 \times 10^{-9}.$$

The above calculation can be interpreted in the following manner. If a man swims a maximum of 5 times a day, and the water he swims in is contaminated with phenol, and the phenol enters the water at a rate of 4.3×10^{-1} (or 0.43) pounds per day (which is the level prior to dilution by the river and lake, i.e. this is not the level of phenol that the swimmer would come in contact with), the MDD to ADI ratio would be 1.05×10^{-9}. This is less than one; hence, he would not be expected to suffer adverse effects from this exposure. MDD to ADI ratios for other chemicals evaluated for Hyde Park based on estimated 70-year average concentrations can be found in Column HH-1 of Table 8, Appendix II.

Scenario HH-2: Swimmer (child) - Noncarcinogens

Dermal contact with water from swimming in the Niagara River or lake Ontario has been identified as a potential exposure for people in the community. For short-term exposures, such as those calculated for noncarcinogens, exposures for children should be estimated since physiological parameters (e.g., body surface area and weight) that affect dose may be different for a child than for an adult. For this assessment, a four-year-old child was modeled, and it was assumed he would swim a maximum of five times a day.

It was further assumed that he would expose his entire body surface (6,950 cm^2: ICRP 1984). Exposure would result in 2 mg water/cm^2 of body surface area (Versar 1984). Absorption was assumed to be 50% for 2,3,7,8-TCDD, PCBs, hexachlorocyclopentadiene, and hexachlorocyclohexane and 1% for all other chemicals. A dilution factor is used because the sampling of the amount of the chemical entering the water is being made at or prior to the Gorge Face, before it enters the Niagara River and Lake Ontario. A swimmer, however, will not come in contact with the chemicals in the water until the chemical is diluted. Thus, a dilution factor of 2,200,000 (approximately 2 million, see Affidavit of Dr. Shifrin) is used.

The Report of the Task Group on Reference Man (ICRP 1984) supplied the following information that is needed for this risk assessment: the average body weight for a 4-year-old child is 17.5 kg.

The resulting MDD to ADI ratio is determined by the following equations, using an absorption coefficient of 1% for phenol:

$$\text{MDD} = \frac{(\text{concentration})\left(\begin{array}{c}\text{total body}\\ \text{surface area}\end{array}\right)\left(\begin{array}{c}\text{water/}\\ \text{area}\end{array}\right)\left(\begin{array}{c}\text{absorption}\\ \text{coefficient}\end{array}\right)(\text{max. swims/day})}{(\text{dilution factor})\ (\text{child's body weight})}$$

$$\text{MDD} = \frac{(c\ \text{mg/kg})\ (6950\ \text{cm}^2)\ (2 \times 10^{-6}\ \text{kg/cm}^2)\ (.01)\ (5)}{(2{,}200{,}000)\ (17.5\ \text{kg})}$$

$$\text{MDD} = (1.8 \times 10^{-11})\ (c)\ \text{mg/kg/day for any concentration of phenol } c \text{ in mg/kg.}$$

Solving for the MDD to ADI ratio for phenol at a concentration of 8.77×10^{-1} mg/kg (or 0.43 lbs/day) with an ADI of 0.01 mg/kg/day:

$$\frac{\text{MDD}}{\text{ADI}} = \frac{1.58 \times 10^{-11}\ \text{mg/kg/day}}{0.01\ \text{mg/kg/day}}$$

$$\frac{\text{MDD}}{\text{ADI}} = 1.58 \times 10^{-9}.$$

The above calculation can be interpreted in the following manner. If a four-year-old child swims a maximum of 5 times a day, and the water he swims in is contaminated with phenol, and the phenol enters the water at a rate of 4.3×10^{-1} (or 0.43) pounds per day (which is the level prior to dilution by the river and lake, i.e., this is not the level of phenol that the swimmer would come in contact with), the MDD to ADI ratio would be 1.58×10^{-9}. This is less than one; hence he would not be expected to suffer effects from this exposure. MDD to ADI ratios for other chemicals evaluated for Hyde Park based on estimated 70-year average concentrations can be found in Column HH-2 of Table 8, Appendix II.

APPENDIX G

INTEGRATED RISK INFORMATION SYSTEMS (IRIS)

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

OFFICE OF
RESEARCH AND DEVELOPMENT

APR 15 1988

Dear Risk Assessor:

I am very pleased to announce the availability of the U.S. Environmental Protection Agency's (EPA) Integrated Risk Information System (IRIS). IRIS is an on-line database of chemical-specific risk information on the relationship between chemical exposure and estimated human health effects. IRIS was developed for EPA staff and contractors to serve as a guide for EPA risk assessments, but because many other parties have indicated how useful IRIS information would be to them, EPA is making the database available outside the Agency.

IRIS provides chemical-specific risk data that represents an EPA scientific consensus. The database presents a summary of information on chemical hazard identification and dose-response assessment, thus, IRIS is not an exhaustive toxicological database.

IRIS translates chemical health effects data into a form which is useful in taking action to protect public health. Thus, IRIS bridges a significant gap in the transmission of information needed to reduce risks to human health. The database provides quantitative risk values and necessary qualitative health effects information which can act as guidance for deciding what action is necessary to protect the public health. Without this combined quantitative and qualitative information, it is often difficult for a risk manager to make decisions on how to best protect human health.

The information in IRIS is an authoritative interpretation of chemical health effects data. The quantitative risk values and supporting explanation has been reviewed and agreed upon by scientists from across the Agency using available studies on a substance. Thus, the information in IRIS represents an expert Agency consensus. This Agency-wide agreement on risk information is one of the most valuable aspects of IRIS.

Currently, there are risk summaries in IRIS for 260 chemicals. IRIS is regularly updated -- new chemicals are added, and existing information on the chemicals is updated as new scientific data is reviewed. Additional risk information will be included on the chemicals to best meet the needs of EPA users. Thus, to ensure use of the most up-to-date chemical information, IRIS is only available on-line. There are several ways to establish on-line access to IRIS. An enclosure explains how to access the IRIS database and who to contact for IRIS training.

We at EPA are encouraged by the demand for IRIS and hope that you find the database useful as you perform risk assessments.

Sincerely,

Wm H Farland

William H. Farland, Ph.D.
Acting Director
Office of Health and Environmental
Assessment

ACCESSING IRIS

IRIS is now available on DIALCOM, Inc.'s electronic mail network, the Public Health Foundation's Public Health Network (PHN), and will soon be on the National Library of Medicine's TOXNET system.

IRIS is housed on the network of DIALCOM Inc., a private telecommunications company. In order to access IRIS, you must obtain an account with DIALCOM, Inc., unless you are eligible to use the Public Health Network (PHN). The account is with DIALCOM, Inc. and not EPA. To obtain a DIALCOM Inc. account, contact Mike McLaughlin at (202) 488-0550 or write to: Mike McLaughlin, DIALCOM Inc., 600 Maryland Avenue SW, Suite 307, Washington DC 20024.

The user must pay only for the cost of accessing IRIS. The user will be billed by DIALCOM, Inc. There is a $25.00 monthly minimum which is applied against a usage fee of $25.00 per hour. In addition to the usage fee, there is a $.05 charge per computer screen accessed. There is no EPA charge for using IRIS.

If you are a state or local health department, it may be possible for you to access IRIS through the Public Health Network (PHN) of the Public Health Foundation. Those choosing to access IRIS via the Public Health Network will be charged at the PHN rate. Contact Paul Johnson at the Public Health Foundation, (202) 898-5600, for information on PHN.

Efforts were recently started to make IRIS available through the National Library of Medicine's TOXNET system. IRIS should become part of TOXNET sometime this summer. On-line messages will be posted on IRIS and TOXNET to announce this availability.

HOW TO GET IRIS TRAINING

Training in using IRIS is being arranged through the ten EPA Regions. This training is for both EPA staff and the public. The Regions are scheduling IRIS training to fit the risk assessment training needs of each particular Region. Thus, IRIS training schedules will vary among the Regions. The following EPA Regional staff are coordinating IRIS training at their Regional offices:

EPA REGION		IRIS CONTACTS
I	Boston	Tom D'Avanzo (617) 565-3222 FTS 835-3222
II	New York	Marian Olson (212) 264-5682 FTS 264-5682

III	Philadelphia	Roy Smith	(215) 597-9857	FTS 597-9857
IV	Atlanta	Gayle Alston	(404) 347-4216	FTS 257-4216
V	Chicago	David Dolan	(312) 886-6195	FTS 886-6195
VI	Dallas	Fred Reitman	(214) 655-2235	FTS 255-2235
		Jill Lyons	(214) 655-7208	FTS 255-7208
VII	Kansas City	Bob Fenemore	(913) 236-2970	FTS 757-2970
VIII	Denver	Jim Baker	(303) 293-1524	FTS 564-1524
IX	San Francisco	Arnold Den	(415) 974-0906	FTS 454-0906
X	Seattle	Dave Tetta	(206) 442-2138	FTS 399-2138
		Dana Davoli	(206) 442-2135	FTS 399-2135

If you have any questions about IRIS, call IRIS User Support at (513) 569-7254 or FTS 684-7254.

IRIS

INTRODUCTION

OVERVIEW OF IRIS

The Integrated Risk Information System (IRIS), prepared and maintained by the U.S. Environmental Protection Agency (EPA), is an electronic data base containing health risk and EPA regulatory information on specific chemicals. IRIS was developed for EPA staff in response to a growing demand for consistent risk information on chemical substances for use in decision-making and regulatory activities. Although IRIS is designed for EPA staff, it is also accessible to state and local environmental health agencies. IRIS is available to libraries, private citizens, and other organizations by means of Dialcom, Inc.'s Electronic Mail telecommunications system. The information in IRIS is intended for EPA staff without extensive training in toxicology, but with some knowledge of health sciences.

The heart of the IRIS system is its collection of computer files covering individual chemicals. These chemical files contain descriptive and quantitative information in the following categories:

- Oral and inhalation reference doses (RfDs) for chronic noncarcinogenic health effects
- Oral and inhalation slope factors and unit risks for chronic exposures to carcinogens
- Drinking water health advisories from EPA's Office of Drinking Water
- EPA regulatory action summaries
- Supplementary data on acute health hazards and physical/chemical properties

To aid users in accessing and understanding the data in the IRIS chemical files, the following supportive documentation is provided:

- Alphabetical list of the chemical files in IRIS and list of chemicals by CAS (Chemical Abstracts Service) number.
- Background documents describing the rationales and methods used in arriving at the results shown in the chemical files.
- A user's guide that represents step-by-step procedures for using IRIS to retrieve chemical information.
- An example exercise in which the use of IRIS is demonstrated.
- Glossaries in which definitions are provided for the acronyms, abbreviations, and specialized risk assessment terms used in the chemical files and in the background documents.

RISK ASSESSMENT AND RISK MANAGEMENT

The information in IRIS is intended for use in protecting public health through risk assessment and risk management. These two processes are briefly explained below.

Risk assessment has been defined as "the characterization of the potential adverse health effects of human exposures to environmental hazards (NRC, 1983, p. 18). In a risk assessment, the extent to which a group of people has been or may be exposed to a certain chemical is determined, and the extent of exposure is then considered in relation to the kind and degree of hazard posed by the chemical, thereby permitting an estimate to be made of the present or potential health risk to the group of people involved.

Risk assessment information is used in the risk management process in deciding how to protect public health. Examples of risk management actions include: deciding how much of a chemical a company may discharge into a river; determining which substances may be stored at a hazardous waste disposal facility; deciding to what extent a hazardous waste site must be cleaned up; setting permit levels for discharge, storage, or transport of hazardous waste; establishing levels for air emissions; and determining allowable levels of contamination in drinking water.

Essentially, risk assessment provides **information** on the health risk, and risk management is the **action** taken based on that information.

A complete risk assessment consists of the following four steps:

1. Hazard identification,
2. Dose-response assessment,
3. Exposure assessment, and
4. Risk characterization,

with risk characterization being the transitional step to risk management.

The following discussion of the four steps of risk assessment was excerpted from "Principles of Risk Assessment: A Nontechnical Review" (U.S. EPA, 1985).

> Hazard identification involves gathering and evaluating data on the types of health injury or disease that may be produced by a chemical and on the conditions of exposure under which injury or disease is produced. It may also involve chararacterization of the behavior of a chemical within the body and the interactions it undergoes with organs, cells, or even part of cells. Data of the latter types may be of value in answering the ultimate question of whether the forms of toxicity known to be produced by a substance in one population group or in experimental settings are also likely to be produced in humans. Hazard identification is not risk assessment; we are simply determining whether it is scientifically correct to infer that toxic effects observed in one setting will occur in other settings (e.g., whether substances found to be carcinogenic or teratogenic in experimental animals are likely to have the same results in humans).
>
> Dose-response assessment involves describing the quantitative relationship between the amount of exposure to a substance and the extent of toxic injury or disease. Data are derived from animal studies, or less frequently, from studies in exposed populations. There may be many different toxic effects under different conditions of exposure.
>
> The risks of a substance cannot be ascertained with any degree of confidence unless dose-response relationships are quantified, even if the substance is known to be toxic.
>
> Exposure assessment involves describing the nature and size of the population exposed to a substance and the magnitude and duration of their exposure. The evaluation could concern past or current exposures, or exposures anticipated in the future.
>
> Risk characterization generally involves the integration of the

assessment process (hazard identification, dose-response assessment, and exposure assessment) to determine the likelihood that humans will experience any of the various forms of toxicity associated with a substance. (In cases where exposure data are not available, hypothetical risk can be characterized by the integration of hazard identification and dose-response assessment data alone.) A framework to define the significance of the risk is developed, and all of the assumptions, uncertainties, and scientific judgments of the preceding three steps are presented.

THE ROLE OF IRIS IN RISK ASSESSMENT/RISK MANAGEMENT

IRIS is a tool that provides hazard identification and dose-response assessment information, but does not provide situational information on instances of exposure. **Combined with specific exposure information, the data in IRIS can be used for characterization of the public health risks of a given chemical in a given situation, which can then lead to a risk management decision designed to protect public health.**

The information contained in Section I (Chronic Health Hazard Assessment for Noncarcinogenic Effects) and Section II (Carcinogenicity Assessment for Lifetime Exposure) of the IRIS chemical files **represents a consensus judgment** of EPA's Reference Dose (RfD) Work Group or Carcinogen Risk Assessment Verification Endeavor (CRAVE) Work Group, respectively. These two Agency-wide work groups include high-level scientists from EPA's program offices (hazardous waste, air, pesticides) and the Office of Research and Development. Individual EPA offices have conducted comprehensive scientific reviews of the literature available on the particular chemical, and have performed the first two steps of risk assessment: hazard evaluation and dose-response assessment. These assessments have been summarized for IRIS and reviewed and revised by the appropriate work group. As new information becomes available, these work groups will re-evaluate their work and revise IRIS files accordingly. For more information, contact IRIS User Support in EPA's Environmental Criteria and Assessment Office, Cincinnati, OH (513/569-7254 or FTS 684-7254).

REFERENCES

NRC (National Research Council). 1983. The Nature of Risk Assessment. In: Risk Assessment in the Federal Government: Managing the Process. National Academy Press, Washington, DC. p. 18.

U. S. EPA. 1985. Principles of Risk Assessment: A nontechnical review. Prepared for a risk assessment workshop. Easton, MD, March 17-18.

LIMITATIONS OF IRIS INFORMATION

The information in the Integrated Risk Information System (IRIS) is most useful if applied in the larger context of risk assessment as outlined by the National Academy of Sciences. IRIS supports the first two steps of the risk assessment process [as summarized in Service Code (menu option) 4]; namely, the hazard identification and dose-response assesssment steps. The primary qualitative and quantitative risk data in IRIS, the reference doses (RfDs) and carcinogen assessments, can serve as guides in evaluating potential health hazards and selecting a response to alleviate a potential risk to human health.

The **reference dose (RfD)** can be used to estimate a level of environmental exposure at or below which no adverse effect is expected to occur. The RfD is an **estimate** (with uncertainty spanning perhaps an order of magnitude) of a daily exposure to the human population (including sensitive subgroups) that is likely to be without appreciable risk of deleterious effects during a lifetime. RfDs are based on an assumption of lifetime exposure and may not be appropriately applied to less-than-lifetime exposure situations. RfDs are also derived for the noncarcinogenic effects of chemicals that are carcinogenic.

The **carcinogen assessments** in IRIS begin with a qualitative weight-of-evidence judgment in the form of a classification as to the likelihood that a chemical may be a carcinogen for humans. This judgment is made independent of consideration of the agent's potency. A quantitative assessment, including slope factor and unit risk, is then presented. The slope factor is an upper-bound **estimate** of the human cancer risk per mg of agent/kg body weight/day. The unit risk, which is calculated from the slope factor, is an **estimate** in terms of either risk per ug/L drinking water, or risk per ug/cu.m air concentration.

In general, risk values, such as those in IRIS, cannot be validly used to predict the incidence of human disease or the type of effects that chemical exposures may have on humans. This is due to the numerous **uncertainties** involved in risk assessment, including those associated with extrapolations from animal data to humans and from high experimental doses to lower environmental exposures. The organs affected and the type of adverse effect resulting from chemical exposure may differ between study animals and humans. In addition, many factors besides exposure to a chemical influence the occurrence and extent of human disease.

Any change to an RfD, slope factor or unit risk as they appear in IRIS (for example, the use of more or fewer uncertainty factors than were applied to arrive at an RfD) invalidates and distorts their application in estimating the potential health risk posed by chemical exposure.

Each reference dose and carcinogen assessment is derived by an interdisciplinary work group of EPA scientists using consistent chemical hazard identification and dose-response assessment methods. These methods are outlined in Background Documents 1 and 2 (Service Code 5). It is important to note that the risk information in IRIS will be revised by these work groups when additional health effects data become available and new developments in risk assessment methods arise.

IRIS Questions & Answers

1) HOW CAN I GET ACCESS TO IRIS?

To obtain an IRIS account call Mike McLaughlin of DIALCOM, Inc. at (202) 488-0550 or write to:

Mike McLaughlin
DIALCOM, Inc.
Federal Systems Division
600 Maryland Avenue SW
Washington DC 20024

IRIS is also available through the Public Health Network (PHN) of the Public Health Foundation. Call Paul Johnson at (202) 898-5600 for more information. PHN is only available to local, state, and federal public health officials.

IRIS will be made available on the NIH National Library of Medicine's TOXNET system sometime during the fall or winter of 1988. At that time, call (301) 496-6531 for details.

2) HOW CAN I OBTAIN A DISK VERSION OF IRIS?

You can obtain a 5 & 1/4 floppy disk version of IRIS from the National Technical Information Service (NTIS). For the disk version call:

Stu Wiseman
NTIS
U.S. Department of Commerce
5285 Port Royal Rd.
Springfield, VA 22161
(703) 487-4807

The IRIS information on the PC disks sent to NTIS is in ASCII form. Since most vendors purchasing the IRIS disks wish to load IRIS on their own database software, only the data itself, and not a database front-end, is on the disks. NTIS has set the cost of the IRIS disks at $125.00. The IRIS disks will be updated quarterly, thus the total cost of the disks is $500.00 per year.

3) **HOW MUCH DOES IRIS COST?**

The user must pay only for the cost of accessing IRIS. The user will be billed by DIALCOM, Inc. There is a $25.00 monthly minimum which is applied against a usage fee of $25.00 per hour. In addition to the usage fee, there is a $.05 charge per computer screen accessed. There is no EPA charge for using IRIS.

Those eligible to access IRIS via the Public Health Network will be charged under a different set of fees. Contact the Public Health Foundation at (202) 898-5600 for more information.

4) **WHO DO I CALL IF I HAVE A QUESTION ABOUT USING IRIS?**

Call IRIS User Support at (513) 569-7254 or FTS 684-7254.

5) **WHO DO I CALL IF I HAVE A SCIENTIFIC OR TECHNICAL QUESTION ABOUT THE REFERENCE DOSES?**

Call the EPA Contact listed at the end of the reference dose section in the IRIS chemical file.

6) **WHO DO I CALL IF I HAVE A SCIENTIFIC OR TECHNICAL QUESTION ABOUT THE CARCINOGEN (CANCER) ASSESSMENTS?**

Call the EPA Contact listed at the end of the carcinogen assessment section in the IRIS chemical file.

7) **WHO DO I CALL IF I HAVE A SCIENTIFIC OR TECHNICAL QUESTION ABOUT DRINKING WATER HEALTH ADVISORIES?**

Call the Safe Drinking Water Hotline at 1-800-426-4791.

8) **WHO DO I CALL IF I HAVE A POLICY OR GENERAL QUESTION ABOUT IRIS?**

Call Rick Picardi at (202) 382-7315 or FTS 382-7315.

9) **HOW CAN MY ORGANIZATION GET TRAINING IN IRIS?**

Call IRIS User Support at (513) 569-7254 or FTS 684-7254.

10) **WHEN WILL (CHEMICAL NAME) BE INCLUDED IN IRIS?**

WHEN WILL THE REFERENCE DOSE FOR (CHEMICAL NAME) BE ADDED TO IRIS?

WHEN WILL THE CARCINOGEN ASSESSMENT FOR (CHEMICAL NAME) BE ADDED TO IRIS?

Call IRIS User Support at (513) 569-7254 or FTS 684-7254.

Occidental Chemical Corporation

NAPL IN BEDROCK BENEATH THE NIAGARA RIVER

ASSESSMENT OF HUMAN ENDANGERMENT

S-Area Remedial Program

CRA 5-0038533

May 1989
Ref. No. 1769

CONESTOGA-ROVERS & ASSOCIATES

OXY
Occidental Chemical Corporation

NAPL IN BEDROCK BENEATH THE NIAGARA RIVER

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S-Area Remedial Program

CRA 5-0038534

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NAPL IN BEDROCK BENEATH THE NIAGARA
RIVER ASSESSMENT OF HUMAN ENDANGERMENT

No. 2-881

CRA 9-0030318