An evaluation of groundwater flow in the freshwater aquifer in Essex County, Ontario, by computer modelling methods.

Jagadish Hebbur. Krishnamurthy
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AN EVALUATION OF GROUNDWATER FLOW
IN THE FRESHWATER AQUIFER IN ESSEX COUNTY, ONTARIO,
BY COMPUTER MODELLING METHODS

by

Jagadish Hebbur Krishnamurthy

A Thesis
submitted to the Faculty of Graduate Studies
and Research through the Department of Geology
in partial fulfillment of the requirements
for the degree of
Master of Science
at
The University of Windsor

Windsor, Ontario, Canada
1991
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ABSTRACT

The "freshwater aquifer" in Essex County, Ontario, Canada is a thin, discontinuous layer of granular material confined between the glacial overburden and the bedrock, plus the fractured bedrock subcrop. The freshwater aquifer is a major source of water supply where about 80% of the domestic wells tap water from it. The main objective of this study is to evaluate groundwater velocity in the freshwater aquifer by using oxygen-18 concentrations in groundwater, a knowledge of temporal variations in oxygen-18 in recharge water, and both the method of characteristics (MOC) and discrete state compartmental (DSC) model.

The aquifer parameters and the variables were discretised from well log records and other relevant documents. The oxygen-18 data were obtained from MacGregor (1985) and Crnkrok (1987, 1991). Initial conditions for the model were derived by using the aquifer parameters in association with isotopic data.

The method of characteristics model (MOC) is a finite difference model. It enables the simulation of groundwater flow and solute transport in two-dimensions. The finite difference matrix for the MOC was prepared using data from approximately 500 domestic wells. Trial and error experimental simulations were performed and the aquifer parameters estimated from the sensitivity analysis of the MOC model were compared with other similar studies of the freshwater aquifer.

The discrete state compartmental (DSC) model is designed on the basis of mixing cell theory used in chemical engineering. It enables the simulation of transportation of energy, mass and fluids in a flow system. The initial conditions for
the DSC model were also derived by using the well log records. The δ¹⁸O values in precipitation and average annual recharge in Essex County were provided by Crnokrak (1991). The DSC model of the study area consisted of 19 cells and was operated under steady state, steady flow and steady volume conditions. The results generated by the model were compared to previous work conducted in the region.

The groundwater velocity in the freshwater aquifer estimated by MOC model varies from 0.55 m/year to 2.6 m/year. The values for groundwater velocity estimated by DSC simulations varies from 0.5 m/year to 1.0 m/year. The average groundwater velocity in the freshwater aquifer in Essex County estimated by Crnokrak (1991) is 1.0 m/year. The average groundwater velocity in the freshwater aquifer in the Sarnia area estimated by Intera (1987) using field derived data is 0.8 m/year. The average groundwater velocity estimated by Long et al. (1988) in the drift aquifer in Bay County area in Michigan, U.S.A. using field derived data is 2.3 m/year.

The average flow across the freshwater aquifer was estimated to be 0.43 m³/year/m. On the basis of this factor, groundwater flow distribution was accomplished and the annual volumetric recharge was estimated to be 33675 m³/ year. This recharge parameter is somewhat more but close to the previous estimate, 28450 m³/year provided by Crnokrak (1991).
DEDICATED

To my sisters,

Jaya and Mangala
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1.0. INTRODUCTION

1.1. Background

The freshwater aquifer is a 1-3 m thick discontinuous layer of sand and gravel plus the upper part of the bedrock subcrop confined between the glacial overburden and the bedrock. The freshwater aquifer generally occurs at a depth of 30-35 m from the surface in the Essex, Kent and Lambton Counties in southwestern Ontario (Dreimanis and Karrow, 1972). In Essex County, the freshwater aquifer is a major source of water supply and about 80 % of the domestic wells tap water from it (Allendorf, 1981). Although major towns in Essex County have their water supplied from Lake St. Clair or Lake Erie, much of the surrounding area still depends on groundwater for domestic uses. In order to assess the susceptibility of the freshwater aquifer to pollution from surface sources, hydrogeological studies relevant to evaluation of flow properties and quality of groundwater have been carried out.

1.1.1. Previous Work

There have been several investigations of the freshwater aquifer in Essex County. Mellary and Nakashiro (1970) sampled the groundwater and produced a groundwater probability map. Hicks (1980) examined the sulphate content and reported higher sulphate concentration in groundwater from deeper zones, especially from the western parts of Essex County. Galinski (1983) examined shallow groundwater and reported lead and cadmium concentrations to exceed the standards set for drinking water. Blazevic (1985) also undertook a similar study and refuted Galinski's findings. However, both the studies concluded that the pollution may be
due to natural and/or anthropogenic sources.

MacGregor (1985) conducted an isotopic and geochemical study of groundwater in Essex County. He observed the co-existence of older glacial water with younger meteoric water in some parts of the study area and suggested that the freshwater aquifer may be susceptible to pollution from surface sources. Crnokrak (1987) focused attention on the areas where freshwater aquifer was susceptible to pollution. She suggested that mixing of waters of different isotopic signatures was probably caused either due to rapid vertical infiltration of precipitation through fractures and/or sand lenses or faulty well construction.

The vertical hydraulic conductivity in the till is reported to vary between $10^{-8}$ cm/s to $10^{-7}$ cm/s and the porewater velocity to be less than 0.53 cm/year (Desaulniers et al., 1981). On the basis of hydrogeological characteristics of the glacial overburden and the distribution of environmental isotopes and major ions, Desaulniers et al. (1981) suggested that the deep groundwater originated under cold climatic conditions during Holocene or Pliocene. Orpwood (1984) conducted an isotopic study and reported the porewater velocity in the glacial till to be in the order of 0.25-3.00 cm/year.

Allendorf (1981) assessed the susceptibility of groundwater to contamination in Essex County (Map S102, Ontario Ministry of Environment). The major factors that were considered in the preparation of Map S102 are type of soil, permeability, thickness of the overburden, influence of shallow aquifers and groundwater use. It has been suggested that, on the basis of a recent drilling investigation conducted by the Ontario Geological Survey, some buried eskers have been noticed in the eastern
parts of Essex County (Morris, 1989). Currently, hydrogeologic studies are being carried out to assess the role of fractured till and buried eskers in conveying meteoric water to the freshwater aquifer (Ainslie, personal communication).

1.2. Objectives

The objectives of the study are as follows:

(a) to characterise the velocity of groundwater in the freshwater aquifer using the method of characteristics model (MOC) and discrete state compartmental (DSC) model.

(b) to characterise the recharge and discharge rates for the freshwater aquifer using the DSC model.

1.2.1. Scope

The calibration of MOC model allows the simulation of groundwater flow and solute transport and the calibration of DSC model allows the simulation of groundwater flow distribution in the study area. The MOC model is commercially marketed by International Groundwater Monitoring Centre and the Water Resources Branch, U.S. Geological Survey. The software for the DSC model was obtained from the author of the model, Dr. Eugene Simpson, Department of Hydrology and Water Resources, University of Arizona.

The pre-requisite for modelling flow in the freshwater aquifer is to obtain isotopic data and use it as a basis to initiate the computer models. The $^{18}$O data were obtained mainly from MacGregor (1985) and Cmokrak (1987, 1991) and also from Ainslie (personal communication) and Ibrahim (personal communication). The
variables for each computer model were prepared by discretising the aquifer parameters from the well log records and in association with the isotopic data, initial conditions were derived. Groundwater samples were collected from 12 domestic wells and were prepared for carbon-14 analysis. The results from isotopic analyses and computer simulations were compared with the results obtained from previous investigations conducted in the region.

1.3. Organisation of This Thesis

This thesis consists of five main chapters. The first chapter provides the introduction, objectives and scope of the study. The second chapter describes the geologic setting and the hydrogeology of the study area. This chapter emphasises the physical aspects of flow in the freshwater aquifer and the direction of the groundwater movement in the study area. The third chapter presents the methods of study and includes theoretical considerations associated with both isotopic and computer modelling methods used in this study. The results of the isotopic study and sensitivity analyses relevant to flow modelling are discussed in the fourth chapter. The fifth chapter gives the conclusions and recommendations for future research.
2.0. THE STUDY AREA

2.1. Location

Essex County is located in southwestern Ontario, on the international border between Canada and United States (Figure 1). It covers an area of approximately 1790 km², excluding Pelee Island, and is bounded by 82°25' W longitude in the east, 83° 25' W in the west, 42° 20' latitude in the north and 42° 00' latitude in the south. Essex County is bounded by Lake St. Clair to the north, Lake Erie to the south, Kent County to the east and Detroit River to the west. The prominent demographic features are the cities of Windsor on the Canadian side and Detroit on the American side.

2.1.1. Climate

The mean temperatures are between 4.2 °C to -2 °C in winter and between 4 °C to 22 °C in summer. The mean annual rainfall is 76 - 84 cm/year and the highest is recorded in June and July. The mean annual snow fall recorded at Windsor Airport is 104.5 cm/year reaching a peak of 25.9 cm in January and February (Sanderson, 1980). The climate of the region is influenced by its proximity to Great Lakes and somewhat by its urban centres. The climate is considered to be humid continental type with warm summers and cold winters (Muller, 1974).

2.1.2. Topography

Essex County is generally flat with an average elevation of 186 m above mean sea level. The region owes its flat terrain to Lake Whittlesey, a glacial lake which covered the region about 13,000 years ago (Chapman and Putnam, 1966). The
highest natural elevation is due to the morainic ridge, near Leamington, which stands approximately 30 m above the local elevation. In general, the topography slopes towards Lake St. Clair in the north however, a small portion in the southern part slopes towards Lake Erie (Vandall, 1965). There are no distinct drainage divides in the area, but the local high directs surface run off. River Canard constitutes the largest river system draining towards the Detroit River, while other stream systems drain either towards Lake St. Clair or towards Lake Erie (ERCA, 1975).

2.1.3. Access

The entire study area has a good network of roads for transportation within the region. The Highways 401, 18, 3, are the major roads and the County Roads 2, 5, 8, 11, 19, 23, 27, 31, 35, 42, 77, some of which are also town lines, extend the access to various points in the study area. Figure 1 is a map showing the geographic location and access within the study area.

2.2. Geology of the Study Area

2.2.1. Bedrock Geology

The study area is located on rim of the Michigan Basin overlapping with the adjacent Appalachian Basin located to the southeast. Essex County and the surrounding areas are seated on the structural flexure between these two Paleozoic basins. The Findlay Arch and the Algonquin Arch are the elements of the flexure. The plunging point of these two arches form the Chatham Sag, running northwest-southeast, is located to the east of the study area (Intera, 1987).
Figure 1. Location and access in the study area.
The bedrock underlying Essex County is composed of limestone and shale belonging to the Middle Devonian age (Hewitt, 1972). There are no reported outcrops but the excavations due to mining and quarrying near Amherstburg expose the Detroit River Group (Sanford, 1957).

The Detroit River Group consists of limestone and dolostone and is predominantly found in the southern parts of the county. The Detroit River Group is overlain by the Dundee Formation, consisting of buff coloured limestones and chert. This formation underlies the northern parts of Essex County. The Dundee Formation is overlain by grey shale and limestone belonging to the Hamilton Group. With the exception of Maidstone and Tilbury Townships, the Hamilton Group Formation is otherwise confined to Kent and Lambton Counties (Freeman, 1979). The subcrop map (after Freeman, 1979) and details relevant to the bedrock geology of Essex County are presented in Appendix 1.

2.2.2. Surficial Geology

The top soil in the study area is comprised of various types of clays, sandy loams and sand. The predominant type of soil is known as Brookston Clay (Chapman and Putnam, 1966). Essex County and other areas adjacent to Lake St. Clair have their bedrock covered by glacial till deposited during the early stages of Wisconsin glaciation (Driemanis and Karrow, 1972). The till is glaciolacustrine in origin and consists of carbonate, quartz, feldspars and shale fragments. The average grain size distribution observed in the till is 40-60 % clay, 30-40 % silt, 5-10 % sand and less than 5 % of gravel (Desaulniers et al., 1981).
The glacial drift varies in thickness from a minimum of 3-4 m near Amherstburg to a maximum of 45 m near Tilbury (Vagners et al., 1973). The glacial till is weathered and fissured at the surface and often exhibits coating due to secondary mineralisation on the fracture surfaces. The average depth of fractures observed in the till overburden in southwestern Ontario is about 5-6 m although, in some places it is thought to go deeper (Hanna, 1966). It is also not uncommon to observe sand lenses occurring close to, or within, the weathered layer. These may considerably affect the local hydrogeologic conditions in areas where they are observed (M.M. Dillon, 1987; Intera, 1987).

The weathered glacial till is underlain by an unweathered zone comprised of blue, grey and brown coloured clay intercalated with silt and fine sand. The unweathered zone extends to a depth of 30-40 m and occasionally includes irregularly distributed lenses of sand and gravel (Vagners et al., 1973). The freshwater aquifer is confined between the glacial till and the bedrock.

2.2.3. Glacial Features

The most common glacial features observed are recessional moraines, striking northwest-southeast, and in a few places east-west directions. A small morainic hill about 25-30 m above the local elevation near Leamington is noted to be the highest natural elevation (Vandall, 1965). A recent drilling investigation conducted by the Ontario Geological Survey indicated the presence of buried eskers striking north and northwest (Morris, 1989). Currently, studies are being carried out to establish the presence of eskers and their influence on the regional groundwater flow (Ainslie,
personal communication).

2.3. Hydrogeology of the Study Area

Groundwater movement in Essex County is affected by the flat topography that imposes a low hydraulic gradient and the low permeability of the glacial till. These two factors contribute towards slow movement of groundwater in the study area. Some locations within the study area, with abundant sand and sandy soils with good infiltration characteristics, constitute recharge areas (Allendorf, 1981). Groundwater recharge occurs from the sandy zones in the southern parts of the county, around Leamington, and it is discharged along the shores of Lake St. Clair, the Detroit River and Lake Erie.

2.3.1. Direction of Groundwater Flow

2.3.1.1. Evaluation of Flow Based on Hydraulic Head Distribution

Figure 2 is a map showing the hydraulic head distribution in the study area. This hydraulic head map was prepared using the data from approximately 500 wells completed in the freshwater aquifer with an average of 40-50 wells selected from each township. The author obtained the details relevant to hydraulic head distribution from the Ontario Ministry of Environment (1974). Since the data in this document is presented in feet/pound/second units, the hydraulic head map is presented in feet above mean sea level. A preliminary investigation of the hydraulic head distribution indicates that the general direction of groundwater flow is towards the north and northwest sections of the study area.
Figure 2. Generalised distribution of hydraulic head in the study area. (units = ft.)
The higher values of hydraulic head indicates that the aquifer is recharged from Mersea and Gosfield South Townships and discharge zones are areas mainly bordering Lake St. Clair and Detroit River. A small component of flow is also directed towards Kent County in the east. The direction of groundwater movement along the border of Essex and Kent Counties is also towards Lake Erie due to recharge from Thames River (Pettapiece, 1988).

2.3.1.2 Evaluation of Flow Based on the Distribution of Electrical Conductivity

Pure water has a low electrical conductivity (EC) but it acquires higher EC values when the total dissolved solid (TDS) content increases. Electrical conductivity is linearly related to the total dissolved solid content of groundwater and is reported in micro siemens (μS/cm) (Eriksson, 1985). Since the chemistry of groundwater evolves along a flow path, both the TDS and EC will gradually increase along the flow path. The EC and TDS will be lowest near the recharge areas and increase along the direction of groundwater movement, reaching a maximum near the discharge areas.

Figure 3 is a map showing the distribution of EC in the study area. The data used in the preparation of the EC map was obtained through the investigations conducted by MacGregor (1985) and Crnokrak (1987, 1991). The EC measurements suggest that the general direction of groundwater movement in the study area is towards the north and northwest direction. It can be noticed that the distribution of EC contours generally concurs with the general direction of groundwater flow.
Figure 3. Distribution of electrical conductivity in the study area. (units = μS/cm) (after Macgregor, 1985 and Crnokrak, 1987, 1991)
2.3.1.3. Evaluation of Flow Based on the Distribution of Oxygen-18 Isotopes

Oxygen-18 ($^{18}$O) is a stable isotope of oxygen whose natural concentrations in groundwater may be used to understand the movement of groundwater in aquifers. The concentration of $^{18}$O in precipitation is directly related to temperature of condensation (Faure, 1977). The variations in $^{18}$O concentration in precipitation has been attributed to factors such as latitude, altitude, distance from the coast, amount of precipitation and seasonal variations of $^{18}$O in the atmosphere (Dansgaard, 1964).

The variations in the $^{18}$O isotope content in groundwater are directly related to the differences in the composition of original recharge water entering the aquifer during recharge events (Davis et al., 1985). The groundwater in the recharge areas reflects the annual average $^{18}$O concentration in precipitation and groundwater in the downgradient direction will be depleted in its $^{18}$O concentration (Fritz et al., 1981). Thus, the distribution of $^{18}$O isotopes can be utilised to interpret the direction of groundwater movement in an aquifer.

Figure 4 is a map showing the $^{18}$O contours of groundwater in the study area (Crnokrak, 1991). The $^{18}$O contours exhibit a depletion of $^{18}$O in the northern sections of the study area, gradually becoming less depleted towards the southern sections. This pattern of depletion in the $^{18}$O concentration towards the north indicates that groundwater is moving towards the north and northwest directions. The distribution of $^{18}$O isotopes also concurs with the general direction of groundwater flow.
Figure 4. Distribution of oxygen-18 isotope in the study area
2.3.1.4. Vertical Movement of Groundwater

The vertical movement of groundwater in the unweathered layer is very slow due to the low permeability of the till and the water table is usually within 2 m from the surface (Allendorf, 1981). The hydraulic conductivity of the till is estimated to be in the order of $10^{-4}$ to $10^{-7}$ m/s (Desaulniers et al., 1981). The porewater water velocity in the till is reported to be in the range of 0.25 - 3.00 cm/year by Orpwood (1984) and less than 0.53 cm/year by Desaulniers et al. (1981).

The vertical activity of groundwater within the bedrock is limited to fractured zones. There are no significant differences in the chemistry and isotopic content of the water within the fractured bedrock and the overlying freshwater aquifer (Dollar et al., 1987). Therefore, this part of the bedrock may also be considered as a part of the freshwater aquifer (Sklash, personal communication). The groundwater in the Dundee formation is somewhat depleted in $^{18}$O and diluted in its chemistry and suggests that there is some infiltration from the freshwater aquifer. The deeper bedrock members are characterised by formation waters which are saline and isotopically very different from that of freshwater aquifer (Dollar et al., 1987).
3.0. METHODS OF STUDY

The pre-requisite for characterising the groundwater velocity is to derive the initial conditions and use them as a basis to model flow in the freshwater aquifer. The initial conditions for method of characteristics (MOC) model and discrete state compartmental model (DSC) were established by discretising the aquifer parameters using the field data. The oxygen-18 ($^{18}$O) data were obtained from MacGregor(1985) and Crnokrak(1987, 1991). The precipitation input $\delta^{18}$O values and corresponding timing of recharge, modified after Edwards and Fritz(1986), were provided by Crnokrak(1991).

In order to establish groundwater ages, a sampling program was undertaken to obtain carbon-14 data. Groundwater samples were obtained from 12 domestic wells and were prepared for $^{14}$C analysis. However, $^{14}$C data were not used because some of the samples were affected by sulphate reduction and methanogenesis (Aravena, personal communication).

3.1. Theoretical Considerations

3.1.1. Environmental Isotopes

Isotopes are atoms of the same element each with the same proton number but with different mass numbers (Faure, 1977). In hydrogeological studies, isotopes are employed for tracing groundwater movement in aquifers. Groundwater tracing studies are conducted by either artificially injecting a tracer into the water or by utilising environmental isotopes. The environmental isotopes are naturally occurring isotopes whose abundance variations may be used in hydrogeologic studies.
Tritium ($^3$H), oxygen-18 ($^{18}$O), deuterium (D) and carbon-14 ($^{14}$C) are some examples of environmental isotopes (Freeze and Cherry, 1979).

The hydrogeological and investigations that widely use environmental isotopes are related to the study of the (a) origin and age of groundwater; (b) transportation of reactive and non-reactive solutes in saturated and unsaturated zones; (c) runoff mechanisms in surface waters; (d) groundwater-surface water interactions; (e) numerical modelling of groundwater flow and solute transport; and, (f) characterisation of aquifer parameters in field and laboratory experiments (Fritz and Fontes, 1980).

3.2. Oxygen-18

Oxygen has three isotopes: 99.673 % are oxygen-16 ($^{16}$O), 0.0375 are oxygen-17 ($^{17}$O), and 0.1995 are oxygen-18 ($^{18}$O) (Hoefs, 1987). Since the concentration of $^{18}$O is low, the ratio of heavy to light species is used to report concentrations. The ratio of heavy to light species, determined by mass spectrometry, is expressed as:

$$R = \frac{^{18}O}{^{16}O} \quad \text{(Faure, 1977)}.$$  

The concentrations are measured with reference to a standard and are reported in delta ($\delta$) units as:

$$\delta\%_\circ = \frac{R_{\text{sample}} - R_{\text{standard}}}{R_{\text{standard}}} \times 1000$$

where, $\%_\circ$ is per mille or parts per thousand. The $R_{\text{standard}}$ is Standard Mean Ocean Water (SMOW) whose $\delta$ value is 0.0 $\%_\circ$ (Craig, 1961).
If a sample is enriched in $^{18}$O relative to the standard then the $\delta$ values are reported with a positive prefix, while a negative prefix indicates depletion of $^{18}$O in the sample relative to the standard.

Due to the vapour pressure difference between the lighter and the heavier species, the process of isotopic fractionation has the lighter isotopes enter the vapour phase and the heavier isotopes enter the liquid phase. The isotopic fractionation in meteoric waters follows the Raleigh distillation process and, as a result of this process, precipitation events become progressively depleted in the heavy isotopes (Faure, 1977).

It has been observed through a network of sampling stations around the world that precipitation events exhibit seasonal variations in the stable isotopic composition. The seasonal variations are produced due to differences in the temperature of condensation. The winter precipitation events show depletion in heavier species relative to the summer precipitation (Gat, 1980). The degree of depletion of $^{18}$O in global meteoric waters has been attributed to factors such as latitude, altitude, distance from the coast, amount of precipitation and seasonal variations of $^{18}$O in the atmosphere (Dansgaard, 1964). The latitude effect over the North American continent is $0.5 \% \delta^{18}O /$ degree latitude (Yurtsever, 1975).
3.2.1. Application of $^{18}$O in Hydrogeologic Studies

A relationship has been established between mean annual $^{18}$O concentration in precipitation and annual temperature as follows:

$$
\delta^{18}O \, \% = 0.69 \, t_{air} - 13.6 \, \% 
$$

where, $t_{air}$ is the air temperature (Dansgaard, 1964). In other words, $^{18}$O concentration in precipitation becomes progressively depleted with decreasing temperature. In confined aquifers, the distribution of $^{18}$O in groundwater can therefore be used to estimate the temperature variations covering the time of recharge.

Investigations of $^{18}$O in shells and wood cellulose conducted in southwestern Ontario show a steady increase in $^{18}$O concentration, and indicate amelioration of atmospheric temperatures in the region (Fritz et al., 1975; Edwards and Fritz, 1986). These studies also show the occurrence of a dramatic increase in the earth’s atmospheric temperature and the enrichment of the stable isotopic composition in precipitation, approximately 10,000 years ago. The groundwater in some parts of southern Ontario exhibits depletion in its $\delta^{18}$O concentration indicating that recharge occurred under colder climatic conditions during Holocene or Pliocene roughly about 10,000 years ago (Desaulniers et al., 1981).

Since groundwater in recharge zones exhibits $\delta^{18}$O values similar to that of meteoric waters in the region (Fritz et al., 1975), it follows that groundwater in the down gradient direction reflects the average annual $\delta^{18}$O values of precipitation events that occurred prior to the recharge. It is suggested that, on the basis of observing depleted $^{18}$O values in the basal till units in southwestern Ontario, groundwater
recharged prior to 10,000 years ago had $^{18}$O concentrations of -16 ‰ to -20 ‰ (Desaulniers et al., 1981). The oldest waters in Essex County have $\delta^{18}$O values of -16 ‰ and the youngest waters have -8 ‰ (MacGregor, 1985; Crnokrak, 1987). The groundwater recharged from the past 10,000 years is suggested to have $\delta^{18}$O values of -9 ‰ to -11 ‰ which is indicative of the present day rainfall (Sklash et al., 1986; Desaulniers et al., 1981).

Thus, based on the results of isotopic studies, it may be assumed that the freshwater aquifer initially contained groundwater depleted in its $^{18}$O concentration that was recharged approximately 10,000 years ago. Since the variations in the $^{18}$O concentration in groundwater are directly related to the differences in the composition of original recharge water entering the aquifer, the distribution of $^{18}$O concentrations may be used to trace groundwater movement in an aquifer (Davis et al., 1985).

The $^{18}$O isotope distribution in the study area shown in Figure 4 (after Crnokrak, 1991), suggests that the general direction of groundwater movement in Essex County is predominantly towards the north and northwest direction and a small component of flow towards the northeast direction. Since the isotopic data from the freshwater aquifer show concentration of $^{18}$O in the past and in the present time, it provides a basis to derive initial conditions to account for the distribution of groundwater flow (Campana, 1975).
3.2.2. $^{18}$O Reaction with the Freshwater Aquifer

$^{18}$O is a stable isotope and is not affected by chemical reactions (Faure, 1977). However, $^{18}$O enrichment in water occurs from isotopic exchange due to water-rock interaction at elevated temperatures (Hoefs, 1987). The enrichment of $^{18}$O resulting from higher temperatures (40 °C - 50 °C) is reported to have occurred in the brines in Michigan Basin and Illinoian Basin (Clayton et al., 1966). It is unlikely to observe enrichment of $^{18}$O in groundwater in the study area as a result of being affected by higher temperatures.

Fritz et al. (1974) reported $\delta^{18}$O values ranging from -16‰ to -19‰ in the Upper Carbonate Aquifer in Central Manitoba. The average depth of the Upper Carbonate Aquifer is reported to be 50 m. These depleted $^{18}$O values, Fritz et al. (1974) suggest, do not show evidence of $^{18}$O enrichment and are typical of recharge events that occurred under cold climatic conditions in central Manitoba. The laboratory experiments conducted by Kennedy et al. (1986) on the composite soil cores collected from the vadose zones have shown that isotopic exchange between water and most minerals is extremely slow under normal ambient conditions.

The $^{18}$O values observed in the freshwater aquifer are indicative of recharge events that occurred under cold climatic conditions (Desaulniers et al., 1981) and the vadose zones in the recharge areas have good infiltration characteristics (Allendorf, 1981). On the basis of all these observations, it may be presumed that $^{18}$O concentration in the freshwater aquifer is not affected by water-rock interactions.
3.3. Time Span of Recharge in the Study Area

The glacial materials in southwestern Ontario were deposited under subaqueous conditions during the early stages of Wisconsinan glaciation (Driemanis and Karrow, 1972). The oldest glacial material comprised of silty clay is suggested to have been deposited during early Wisconsinan stage (Morris, 1988). The radiocarbon age measurements of the Cedar wood contained in the beach sands overlying the glacial deposits display ages of approximately 10,000 years before present (Morris, 1989).

The glacial overburden in Essex County is suggested to be smoothed out by Lake Whittlesey. Following this stage, the region was submerged under Lake Warren which prevailed approximately 13,000 years before present (Chapman and Putnam, 1984). Essex County and the surrounding regions were exposed following the Port Bruce advance during Lake Iroquis - Lake Grassmere levels and the radiocarbon dates of sediments deposited during this stage show ages between 13,000 to 12,500 years before present (Chapman and Putnam, 1984).

Therefore, it may be presumed that the meteoric waters have infiltrated into the freshwater aquifer over the last 12,500 years. The $^{18}$O concentration in Essex County is suggested to have been $-18\%$ about 12,500 years before present and it follows that the freshwater aquifer initially contained water having $-18\%$ or more depleted $\delta^{18}$O values. On the basis of this knowledge, a time span of 12,500 years which will accommodate changes in $\delta^{18}$O values from $-18\%$ to $-8\%$ will be used for the computer simulations.
3.4. The MOC Model

The method of characteristics (MOC) model was developed by Konikow and Bredehoeft (1979) for the U.S. Geological Survey to enable the simulation of groundwater flow and solute transport in an aquifer. The working principle of the MOC model is based on finite difference modelling methods. The model is programmed to simulate two dimensional flow under steady state or transient flow conditions in an aquifer which may be either or both heterogeneous and anisotropic.

The model is capable of computing changes in the initial concentration of a solute produced over time by physical processes such as advective transport, hydrodynamic dispersion and mixing from other bodies of groundwater. In addition, changes in the initial concentration of the solute produced due to chemical processes such as retardation, radioactive decay, linear and non-linear sorption and ion exchange reactions may also be computed. Properly calibrated models can be employed to project changes in the groundwater quality in an aquifer on a spatio-temporal context.

The first version of MOC (Konikow and Bredehoeft, 1979) was limited to modelling the flow of groundwater and transportation of non-reactive contaminants within an aquifer. The updated version of MOC (Konikow and Goode, 1989), is somewhat more flexible in its applicability and allows the simulation of both reactive and non-reactive solute transport. The modifications in the updated version incorporate solutions for first order reactions, irreversible rate-reactions, linear and non linear equilibrium-controlled sorption, and equilibrium-controlled ion exchange.
The first version allows a 20 by 20 grid size and the updated version allows the usage of 40 by 40 grid size and enables the inclusion of larger portions of a study area.

The finite difference equations describing groundwater flow and solute transport are coupled and solved by numerical approximation procedures. The computer program uses the alternating direction implicit (ADI) or strongly implicit procedure (SIP) to solve the finite difference approximation for groundwater flow. The SIP is used to solve flow equations when areal discontinuities in transmissivity exist or when the ADI solution does not converge. The solute transport equations are solved by the method of characteristics.

3.4.1. System Requirements

The minimum requirements for PC versions of MOC are:

(a) IBM-PC, XT or AT (b) 640K RAM (c) DOS 2.0 or higher and, (d) 80287 or 80387 Math co-processor. The minimum requirements for the mainframe versions are: (a) Fortran 77 compiler (b) 132 column dot matrix printer.

3.4.2. The PREMOC Program

The MOC package includes a preprocessor, PREMOC, that can be used to input the data into the main program. Alternatively, the data can be input using any suitable ASCII text editor. The PREMOC version 3.4 written by Srinivasan (1989), allows the user to prepare or edit a data file in an interactive mode and transfer it into the main program. A help module built into the PREMOC is made easily accessible at any stage of data file preparation. The program documentation includes the format for all the variables that are specified from PREMOC into the MOC program.
The data file prepared from PREMOC has to be completed carefully in order to avoid errors and to facilitate easy execution of the subroutines.

3.4.3. Equation Describing Groundwater Flow

The equation describing the transient two-dimensional flow of a homogeneous compressible fluid flow through a non-homogeneous anisotropic aquifer written in cartesian tensor notation (after Pinder and Bredehoeft, 1968., quoted in Konikow and Bredehoeft, 1979) is

\[
\frac{\partial}{\partial x_i} \left[ T_{ij} \frac{\partial h}{\partial x_j} \right] - S \frac{\partial h}{\partial t} = w \quad i, j = 1, 2
\] (1)

where:

- \( T_{ij} \) is the transmissivity tensor, \( L^2/T \)
- \( h \) is the hydraulic head, \( L \)
- \( S \) is the storage coefficient, (dimensionless);
- \( t \) is the time, \( T \);
- \( W = W(x, y, t) \) is the volume flux per unit area, \( L/T \)

(positive sign for outflow and negative for inflow)

- \( x_i \) and \( x_j \) are Cartesian coordinates, \( L \).

When fluxes such as withdrawal or recharge due to pumpage, well injection or evaporation and steady leakage into or out of the aquifer are taken into account, then \( W(x, y, t) \) can be expressed as (Konikow and Bredehoeft, 1979)

\[
W(x, y, t) = Q(x, y, t) - \frac{K_f}{m} (H_o - h)
\] (2)
where:

$Q$ is the rate of withdrawal (positive) or recharge (negative), L/T;

$K$ is the vertical hydraulic conductivity, L/T;

$m$ is the thickness of the confining layer, streambed or lakebed, L;

$H_s$ is the hydraulic head in the streambed or the sourcebed, L;

3.4.4. Equation Describing Solute Transport

When constant and uniform porosity and fluid density in two-dimensions are assumed, the equation describing solute transport may be expressed as (after Konikow and Grove, 1977):

$$
\frac{\partial C}{\partial t} - \frac{1}{b} \frac{\partial}{\partial x_i} \left( D_{ij} \frac{\partial C}{\partial x_j} \right) - V_i \frac{\partial C}{\partial x_i} + \frac{W(C-C')}{\varepsilon b} + \frac{\text{CHEM}}{\varepsilon} \tag{3}
$$

where:

$C$ is the concentration of the solute, M/L$^3$;

t is the time, T;

$b$ is the aquifer thickness, L;

$D_{ij}$ is the dispersion tensor, L$^2$/T, with implied summation for $i=1,2, j=1,2$;

$x_i$ are the spatial coordinates, L;

$V_i$ is the fluid seepage velocity, L/T;

$W$ is the source fluid flux into the ($W<0$) aquifer, L/T;

$\varepsilon$ is the porosity, (dimensionless);

$C'$ is the chemical reaction source (+)/sink (-) per unit volume of the aquifer, M/L$^3$;

CHEM is the type of chemical reaction source or sink, M/L$^3$/T.
For a detailed discussion of the flow and transport equations, the reader is referred to (a) Techniques of Water Resources Investigation Book 7, Chapter 2, (Konikow and Bredehoeft, 1979) and, (b) Water Resources Investigations Report 89-4030, U.S. Geological Survey (Konikow and Goode, 1989).

The equations describing groundwater flow are partial differential equations and exact analytical solutions cannot be obtained because of the complex boundary conditions and variability within the physical framework of the aquifer. The flow equation is written in a finite difference form by considering the principal directions of the transmissivity tensor. The finite difference equation describing groundwater flow is solved by the iterative alternating implicit procedure (ADI) or strongly implicit procedure (SIP) (Konikow and Bredehoeft, 1979). The equation describing solute transport is a hyperbolic equation and cannot be solved directly on a digital computer. Instead, a system of equivalent linear equations that are analogous with the transportation equation are devised and then solved by numerical approximation using the method of characteristics (Konikow and Goode, 1989).

The MOC model is based on a block-centred, rectangular finite difference grid which is overlain on the area of interest. The nodes of the finite difference grid are located at the centre of the cells to represent the average values of the hydrogeologic parameters such as transmissivity, aquifer thickness and hydraulic conductivity for the area enclosed by a cell. The physical parameters of the aquifer are specified to the model in the form of matrices whose elements vary depending on the type of physical character represented by a particular matrix. The grid system actually represents the
physical framework of the aquifer and provides the matrix form to the model.

The initial conditions such as thickness, hydraulic head, transmissivity, reactive or non-reactive solute, etc., are specified by discretising the field data for all the cells in the grid system. The boundary conditions assumed by the model, either constant-head or constant-flux, may be implemented by setting up zero transmissivity in the outer cells of the grid system.

3.4.5. Particle Tracking

The method of characteristics employs the particle tracking procedure (Konikow and Bredehoef, 1979) as a basis to solve the solute transport equation. Figure 5 shows a section of the finite difference grid and the particle tracking procedure. A number of particles, pre-determined to avoid high density, are introduced in a uniform pattern into the grid system. Initially, the particles are placed in each of the cells and the locations of these particles will be defined by using the spatial co-ordinates. Each particle is temporarily assigned a concentration value before introducing it into the system. The initial concentration associated with all the particles in a given cell will describe the initial concentration of the node in that cell. The particles are allowed to move a small distance proportional to the velocity at that point and length of time increment for that iteration.

At each step of the iterative procedure changes in the concentration are recorded and the nodes are re-assigned the average concentration value computed from the particles present within the cell.
Figure 5. A hypothetical finite difference grid showing the particle tracking procedure (after Konikow and Bredehoeft, 1979)
New particles are introduced into the system at regular intervals and the changes in concentration of these particles are tracked until they are flushed out of the system due to discharge. In effect, these moving particles simulate convective transport because the concentration of each node varies as different particles with different concentration enter and leave the system (Konikow and Bredehoefit, 1979; Konikow and Goode, 1989).

The changes in the locations of the particles are computed by observing the differences in the X and Y coordinates of the particle prior to and after every particle movement. The X and Y velocities of a particle are calculated using bilinear interpolation over half the area of the cell using the X and Y velocities calculated at adjacent nodes and cell boundaries. The changes in the chemical concentration are calculated by method of characteristics and matrix methods.

3.4.6. Model Assumptions

Some of the important assumptions included in the MOC model are:

1. Darcy’s law is valid and hydraulic head gradients alone are responsible for fluid flow.

2. Hydraulic conductivity of the aquifer is constant and porosity is uniform through space and time.

3. The velocity distribution is not affected by gradients of fluid density, viscosity, and temperature.

4. The fluid properties and aquifer properties are not affected by chemical reactions.

5. The vertical variations in head and concentration are negligible.
(6) The changes in the total dispersive flux due to ionic and molecular diffusion are negligible.

(7) The aquifer parameters are homogeneous and isotropic and coefficients of longitudinal and transverse dispersivities remain constant.

For complete details on other model assumptions, the reader is referred to Konikow and Bredehoeft (1979) and Konikow and Goode (1989).

3.4.7. Stability Criteria

There are several stability criteria built into the program to control errors. The iterative procedures in the finite difference technique usually introduce some errors due to the 'numerical dispersion'. By using the method of characteristics to solve the solute transport equation, the oscillations of numerical dispersion are smoothed. The program computes mass balance errors caused due to variation in the number of particles in the system and only accepts less than 10% error to solve the transport equation.

The increments in the time step intervals are automatically optimised and smaller time steps are calculated by the program when the time input parameter is too high. The program also takes care of the concentration changes due to the deviation of particle flow path, over-crowding in a cell and the maximum number of cells that can be devoid of particles during the iterations (Konikow and Bredehoeft, 1979).

3.4.8. The Computer Program

The source code is written in Fortran 77 and requires a Fortran compiler for editing purposes. The first version has eight subroutines. The updated version
maintains the same structure, however, two more subroutines are added to the main
version to perform corrections for the effect of chemical changes on solute transport
(Konikow and Goode, 1989). The flow chart of the original program and the updated
portion is presented in Appendix 2. The software package includes program listing
and definitions of selected variables. The program documentation in the PREMOC
provides information on data input procedure.

3.4.9. Model of the Study Area

Figure 6 shows the finite difference grid map of the study area and the
distribution of the cells in the matrix consisting of 20 columns and 15 rows. The grid
system has 300 cells of which 101 cells are located outside the boundary of the study
area. Due to lack of data, parts of Tilbury North and Point Pelee peninsula are not
included in the model. The length of a cell was arbitrarily set to 3 km on each side
of the cell.

The three basic types of cells shown in the Figure 6 are inactive cells, active
cells and source cells. The source cells represent recharge areas through which water
and solutes enter the aquifer. The recharge is assumed to enter the aquifer
instantaneously. The active cells are those that take part in groundwater flow and
solute transport and record changes during particle tracking procedure. The inactive
cells lie on the fringes of the finite difference grid and form the boundary cells or
zero transmissivity cells and do not take part in flow simulation. The nodal value of
the cells represents the arithmetic average of the parameters observed from the well
log records for wells located in each of the cells.
Figure 6. The finite difference grid map of the study area.
The data were taken from approximately 70 wells from each township and at least 6-7 wells should occur within each cell. The thickness value specified in each cell is that of the sand and gravel aquifer in that cell plus 1 m of the underlying bedrock. The bedrock is partially weathered and fractured within the top and actively participates in the flow. It maintains continuity of groundwater flow at some spots where the sand and gravel aquifer is absent. Besides, chemically and isotopically, the water in this zone is not different than that of the draping sand and gravel layer. Therefore, the upper 1 m of the bedrock was considered to be a part of the freshwater aquifer for the simulations.

3.4.9.1. Input Parameters

Data input was accomplished using the PREMOC program. When the PREMOC program is used to specify the parameters into the model, some data sets related to the physical framework of the aquifer need be specified once only. The data specified only once included the following:

a) aquifer thickness and static water levels.

b) number of columns and rows, 20 and 15, with cell dimension of 3 km on each side. The choice of this grid size allowed the utilisation of maximum number of data points.

c) an initial pumping period of 500 years followed by 12 pumping periods each for a duration of 999 years. The output from the initial pumping period was used to specify initial concentration for the 12 pumping periods.

d) specification of $^{18}$O concentration. The $^{18}$O concentration of precipitation in
southwestern Ontario was -18% and the $^{18}$O concentration in the present day precipitation is -8%. The input concentration for each pumping period was specified based on the $^{18}$O variation observed in the study area. Figure 7 shows the variation of $^{18}$O input in the meteoric water in the study area.

3.4.9.2. Sensitivity Analysis of MOC

The data that were modified during the simulations are hydraulic conductivity, dispersivity and porosity. The sensitivity of the MOC model to variations in these parameters was used to estimate the best values for the model of the study area. During the initial stages, various values of hydraulic conductivity were specified to the model. Based on the results obtained, the best value of hydraulic conductivity was estimated for the freshwater aquifer in the study area. Modifications in the dispersivity values were made to improve the results generated by the model. The model sensitivity to variations in porosity was tested after best estimates for hydraulic conductivity and dispersivity were obtained.

Following the estimation of hydraulic conductivity, dispersivity and porosity values, the groundwater velocity in the study area was characterised.

3.4.9.3. Discussion of Validity of MOC Assumptions

The concentration gradients of TDS and $^{18}$O isotopes exist within the freshwater aquifer. However, these gradients are not significant enough to become major driving forces to cause flow of groundwater. Therefore Darcy’s Law may be considered valid and hydraulic head gradients alone are responsible for flow.
Figure 7. Variation of $^{18}$O input concentration in the meteoric water in the study area (after Crnokrak, 1991).
The values of hydraulic conductivity reported for the freshwater aquifer are in the range of $10^{-5}$ m/s and these values are representative of K values on a local scale. Therefore, a constant hydraulic conductivity may be assumed while characterising groundwater flow on a regional context.

Fluid density, viscosity and temperature variations are taken into account while modelling multi-phase fluid flow. Since this study is aimed towards modelling flow of groundwater, fluid properties do not affect velocity distribution. The dissolution-precipitation reactions do not affect the fluid and aquifer properties. However, the infinitesimal changes due to chemical reactions may be considered insignificant while modelling flow in the freshwater aquifer on a regional context.

The average linear velocity in sand gravel aquifers is reasonably high and it may be assumed that changes in the dispersive flux due to molecular and ionic diffusion are negligible. The freshwater aquifer is 1 to 3 m in its thickness and is fully saturated and vertical variations in hydraulic head may be considered insignificant since withdrawal of water due to pumpage is not taken into account. Since the flow field homogenises the isotopic signature, vertical variations in concentration may also be considered negligible.

3.4.9.4. Order of Magnitude Analysis

The influence of advective transport and the dispersive mechanism on the changes produced through time in the initial concentration of the solute is discussed in Appendix 2.
3.5. Discrete State Compartmental Model (DSC)

The DSC model is designed on the basis of mixing cell theory used in chemical engineering to simulate the mixing of chemical substances within and among reactor vessels. By utilising the mixing cell theory, it is possible to simulate the transportation of energy, mass and fluids in a flow system by applying appropriate algorithms (Campana, 1975).

A flow system under study may be arbitrarily divided into a series of interconnected cells of any shape and size. The cells may be arranged in one, two or three dimensional arrays depending on the nature of the flow field and a tracer is allowed to pass through the flow field. The input tracer is allowed to mix with the contents of the cells, the aquifer material, and the changes in its chemical concentration as it passes through the cell network are computed after a certain time.

The concentration of the input in any cell after a certain time can be computed if the cell parameters, volume of water flowing through the cells, and the initial concentration of the input are known (Simpson and Duckstien, 1973). The DSC model is somewhat similar to a continually evolving chemical system in which the changes in the concentration of a tracer introduced at some time may be monitored within the entire system at a discrete time. An analogy will be presented here to simplify the concept of the DSC model.

Figure 8(a) shows a schematic diagram of a flow tube arbitrarily divided into 6 cells of the same size. If the porosity of the material inside the tube is uniform then, the effective volume (VOL) of all the cells will be equal.
Figure 8. A schematic diagram to explain the mixing cell theory using a flow tube
If volume of water entering the tube $Q_m$ is equal to the volume of water leaving the tube $Q_{out}$, then the tube is said to have steady flow conditions. A tracer of known concentration, $C$, is introduced into the flow tube and, after a certain time period, $T$, the concentration of the tracer discharged by the tube, $C_o$, is noted at the discharging end. Assuming that the volume of water passing from one cell to the other is constant, changes in the initial concentration of the tracer over time $T$ caused by the physical and chemical processes may be accounted for by application of the equation of continuity (Campana, 1975).

Figure 8 (b) shows the same tube with six cells showing the changes in the initial concentration $C$ evolving through six intermediate phases, $C_1$ through $C_6$, before exiting the flow tube in the form of $C_o$, the discharge concentration. Thus, if the volume of water entering the flow tube $Q_m$, the effective volumes of the cells, VOL, concentration of the input, $C$, are known then, the concentration of the tracer in any cell after a certain time may be computed by using appropriate mixing cell algorithms (Simpson and Duckstein, 1973).

By applying the same logic, a hydrogeologic or hydrologic system may be arbitrarily divided into one, two or three dimensional array of cells. If the flow pattern within the aquifer is known then, the changes in the concentration of a tracer caused by physical or chemical processes over time within any or all the cells can be computed by using mixing algorithms. Alternatively, if the areal distribution of a tracer, any environmental isotope, is known then the distribution of groundwater flow may be computed within any or all the cells of the aquifer.
The calibration of the DSC model for an aquifer may be done by arbitrarily dividing the aquifer into a series of interconnected cells whose parameters can be determined from the field data. The input tracer concentration is specified by obtaining the areal distribution of isotopes such as $^{18}$O, $^{14}$C, $^3$H from the study area. The data from water balance studies and/or rainfall records may be used to compute the volume of water entering the DSC through the recharge cells.

By matching the concentration changes computed by the DSC for each cell, after a certain number of iterations, with the areal distribution of the isotopes, the modeller would be simulating the groundwater flow distribution and solute transport within the aquifer. DSC models are not hydraulic models and do not include hydrogeologic parameters such as hydraulic conductivity, dispersivity, etc., and they do not utilise rigorous flow equations. They are not predictive models; rather they are interpretive models. Properly calibrated DSC models provide information such as recharge rates, residence times, storage volumes and general flow directions (Campana, 1984).

3.5.1. System Requirements

The source code for the model is written in Fortran IV and can be used on mainframe systems equipped with a Fortran compiler. Alternatively, the executable file of the program may be used on an IBM or any compatible computer equipped with an Intel 8087 Math Co-Processor. The data can be input in the DOS format by using Word Perfect or any other suitable word processor. The program operates with a minimum of 11 lines of data entry, however, more lines may be added if necessary.
The program documentation provided with the software package describes the input format for all the lines and the number of variables allocated to each line. The output file may be printed using Word Perfect.

The DSC model was first devised by Simpson and Duckstein (1973). After minor modifications it was renamed Finite State Mixing model (FSM) by Campana (1975). The modifications in the FSM were maintained but the terminology was changed back to DSC since the term finite state conveys a meaning that is different from the working principle of the model (Campana and Simpson, 1984). Since 1975, the source code has been updated several times and some subroutines have been incorporated into the main program to improve its flexibility and, the source code used in this study was last updated in April 1989 (Simpson, personal communication).

3.5.2. Initiation of the DSC

The initiation of the DSC model begins with the introduction of a tracer, for example, any environmental isotope whose concentration is known, into a cell. The tracer is dispersed throughout the entire volume of the cell and is allowed to mix with its contents before it passes into the other cells. The process of mixing, simple type for dispersive flow and modified type for piston flow, must be specified before starting the iterations (Simpson et al., 1973).

It is imperative to have only one type of mixing within the entire DSC system for any given iteration and a transition from one type to the other is allowed only between the iterations. The changes in the concentration of the input due to advection
are computed initially and later on adjusted with changes caused by first order reactions such as radioactivity. The final concentrations in each cell are computed by considering the changes produced from both the processes. The changes in the concentration of the input within each cell will be computed until the tracer is flushed out of the system.

The parameters required to operate the DSC are:

(a) initial concentration of the tracer in each cell;
(b) value of all the inputs as a function of time;
(c) the initial effective volumes of each cell;
(d) the locations of all the inputs and outputs from the DSC;
(e) the flow paths within the DSC;
(f) the spatial distribution of the volumetric outputs from the cells and the fraction of volumetric output associated with each flow path in the DSC (Campana, 1975).

3.5.3. Continuity Equation

The transportation of dissolved matter and water in the DSC is represented by a series of finite states and transformation from one state to the other is governed by a set of recursive equations. The recursive equations are used to represent the concentration of matter, including changes due to radioactivity in the cells of the DSC system.

The basic mathematical equation describing the flow, a discrete form of a continuity equation, is as follows:

\[ S(N+1) = S(N) + BRV(N+1) \times BRC(N+1) - BDV(N+1) \times BDC(N+1) \pm R(N+1) \]
where,

\[ S(N+1) = \text{the cell state or the amount of matter in the cell at iteration } N+1; \]

\[ S(N) = \text{cell state at iteration } N; \]

\[ N = \text{the iteration number} \]

\[ \text{BRV}(N+1) = \text{boundary recharge volume at iteration } N+1, \text{ the volume of water entering the cell;} \]

\[ \text{BRC}(N+1) = \text{boundary recharge concentration at iteration } N+1, \]

\[ \text{BDV}(N+1) = \text{boundary discharge volume at iteration } N+1, \text{ the volume of water leaving the cell;} \]

\[ \text{BDC}(N+1) = \text{boundary discharge concentration at iteration } N+1, \]

\[ R(N+1) = \text{the source or sink term for iteration } N+1; \]

This equation states that the amount of material in the cell at iteration \( N+1 \) equals the amount of material in the cell at iteration \( N \) plus the amount of material that entered the cell at iteration \( N+1 \) minus the amount of material that left the cell at iteration \( N+1 \) minus the amount of material that was added or subtracted within the cell at iteration \( N+1 \) (Campana, 1975).

3.5.4. The DSC Regimes

The transportation of material in the DSC is computed based on the knowledge of: (a) the effective volume of the cells, \( \text{VOL} \); (b) volumetric recharge, \( \text{BRV} \), and discharge, \( \text{BDV} \), of water from each cell; and, (c) the concentration of the input, \( \text{BRC} \), and the concentration of the output, \( \text{BDC} \), of the cells. The DSC model allows six possible ways to compute transportation of material which are combinations of
steady or unsteady regimes (Campana, 1975). The steady state regime will have steady volume, steady flow conditions where the volume and flow remain unaltered. The state of the cell in the initial stages will be unsteady and will become steady after sufficient number of iterations. In this case, state is meant to represent the absolute amount of material in a cell (Campana and Simpson, 1984).

If steady flow and steady volume is specified for a particular model, where $BDV = BRV$, then the state of the cell may be steady or unsteady and the only unknown item on the right hand side of the continuity equation is $BDC(N+1)$. This quantity can be calculated depending on the type of mixing that occurs within the cell for a given iteration. The types of mixing allowed within the DSC model are simple mixing cells (SMC) and modified mixing cells (MMC).

3.5.4.1. Mixing Cells

Figure 9 is schematic diagram of the mixing cell types for both simple mixing cell and modified mixing cell configurations allowed by the model (Simpson and Duckstein, 1976). Simple mixing occurs when a cell expands to accommodate the incoming boundary recharge volume ($BRV$) and allows the contents within the cell to mix completely with the incoming boundary recharge concentration ($BRC$) after which the cell returns to its original size by expelling an equal volume of water. The SMC is also called the 'in-mix-out' type and the algorithm for the discharge concentration is (after Campana, 1975):

$$BDV(N+1) = \frac{S(N) + BRV(N+1) \times BRC(N+1)}{VOL + BRV(N+1)}$$
Figure 9. Types of mixing cells in the DSC model

(a) Simple mixing cell  (b) Modified mixing cell

(after Campana, 1975)
BDC(N+1) = boundary discharge concentration at N+1;
S(N) = state of the cell at iteration N;
BRV = boundary recharge volume;
BRV(N+1) = boundary recharge volume at iteration N+1; and,
VOL(N) = the volume of the cell at iteration N.

Modified mixing cells are rigid cells and do not expand. Instead, an equal volume of water is simultaneously expelled from the MMC cell as the recharge water enters the cell (Campana, 1975). This type of mixing is also known as the 'in-out-mix' type and the algorithm for the discharge concentration is:

\[ BDC(N+1) = \frac{S(N)}{VOL} \]

the accuracy of results from the model may be checked by using one or both of the mixing methods. It should be noted that for a steady state regime where SMC is specified, the mixing approaches MMC type if the volume of water entering a cell (BRV) is larger than the effective volume (VOL) of the recipient cell.

3.5.5. Mean Ages and Residence times

The DSC model uses the Impulse Response method (Campana, 1975) to compute residence times and groundwater ages. The distribution functions of the fluid elements are used to determine the residence times and mean ages of groundwater in the DSC system. The water recharged into the DSC system is designated into an infinite number of fluid elements. The fluid elements are characterised by a finite and constant volume which retain their identity and volume as they pass through all the cells of the DSC model.
At the time of entry, a fluid element displays an integer as its identity whose value increases by one for every iteration until it is discharged from the DSC system. The integer displayed by the fluid element still remaining within the DSC system is called as the "age number", while the integer value displayed at the point of discharge is called as the "transit number". Both the age number and transit number are functions of the iteration number which is a measure of the amount of time spent by any fluid element within the DSC. The age number indicates the number of iterations through which the fluid element has remained in the DSC while the transit number indicates the iteration number at which the fluid element exited from the DSC (Campana, 1975).

The fluid elements collected from within the DSC can be divided into various groups. Each group will display its age number and the fraction of fluid elements within it. Analogously, fluid elements collected at the discharge area will indicate the transit numbers of each group and the fraction of fluid elements within each group. The mean age number and the mean transit number may then be obtained by taking the first moments of their respective distributions.

The mean age numbers and the mean transit numbers can be converted into real time quantities by multiplying them by the time factor, a constant for each iteration. The time factor may be chosen as one month if mean monthly recharge data is available or as one year if average annual recharge data is available. It is usually convenient to use the average annual rainfall and recharge data to calibrate the DSC for a given aquifer system.
For more details on the Impulse Response method, the reader is referred to FSM model and transport phenomenon in hydrologic systems by Campana (1975).

3.5.6. DSC Model of the Study Area

The freshwater aquifer in the study area was initially divided into 14 cells for the DSC model and was recalibrated into 19 cells to augment the precision of the age distributions generated by the model. Since $^{14}$C data were not available due to the complex geochemistry of the aquifer, modelling the flow in the study area was conducted by using the $^{18}$O isotopic distribution.

3.5.7. Input Parameters

Figure 10 shows the configuration of cells in DSC model of the study area. The rationale behind choosing the cell configuration and the connections between the cells was based on the general direction of groundwater flow. The input data were prepared in compliance with the program code of the model and the aquifer parameters were specified in the form of integers or real numbers. To accomplish this, an Unit Reference Volume (URV) was chosen and all the parameters were specified either as fractions or as multiples of the URV. In this study, a suitable URV was found to be $1 \times 10^7$ m$^3$.

The variables for the model were prepared by discretising the field data for each cell from the well log records and later on converted into fractions or multiples of the URV. Table 1 lists the area, average thickness, and effective volumes of the cells for the DSC model of the study area. The effective volume of each cell was computed by multiplying the volume of each cell by the porosity value.
Figure 10. Configuration of cells in the DSC model of the study area.
Table 1. Summary of the parameters specified for the DSC model of the study area.

<table>
<thead>
<tr>
<th>Cell</th>
<th>Area (km²)</th>
<th>Thickness (m)</th>
<th>Volume ($10^4$ m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>90</td>
<td>2.34</td>
<td>0.64</td>
</tr>
<tr>
<td>2</td>
<td>117</td>
<td>2.86</td>
<td>1.01</td>
</tr>
<tr>
<td>3</td>
<td>90</td>
<td>2.34</td>
<td>0.64</td>
</tr>
<tr>
<td>4</td>
<td>144</td>
<td>2.49</td>
<td>1.07</td>
</tr>
<tr>
<td>5</td>
<td>81</td>
<td>2.47</td>
<td>0.60</td>
</tr>
<tr>
<td>6</td>
<td>81</td>
<td>2.66</td>
<td>0.64</td>
</tr>
<tr>
<td>7</td>
<td>108</td>
<td>3.42</td>
<td>1.10</td>
</tr>
<tr>
<td>8</td>
<td>108</td>
<td>2.56</td>
<td>0.83</td>
</tr>
<tr>
<td>9</td>
<td>108</td>
<td>1.93</td>
<td>0.63</td>
</tr>
<tr>
<td>10</td>
<td>81</td>
<td>2.30</td>
<td>0.56</td>
</tr>
<tr>
<td>11</td>
<td>81</td>
<td>3.11</td>
<td>0.75</td>
</tr>
<tr>
<td>12</td>
<td>108</td>
<td>2.79</td>
<td>0.91</td>
</tr>
<tr>
<td>13</td>
<td>108</td>
<td>2.05</td>
<td>0.67</td>
</tr>
<tr>
<td>14</td>
<td>108</td>
<td>1.52</td>
<td>0.50</td>
</tr>
<tr>
<td>15</td>
<td>54</td>
<td>2.69</td>
<td>0.44</td>
</tr>
<tr>
<td>16</td>
<td>54</td>
<td>2.51</td>
<td>0.40</td>
</tr>
<tr>
<td>17</td>
<td>40</td>
<td>2.55</td>
<td>0.30</td>
</tr>
<tr>
<td>18</td>
<td>81</td>
<td>1.82</td>
<td>0.44</td>
</tr>
<tr>
<td>19</td>
<td>72</td>
<td>1.33</td>
<td>0.29</td>
</tr>
</tbody>
</table>
The porosity value suitable for the freshwater aquifer was assumed to be 30% since sand and gravel materials have a porosity of 25-50% (Freeze and Cherry, 1979). Also, the porosity value of 30% was found to be suitable for freshwater aquifer through the simulations of the MOC model. The factor relating the model iterations to the real time was chosen on the basis of rainfall data available in an area. In this study, a suitable time value for real time between iterations was found to be one year. The estimates for average annual volumetric recharge entering the freshwater aquifer for this study were provided by Cmokrak (1991).
4.0. RESULTS AND DISCUSSION

4.1. Simulation of the MOC model.

4.1.1. Specification of Initial Conditions

The thickness values input to the model shown in Figure 11 represent the sum of the average thickness of the freshwater aquifer in that cell plus about 1 m from the bedrock. The static water levels input to the model are shown in Figure 12. Both the thickness map and the static water level map data are input to the model in FPS units; therefore, the maps are also shown in the same units of measurement. The hydraulic head map of the study area was used as a basis to input static water levels and to choose the source or recharge cells.

The porosity for sand and gravel varies between 25-50 % and for the bedrock, between 0-20 %. The hydraulic conductivity (K) of the sand and gravel material is between $1 \times 10^{-3}$ m/s to $1 \times 10^{2}$ m/s and the average hydraulic conductivity for the bedrock is between $1 \times 10^{9}$ m/s to $1 \times 10^{5}$ m/s (Freeze and Cherry, 1979). Initial assumed porosity and hydraulic conductivity values specified to model of the study area were 30 % and $5.0 \times 10^{5}$ m/s respectively.

Since the aquifer parameters specified to the model represent average values obtained from data points, a considerable margin of statistical error may affect the simulations. Therefore, trial and error simulations were conducted and the results from these experimental runs were used to assess the model sensitivity. The aquifer parameters affecting the performance were modified in a progressive manner through the course of experimental simulations.
Figure 11. Finite difference grid map of the study area showing the input of aquifer thickness. (units = ft.)
Figure 12. Finite difference grid map of the study area showing the input of static water levels (units = ft.)
The distribution of $^{18}$O in the study area superimposed on the finite difference grid map is shown in Figure 13 (after Macgregor, 1985 and Crnokrak, 1991). The spatial distribution of $^{18}$O values generated from the experimental simulations was compared with the observed distribution of $^{18}$O in the study area. The aquifer parameters affecting the performance of the model were changed in a systematic manner and the simulations were conducted until the model-generated $^{18}$O distribution was close to the observed distribution. The summary of parameters that were varied during the simulations is presented in Appendix 2.

4.1.2. Variations in Hydraulic Conductivity

During the initial stages of simulation the behaviour of the model was tested for its sensitivity to changes in hydraulic conductivity, while, porosity and dispersivity were kept constant. The parameters specified in the initial test were: hydraulic conductivity $= 5.0 \times 10^{-5}$ m/s; porosity $= 30\%$; longitudinal dispersivity $= 5000$ m; and, transverse dispersivity $= 1500$ m. Figure 14 shows the results from the initial simulations. The distribution of $^{18}$O values shown in Figure 14 are not similar to the observed distribution and a good match exists for 42% of the data points (10/24).

Several reasons may be responsible for the mismatch: (a) low porosity value; (b) low dispersivity values; (c) low hydraulic conductivity; and, (d) a combination of one or two parameters or all of the above. Porosity values for sand and gravel vary between 25-50% (Freeze and Cherry, 1979). The porosity values estimated by previous studies in the study area vary between 30-35% (M.M.Dillon, 1987).
Figure 13. Finite difference grid map superimposed on oxygen-18
distribution in the study area
Figure 14. Results from an initial simulation of the MOC model

\[ K = 5.0 \times 10^{-5} \text{ m/s}, \]

longitudinal dispersivity = 5000 m

Transverse dispersivity = 1250 m
Thus, an increase in the porosity values beyond 35 % would not be realistic. The values of longitudinal and transverse dispersivity are usually in the proportion of 1 : 0.3 and the dispersivity values vary somewhat linearly with the distance of groundwater movement (Anderson, 1984). Therefore, simulations performed with increases in the dispersivity values, for a constant and low value of hydraulic conductivity will produce the same results as simulations conducted with low dispersivity values and high hydraulic conductivity values.

Since longitudinal dispersivity of 5000 m and transverse dispersivity of 1500 m for the freshwater aquifer are not unwarranted, (Hyde, personal communication), the next set of simulations were conducted by varying the hydraulic conductivity values. The initial set of simulations were conducted by progressively decreasing the values from $5.0 \times 10^{-5}$ m/s to $1.0 \times 10^{-5}$ m/s. Since a decrease in the $K$ values did not produce the desired match between the observed and simulated distribution, the next set of simulations were performed by increasing the hydraulic conductivity progressively until the system displayed a good match between observed and simulated distribution of $^{18}O$ values.

Figure 15 shows the distribution of $^{18}O$ values when the simulation was conducted with a hydraulic conductivity value of $7.5 \times 10^{-5}$ m/s. The distribution of $^{18}O$ values in Figure 15 indicates that the parameters specified to the model are more reasonable in that the model simulation shows improvement. The match between observed and simulated data points increased from 10 to 14.
Figure 15. Results from the simulation for a higher value of hydraulic conductivity

\[ K = 7.5 \times 10^{-3} \text{ m/s} \]

longitudinal dispersivity = 5000 m
transverse dispersivity = 1250 m
During the next simulation, the system was tested with hydraulic conductivity values of $8.5 \times 10^{-3}$ m/s and $9.5 \times 10^{-3}$ m/s. In both cases the advection front was found to have moved faster and the placement of $^{18}$O values suggested that the transmissivity values were incorrect for the freshwater aquifer.

Figure 16 shows the model sensitivity to variations in hydraulic conductivity. The hydraulic conductivity value estimated from this study was found to be within the threshold of K values specified for freshwater aquifer in southwestern Ontario. The values estimated by computer simulations for the freshwater are in the following manner: (a) in Essex County, $K = 1.56 \times 10^{-5}$ m/s (Crnokrak, 1991); (b) in Kent County, $K = 1.0 \times 10^{-5}$ m/s (Pettapiece, 1988); and, (c) in Lambton County, $K = 5.0 \times 10^{-5}$ m/s (Hyde, 1987). The values for hydraulic conductivity determined by pump tests for the freshwater aquifer in Lambton County vary between $2.0 \times 10^{-5}$ m/s to $7.0 \times 10^{-5}$ m/s (Intera, 1987). Thus, a hydraulic conductivity value of $7.5 \times 10^{-5}$ m/s was assumed to be optimum for the freshwater aquifer in Essex County.

4.1.3. Variations in Dispersivity

To improve the match between observed and simulated distribution of $^{18}$O values, sensitivity of the model to variations in dispersivity, a fine tuning mechanism, was tested by modifying dispersivity values, while the other parameters were kept constant. Initially, the simulations were performed with low dispersivity values. However, the values were progressively increased as the simulations continued.
Figure 16. Sensitivity analysis of MOC model to variations in hydraulic conductivity.
The values of longitudinal and transverse dispersivity are usually in the proportion of 1 : 0.3 and the dispersivity values vary somewhat linearly with the distance of groundwater movement (Anderson, 1984). The movement of the advection front was noticed to be somewhat faster for increased values of dispersivity. The results of simulation when the longitudinal dispersivity = 7500 m and transverse dispersivity = 1875 m were specified are shown in Figure 17. A small increase in the match between simulated and observed data points was noticed.

These values are considered to be a good estimate for the longitudinal and transverse dispersivity in the freshwater aquifer. The dispersivity values estimated for the freshwater aquifer are in the following manner: (a) in Lambton County, longitudinal dispersivity = 5000 m and transverse = 1250 m (Hyde, 1987); (b) in Kent County, longitudinal dispersivity = 7000 m and transverse = 1750 m (Pettapiece, 1988). Figure 18 shows the model sensitivity to variations in dispersivity values. Figure 19 shows the plot of dispersivity and distance relationship estimated by Anderson (1984) and the plot of dispersivity value estimated in this study.

4.1.4. Variation in Porosity

During the next stages of simulation, porosity values were varied from 25 % to 40 % while the other parameters remained unchanged. Fracture porosity in the bedrock was not characterised due to lack of data. The increase in porosity did not produce any significant improvement in the results, however, the advection front seemed to move faster for porosity value lower than 30 %.
Figure 17. Result of MOC simulation for higher dispersivity value.

\[ K = 7.5 \times 10^{-5} \text{ m/s} \]

longitudinal dispersivity = 7500 m

transverse dispersivity = 1875 m
Figure 18. Sensitivity of MOC model to variations in dispersivity.
Figure 19. Dispersivity values in relation to distance

(from Anderson, 1984) (after Hyde, 1987)
Porosity of 35% was found to be the best value for the freshwater aquifer.
The porosity values for the freshwater aquifer are estimated to be in the range of 30-35% (Hyde, 1987; Pettapiece, 1988; Crnokrak, 1991). Figure 20 shows the sensivity of the MOC model to variations in porosity.

4.1.5. Final Simulation

The parameters input to the model were slightly changed to accommodate a better match between observed and simulated $^{18}$O distribution. Since the aquifer thickness specified cells were the average values estimated from 6-7 wells located within the cells, some ambiguity would invariably exist between the actual thickness of the aquifer and the input values. The thickness values input to the model were modified in some cells of the finite difference grid to optimise the transmissivity of the aquifer within that cell.

Figure 21 shows the results of the final simulation. The parameters specified to the model are: (a) hydraulic conductivity = $7.5 \times 10^{-5}$ m/s; (b) longitudinal dispersivity = 7500 m and transverse dispersivity = 1875 m; and, (c) porosity = 0.35. The percentage in the ratio of number correct and total includes 4 simulated points within ± 1% to the observed value. The match between the observed and simulated points in the final simulation is 16/25 (66%).
Figure 20. Sensitivity of MOC model to variations in porosity.
Figure 21. Results from the final simulation of MOC model

\[ K = 7.5 \times 10^{-5} \text{ m/s} \]

longitudinal dispersivity = 7500 m

transverse dispersivity = 1875 m
4.2. Simulation of the DSC Model

The initial conditions for the DSC model of the study area were determined from the field data. The model was operated under steady state, steady flow and steady volume conditions. The satisfactory operation of steady volume and steady flow DSC model requires boundary recharge equals discharge for all the iterations while the model computes transformation in the state of the material. It should be noted here that state is meant to represent the absolute amount of material in a cell.

The following assumptions were made in order to maintain steady flow conditions in the model: (a) precipitation enters the aquifer instantaneously and, (b) fluxes due to pumpage are negligible. The first assumption facilitates exchange of water between cells only after recharge enters the aquifer. The second assumption helps retain the actual volume of water recharged into the aquifer by not allowing any loss due to well pumpage. Thus, the distribution of water within the system is not affected and the volume of water recharged will be equal to the volume of water discharged from the system.

The average annual recharge entering the freshwater aquifer, estimated by computer simulations and by flow net analysis is reported to be 28450 m$^3$ per year (Crnokrak, 1991). In order to compute the distribution of groundwater flow between the cells, the estimates provided by Crnokrak (1991) were initially used and modified later. During the process of sensitivity analysis, it was found that the DSC model did not operate under steady flow conditions since some cells received less recharge.
When the concept of the DSC model was demonstrated using the flow tube, it was assumed that all the cells in the flow tube were initially saturated with water. This assumption can also be extended into the systems such as the freshwater aquifer because they are also initially saturated with water. The volume of water entering the DSC actually represents the annual volumetric recharge entering the aquifer system. It is designated into an infinite number of fluid elements which are representative of water and dissolved solutes. During the first iteration, all the cells in the DSC system receive fluid elements that enter the system in the form of recharge. This implies that the cells located near the discharge areas also receive fluid elements during the same iteration and that the fluid elements leave the system when the next iteration begins.

Since the velocity of groundwater is very slow in most real world systems, it is unlikely to observe water from a particular recharge event entering and leaving the aquifer within one year. In the DSC model of the study area, the cells located near the discharge areas will not receive water that was recharged in the recent years if the enormity of the cell sizes and the slow movement of groundwater across the cells are taken into consideration.

However, the fluid elements also represent the concentration of material dissolved in water and the cells located near the discharge areas receive fluid elements having the least amount of dissolved matter in them. The input concentration is specified prior to starting the iterations and it is zeroed for all the iterations that follow later. Since the DSC model computes the 'state' of the cells, which is representative of the absolute amount of material, the cells near the discharge areas
will have the lowest state. The state of each cell is converted into concentration by dividing the state of each cell by its effective volume. During the initial stages, the system will be in an unsteady state and will attain steady state as the iterative procedure continues. Under steady state conditions, the amount of material entering a cell will be equal to the amount of material leaving the cell.

In order to accomplish steady state conditions within the system, the DSC has to be operated under steady flow conditions in that the volume of water entering a cell should be equal to the volume of water leaving a cell. After the DSC is operated under steady state and steady flow conditions for a certain number of iterations, the mean ages for groundwater in all the cells are generated by the model. The model-generated mean ages have to be compared with estimated ages to check the degree of correlation between them. The model-generated mean ages are calculated from a collection of fluid elements, while the estimated ages represent the ages obtained through the conversion of spatial distribution of isotopic values. If the estimated ages and model-computed ages exhibit a good correlation, then the flow distribution within the model will be reflecting the flow distribution in the real world system.

The correlation between the estimated ages and model generated ages was checked during each step of the iterative procedure. In order to reduce the disparity between estimated ages and computed ages, the volumetric flow distribution across the freshwater aquifer was re-evaluated by progressively changing the values used. After some trial and error experimental runs, a suitable factor to distribute volumetric exchange was found to be 0.432 m³/year/m. Based on this factor, the recharge was
found to be somewhat less to maintain steady flow conditions in the DSC. This condition prompted the evaluation of the average annual recharge entering the freshwater aquifer.

4.2.1. Estimation of Recharge

Since the DSC model facilitates the estimation of volumetric recharge entering the aquifer when BRV = BDV, the differences between the BRV and the BDV of a cell provides a rough estimate of the recharge deficit. It was found that steady flow conditions (BDV=BRV) were prevalent in all the cells except cells 3 and 4, which were discharging more than the incoming recharge. The volume of water recharged into the DSC was systematically increased so that steady flow conditions were established for cells 3 and 4.

The estimated ages and the computed ages in all the cells were compared at each step to see if they concurred with each other. The simulations were continued until the computed ages fell within the range of estimated ages for all the cells. After a close correlation between the two was observed, it was assumed that steady flow conditions became prevalent in cells 3 and 4. The model was assumed to have approached steady flow conditions because: (a) the volume of water associated with each flow path, when properly allocated, reflects the distribution of groundwater flow in the aquifer which has a steady state flow; and, (b) comparison of estimated isotopic ages and model-generated ages is the only basis from which it is possible to check whether groundwater distribution is done correctly.
Based on the model estimation, there are deficits of approximately 5226 m$^3$/year of recharge into the freshwater aquifer. The total volumetric recharge into and total volumetric discharge from the freshwater aquifer in Essex County is estimated to be 33675 m$^3$/year. The total volumetric recharge into the freshwater aquifer estimated by Crnokrak (1991) is 28449 m$^3$/year.

4.2.2. Physical Conditions in Favour of Recharge

Cell #3 lies under the Malden and Anderdon Townships, which have a thin and fissured overburden, especially around the Amherstburg area (Vagners et al., 1973). Cell #4 lies under Colchester South Township, which is characterised by the presence of sandy material at the surface. Favourable conditions for infiltration exist in these parts of Essex County and it has already been stated that the Harrow area is rated highly susceptible for groundwater pollution (Allendorf, 1981).

The $^{18}$O analyses of water from these subregions show the presence of recently recharged water in these areas. These factors together make the cells 3 and 4 very likely candidates to contribute additional recharge to the aquifer other than the main recharge area. The recharge estimate claimed through the model cannot be substantiated by providing evidence through water level measurements because the observation wells (Well no.170 and 171, S.Colchester; Observation Well Records) do not lie within the area outlined by Allendorf (1981) where, infiltration is rated to be high. Besides, areas near Amherstburg and areas south of Harrow have not been monitored for water level fluctuations.
The absence of water level data and not having monitoring wells do not constitute a valid argument to accept the model-generated recharge figure as authentic. However, it is not known what argument may be used as a basis to refute the estimation. Although the DSC model comes with lack of mathematical rigor, it still provides a good assessment of the volumetric inflow and outflow in an aquifer. The recharge estimated through the DSC model may be cross-checked against a hydraulic model for the study area. But nevertheless, constructing a hydraulic model was outside the scope of this investigation and a comparative study was not pursued. In the light of all the pros and cons, the author considers the model-generated estimates of recharge as only provisional and not determinative.

4.2.3. Distribution of Volumetric Flow in the DSC

Tables 2 and 3 present the volumetric flux between the cells in DSC of the study area. This also represents the distribution of groundwater in the study area. The amount of water associated with each flow path was computed by multiplying the average flow across the aquifer into the boundary length affecting the flow between the cells. The boundary length between the adjacent cells was computed for most cell connections and was estimated for some other cells. Table 4 is a list of the volumetric flux associated with each flow path, expressed as fractions of the total BDV of a cell.
Table 2. Volumetric recharge into the DSC and the volume of water associated with each flow path between the cells.

<table>
<thead>
<tr>
<th>SBRV</th>
<th>Volume * E+03 (m³/year)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>10.4</td>
</tr>
<tr>
<td>2</td>
<td>14.2</td>
</tr>
<tr>
<td>3</td>
<td>3.2</td>
</tr>
<tr>
<td>4</td>
<td>5.8</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Source Cell</th>
<th>Recipient Cell</th>
<th>BRV * E+03 (m³/year)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
<td>3.9</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>2.6</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>3.9</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>1.3</td>
</tr>
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<td></td>
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<tr>
<td>5</td>
<td>11</td>
<td>3.9</td>
</tr>
<tr>
<td>7</td>
<td>12</td>
<td>3.9</td>
</tr>
<tr>
<td>8</td>
<td>13</td>
<td>3.9</td>
</tr>
<tr>
<td></td>
<td>14</td>
<td>2.6</td>
</tr>
<tr>
<td>9</td>
<td>14</td>
<td>3.9</td>
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<tr>
<td>10</td>
<td>15</td>
<td>1.3</td>
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<td>3.9</td>
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<td>2.6</td>
</tr>
<tr>
<td></td>
<td>18</td>
<td>1.3</td>
</tr>
<tr>
<td>13</td>
<td>18</td>
<td>2.6</td>
</tr>
<tr>
<td></td>
<td>19</td>
<td>1.3</td>
</tr>
<tr>
<td>14</td>
<td>19</td>
<td>3.9</td>
</tr>
</tbody>
</table>
Table 3. Volume of water discharged from the DSC to the outside environment.

<table>
<thead>
<tr>
<th>Discharge Source</th>
<th>To</th>
<th>Volume of water discharged * E+03 (m³/year.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Lake Erie</td>
<td>3.9</td>
</tr>
<tr>
<td>2</td>
<td>Lake Erie</td>
<td>2.6</td>
</tr>
<tr>
<td>3</td>
<td>Lake Erie</td>
<td>1.3</td>
</tr>
<tr>
<td>4</td>
<td>Lake Erie</td>
<td>1.3</td>
</tr>
<tr>
<td>5</td>
<td>Kent County</td>
<td>1.3</td>
</tr>
<tr>
<td>9</td>
<td>Detroit River</td>
<td>2.6</td>
</tr>
<tr>
<td>10</td>
<td>Kent County</td>
<td>1.3</td>
</tr>
<tr>
<td>14</td>
<td>Detroit River</td>
<td>2.6</td>
</tr>
<tr>
<td>15</td>
<td>Lake St.Clair</td>
<td>1.3</td>
</tr>
<tr>
<td>16</td>
<td>Lake St.Clair</td>
<td>3.9</td>
</tr>
<tr>
<td>17</td>
<td>Lake St.Clair</td>
<td>2.6</td>
</tr>
<tr>
<td>18</td>
<td>Lake St.Clair</td>
<td>3.9</td>
</tr>
<tr>
<td>19</td>
<td>Detroit River</td>
<td>5.2</td>
</tr>
</tbody>
</table>
Table 4. Volume of water associated with each flow path expressed as fractions of the total BDV of each cell.

<table>
<thead>
<tr>
<th>From</th>
<th>To</th>
<th>% BDV</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>0.26</td>
</tr>
<tr>
<td>0</td>
<td>2</td>
<td>0.32</td>
</tr>
<tr>
<td>0</td>
<td>3</td>
<td>0.10</td>
</tr>
<tr>
<td>0</td>
<td>4</td>
<td>0.16</td>
</tr>
<tr>
<td>1</td>
<td>5</td>
<td>0.38</td>
</tr>
<tr>
<td>1</td>
<td>6</td>
<td>0.22</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>0.19</td>
</tr>
<tr>
<td>2</td>
<td>6</td>
<td>0.10</td>
</tr>
<tr>
<td>2</td>
<td>7</td>
<td>0.34</td>
</tr>
<tr>
<td>2</td>
<td>8</td>
<td>0.15</td>
</tr>
<tr>
<td>3</td>
<td>9</td>
<td>0.65</td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td>0.13</td>
</tr>
<tr>
<td>4</td>
<td>8</td>
<td>0.27</td>
</tr>
<tr>
<td>4</td>
<td>9</td>
<td>0.24</td>
</tr>
<tr>
<td>5</td>
<td>10</td>
<td>0.55</td>
</tr>
<tr>
<td>6</td>
<td>11</td>
<td>1.00</td>
</tr>
<tr>
<td>7</td>
<td>12</td>
<td>1.00</td>
</tr>
<tr>
<td>8</td>
<td>13</td>
<td>0.45</td>
</tr>
<tr>
<td>8</td>
<td>14</td>
<td>0.27</td>
</tr>
<tr>
<td>9</td>
<td>14</td>
<td>0.37</td>
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<td>10</td>
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<td>0.70</td>
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<tr>
<td>11</td>
<td>16</td>
<td>1.00</td>
</tr>
<tr>
<td>12</td>
<td>17</td>
<td>0.65</td>
</tr>
<tr>
<td>12</td>
<td>18</td>
<td>0.35</td>
</tr>
<tr>
<td>13</td>
<td>18</td>
<td>0.65</td>
</tr>
<tr>
<td>13</td>
<td>19</td>
<td>0.35</td>
</tr>
<tr>
<td>14</td>
<td>19</td>
<td>0.35</td>
</tr>
</tbody>
</table>

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4.2.4. Input of Isotopic Data

In order to accomplish proper calibration, groundwater ages must be estimated from the spatial distribution of isotopic data. The samples for isotopic data have to be obtained from wells located approximately in the centre of each cell. The ages estimated from the isotopic data are assumed to be representative of the average age of groundwater within each cell (Campana, 1975).

Since $^{18}$O data collection was not one of the objectives of this study, and neither was data collection in earlier studies done with an objective to suit this investigation, all the available isotopic data had to be used from the data base as is. The estimated ages were obtained from the $^{18}$O isotopic distribution, which is representative of $\delta^{18}$O values in precipitation events that occurred years before present. Therefore, estimated ages in some cells do not correlate with the model-generated mean age of groundwater within the entire cell; rather they are older than the mean ages in some cells.

This factor alone contributes more to the improper distribution of groundwater since modifications in flow distribution can only be done by comparing estimated and calculated ages, besides other factors relevant to improper calibration.

4.2.5. Operational Aspects of DSC model

Table 5 is a list of estimated ages and calculated ages for groundwater in all the cells of the DSC. The estimated ages for the DSC cells represent the ages converted from $^{18}$O values obtained in the study area and, the relevant details are presented in Appendix 3.
Table 5. List of ages estimated from $^{18}$O concentrations and mean ages and residence times computed by the DSC.

<table>
<thead>
<tr>
<th>Cell</th>
<th>Estimated Ages (years B.P.)</th>
<th>Model-generated Mean Ages in years</th>
<th>Residence time within the cells in years</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Modern</td>
<td>651</td>
<td>651</td>
</tr>
<tr>
<td>2</td>
<td>Modern</td>
<td>917</td>
<td>916</td>
</tr>
<tr>
<td>3</td>
<td>Modern</td>
<td>2,110</td>
<td>2,020</td>
</tr>
<tr>
<td>4</td>
<td>Modern</td>
<td>2,040</td>
<td>1,990</td>
</tr>
<tr>
<td>5</td>
<td>11,950</td>
<td>2,230</td>
<td>2,190</td>
</tr>
<tr>
<td>6</td>
<td>?</td>
<td>2,650</td>
<td>2,550</td>
</tr>
<tr>
<td>7</td>
<td>Modern</td>
<td>3,120</td>
<td>2,900</td>
</tr>
<tr>
<td>8</td>
<td>11,450</td>
<td>3,840</td>
<td>3,350</td>
</tr>
<tr>
<td>9</td>
<td>10,950</td>
<td>3,900</td>
<td>3,490</td>
</tr>
<tr>
<td>10</td>
<td>11,950</td>
<td>4,880</td>
<td>3,980</td>
</tr>
<tr>
<td>11</td>
<td>7,500</td>
<td>4,780</td>
<td>4,030</td>
</tr>
<tr>
<td>12</td>
<td>10,950</td>
<td>5,670</td>
<td>4,230</td>
</tr>
<tr>
<td>13</td>
<td>11,950</td>
<td>7,490</td>
<td>4,130</td>
</tr>
<tr>
<td>14</td>
<td>11,950</td>
<td>6,120</td>
<td>4,400</td>
</tr>
<tr>
<td>15</td>
<td>12,450</td>
<td>7,910</td>
<td>4,310</td>
</tr>
<tr>
<td>16</td>
<td>12,450</td>
<td>7,020</td>
<td>4,590</td>
</tr>
<tr>
<td>17</td>
<td>12,450</td>
<td>7,000</td>
<td>4,590</td>
</tr>
<tr>
<td>18</td>
<td>12,450</td>
<td>9,020</td>
<td>4,020</td>
</tr>
<tr>
<td>19</td>
<td>12,450</td>
<td>9,120</td>
<td>4,050</td>
</tr>
</tbody>
</table>

B.P. before present.

The estimated ages represent $\delta^{18}$O values years before present. The values for the study at a point were modified by Crnokrak (1991) after Edwards and Fritz (1986).

Modern - The isotopic composition in the water sample resembles the isotopic composition of modern day precipitation.

Model-generated ages represent the mean ages of groundwater in the cells and is computed by the model by Impulse Response method.
The relative ages for various $^{18}$O values were computed by Edwards and Fritz (1986) for Brampton, Ontario based on observing the isotopic composition in wood cellulose samples. The $\delta^{18}$O values ages were subsequently modified by Crnokrak (1991) for Essex County and surrounding areas by considering the relationship between $\delta^{18}$O values and the temperature of condensation in a region and other factors affecting $^{18}$O concentration in precipitation.

It can be seen that the mean ages calculated for the cells 1 through 4 agree quite well with the estimated ages. Both the computed mean ages and estimated ages suggest the presence of young groundwater in the cells 1 through 4. The term "modern" means that the concentration of $^{18}$O in groundwater is similar to the $^{18}$O values observed in modern day precipitation. The average age of groundwater in cells 1 through 4 is affected by their proximity to the recharge zone from which fluid elements with new identity enter the aquifer regularly. Therefore, calculated mean ages falling within the threshold of modern ages described by $^{18}$O data are acceptable.

Cells 5 and 10 are located at the border of Essex and Kent County. Recharge from Thames River is discharged along Lake Erie (Pettapiece, 1988), while a small component of recharge from Essex County moves towards Kent County. The groundwater in this fringe zone is perhaps affected by mixing of the recharge components from Essex and the Thames River. Therefore, it is not unlikely to observe depleted $^{18}$O values in groundwater along this zone. Thus, estimated ages for cells 5 and 10 are much higher than calculated mean ages.
The calculated age and estimated age for cell 7 shows good agreement while cell 6 does not have any isotopic data to draw a comparison. Since the cells 6 and 7 are recharged from cells 1 and 2, and that 7 shows a good agreement it may be assumed that the computed mean age for cell 6 is acceptable.

The calculated ages for cells 8 and 9 differ from the estimated ages by three to four times. The isotopic data for cells 8 and 9 was obtained from wells located near the upper fringes, once again representative of older groundwater. The mean age calculated for the cell 11 is close to the estimated age. This cell encloses the area where buried esker is suspected to influence the groundwater regime (Morris, 1989). The isotopic data provides a generalised idea on the observed ages for cells 12, 13 and 14, in that they have water recharged approximately 11000 years before present. The calculated ages for these cells are 5600, 7490 and 6120 years respectively. Since a degree of uncertainty is present in the observed ages, no attempts are made to characterise its relation with the calculated ages.

Cells 15 and 16 have water very depleted in its \(^{18}\text{O}\) content suggesting the presence of very old groundwater. There is no data for cells 17, 18 and 19 due to lack of suitable sampling points in Windsor and its suburbs. However, it can be presumed that groundwater under these areas is oldest in comparison with the rest of the area due to its proximity to the discharge zones. The calculated and estimated ages for cells 15 and 18 show excellent agreement, while the same is not true for cell 16 and cell 17. The mean age for cell 19 is acceptable because the computed age is close to what would have been the estimated age supposing the data was available.
4.2.6. Model Assumptions Affecting the Results.

When the simple mixing regime (SMC) is specified, the incoming recharge water is supposed to completely mix with the contents of the cell. If real time is chosen to be one year then, the modeller will be assuming that the cell contents will undergo complete mixing with the incoming recharge within one year before discharge is expelled. This assumption is unrealistic when the enormity of the cell sizes are taken into consideration. The DSC model permits more iterations for a given time interval to enable the modeller to accommodate enough time for the system to reach equilibrium. In such cases, the modeller will be allowing more water to pass through the system than what is supposedly passing. These are some factors affecting the computed ages.

The model does not offer any hints to modify either the cell sizes or the volumetric recharge entering into a cell. Often, the cell sizes may be reduced to suit the incoming BRV such that the cell experiences the expansive effects of SMC algorithms. In the DSC model of the study area, the effective volumes of the cells 7, 8, 9, 12, 13 and 14 are much higher than the volume of water entering these cells and these cells do not experience the expansive effects of SMC regime.

The effective volumes of cell 16 and 17 are smaller compared to the incoming BRV and in effect, dispersive flow probably approaches one of piston flow resulting in younger mean ages for these cells. In contrast to the SMC algorithm, the MMC algorithm used under piston flow cases in reality does not simulate flow distribution between two cells of large dimensions. Since the average linear velocity of
groundwater is low even under piston type of flow, the volume of water exchanged between two large cells in MMC simulations cannot be justified. These factors may also be partially responsible for disparities between computed mean ages and estimated ages for these cells.

The other possibilities for error arise from the volumetric inflow and outflow associated with each flow path. In this study, the volumetric flow with each flow path was calculated by multiplying the average volumetric flow rate into the boundary length of the adjacent cells. The boundary lengths affecting the flow between the cells were computed for some cells and estimated for others.

4.3. Computation of Groundwater Velocity

The MOC model uses the particle tracking procedure to compute the velocity of groundwater. The X and Y velocities of a particle are calculated using bilinear interpolation over half the area of the cell using the X and Y velocities calculated at adjacent nodes and cell boundaries. Figure 22 is a finite difference grid showing areas over which bilinear interpolation is used to compute velocity at a point.

Figure 23 shows the distribution of resultant velocities in the finite difference grid of the study area. The lowest value of velocity in the study area is 0.55 m/year and the highest value is 2.56 m/year.
Figure 22. Hypothetical finite difference grid showing area over which bilinear interpolation is used to compute groundwater velocity. (after Konikow and Bredehoeft, 1979)

- location of a particle P

  o is the node of the finite difference grid

- area of influence for interpolating X velocity of particle P

- area of influence for interpolating Y velocity of particle P
Figure 23. Resultant groundwater velocity distribution in the study area (units = m/year)
The average linear groundwater velocity in the freshwater aquifer was computed by using the results from the DSC simulations in association with the Darcy flux equation of the form:

\[ v = \frac{Q}{nA} \]

where, \( v \) is the average linear velocity;

\( Q \) = the volumetric flux across the cells obtained from DSC simulations;

\( A \) = the area of cross-section affecting the flow between the cells; and,

\( n \) = the porosity value.

The volumetric fluxes across the cells in the DSC model of the study area are listed in Table 2. The average velocity computed between the cells is shown in Table 6.

4.4. MOC Versus DSC

In comparison to DSC, the MOC model is more versatile and sophisticated in terms of its applicability to simulate groundwater flow and contaminant transport within the freshwater aquifer. The DSC model can be viewed as a precursor to higher order sophisticated models. The DSC model is not well suited to simulate flow in Essex County because the thickness of freshwater aquifer is insufficient to be compatible with the mixing algorithms. On the contrary, since MOC is a finite difference model, it can handle thickness variations in both the lateral and vertical dimensions.

The recharge estimates generated by DSC model are more abstract rather than factual since the concept of fluid elements and its relation to groundwater age does not always remain consistent.
Table 6. Summary of average linear groundwater velocity between the cells in the DSC model of the study area.

<table>
<thead>
<tr>
<th>Cells</th>
<th>Area of cross-section (m²)</th>
<th>Volumetric flux (m³/year)</th>
<th>Average linear velocity (m/year)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-5</td>
<td>5778</td>
<td>3888</td>
<td>0.67</td>
</tr>
<tr>
<td>2-7</td>
<td>9216</td>
<td>5184</td>
<td>0.56</td>
</tr>
<tr>
<td>4-8</td>
<td>6183</td>
<td>3888</td>
<td>0.63</td>
</tr>
<tr>
<td>3-9</td>
<td>6048</td>
<td>3888</td>
<td>0.65</td>
</tr>
<tr>
<td>5-10</td>
<td>4086</td>
<td>2592</td>
<td>0.65</td>
</tr>
<tr>
<td>6-11</td>
<td>6669</td>
<td>3888</td>
<td>0.58</td>
</tr>
<tr>
<td>7-12</td>
<td>8424</td>
<td>3888</td>
<td>0.46</td>
</tr>
<tr>
<td>8-13</td>
<td>6912</td>
<td>3888</td>
<td>0.64</td>
</tr>
<tr>
<td>9-14</td>
<td>6372</td>
<td>3888</td>
<td>0.61</td>
</tr>
<tr>
<td>10-15</td>
<td>1935</td>
<td>1296</td>
<td>0.67</td>
</tr>
<tr>
<td>11-16</td>
<td>7527</td>
<td>3888</td>
<td>0.51</td>
</tr>
<tr>
<td>12-17</td>
<td>4842</td>
<td>2592</td>
<td>0.53</td>
</tr>
<tr>
<td>13-18</td>
<td>3690</td>
<td>2592</td>
<td>0.70</td>
</tr>
<tr>
<td>14-19</td>
<td>4104</td>
<td>3888</td>
<td>0.95</td>
</tr>
</tbody>
</table>
If the cell configuration in the DSC model of Essex County is changed from just one cell to one hundred cells, the concept of fluid elements fails. The ages generated by the model in both cases will bear absolutely no relationship to the real world system. The author opines that the DSC models are best suited to simulate flow distribution and transportation of contaminants in large bodies of surface water since the mixing algorithms are well suited for rapid mixing scenarios.

4.5. Summary of Results

4.5.1. Results From MOC Simulations

1) The hydraulic conductivity (K) for the freshwater aquifer is suggested to be $7.5 \times 10^{-5}$ m/s. The K values estimated in the freshwater aquifer, in Essex County, by Crnokrak (1991) is $1.56 \times 10^{-5}$ m/s, in Kent County, by Pettapeice (1988) is $1.0 \times 10^{-4}$ m/s, in Lambton County, by Hyde (1987) is $5.0 \times 10^{-5}$ m/s and by Intera (1987) is between $2.0 \times 10^{-5}$ m/s to $7.0 \times 10^{-5}$ m/s. Thus, the K value estimated is also within the range of K values estimated in the freshwater aquifer from previous studies.

2) The dispersivity values estimated for the freshwater are: longitudinal dispersivity $= 7500$ m and transverse dispersivity $= 1875$ m. These values are within the range of dispersivity values estimated by MOC model for the freshwater aquifer in Kent County (Pettapeice, 1988) and Lambton County (Hyde, 1987).

3) The groundwater velocity varies between 0.55 m/year to 2.56 m/year. The velocity values estimated from this study is in the range of velocity values estimated by Crnokrak (1991).
4.5.2. Results From DSC Simulations

1) The volumetric flow across the freshwater aquifer is estimated to be 0.432 m³/y/m.

2) The model estimates indicate recharge of approximately 5000 m³/year for Malden and Colchester South townships. The total recharge estimated in this study in order to maintain steady flow conditions is 33675 m³/year. This value is slightly more than the estimate provided by Crnokrak (1991).

3) The average groundwater velocity calculated for a majority of cells is somewhat low and ranges between 0.5 m/year - 0.95 m/year.
5.0. CONCLUSIONS AND RECOMMENDATIONS

5.1. Conclusions

The conclusions drawn from computer simulations are as follows:

1) The average groundwater velocity estimated by MOC model varies between 0.55 m/year to 2.56 m/year.

2) The average groundwater velocity estimated by DSC simulations lies in the range of 0.5 m/year - 0.95 m/year. The velocity values estimated by DSC simulations are somewhat low.

The velocity values estimated from this study are in the range of velocity values between 0.80 - 1.18 m/year estimated by Crnokrak (1991). The average linear groundwater velocity in the drift aquifer in Bay County, East Central Michigan by Long et al., (1988) is 2.3 m/year.

3) The total recharge estimated in this study by DSC simulations is 33675 m³/year. This estimate is more than the estimate provided by Crnokrak(1991). The volumetric flow across the freshwater aquifer is estimated to be 0.432 m³/year/m. The model estimates indicate recharge of approximately 5000 m³/year for Malden and Colchester South Townships.

4) The longitudinal dispersivity = 7500 m and transverse dispersivity = 1875 m. These values are within the range of dispersivity values estimated by MOC model for the freshwater aquifer in Kent County (Pettapiece, 1988) and Lambton County (Hyde, 1987).
5) The hydraulic conductivity (K) for the freshwater aquifer is suggested to be $7.5 \times 10^{-3}$ m/s. The K values estimated in the freshwater aquifer by computer simulations are: in Essex County $K = 1.56 \times 10^{-3}$ m/s (Crnokrak, 1991); in Kent County, $K = 1.0 \times 10^{-4}$ m/s (Pettapeice, 1988); in Lambton County, $K = 5.0 \times 10^{-5}$ m/s (Hyde, 1987). The hydraulic conductivity values estimated from pump tests by Interar(1987) are in the range of $2.0 \times 10^{-5}$ m/s to $7.0 \times 10^{-5}$ m/s. On the basis of the previous observations, it is concluded that the K value estimated in this study is applicable to the freshwater aquifer.

6) The total dissolved carbon content in groundwater has carbon contributed by sulphate reduction and methanogenesis, the dilution in the initial activity of carbon-14 due to geochemical processes cannot not be estimated. Therefore, carbon-14 isotopes are considered not conducive for groundwater tracing in the study area.

5.2. Recommendations

1) The role of the overlying till in conveying meteoric water to the aquifer should be investigated. This study will help delineate some more areas where pollution from surface sources is possible.

2) A majority of the finite difference packages are limited to model flow under isotropic and homogeneous conditions. The results generated by such models may find wide acceptance only if field data is available to substantiate the model estimates. Therefore, the velocity of groundwater in the freshwater aquifer needs to investigated by field methods.
3) Since freshwater aquifer is confined and relatively thin, finite element modelling approach is recommended to augment the precision of groundwater flow distribution.

4) The accuracy of modelling flow in freshwater is somewhat limited by the number of data points available for simulating flow. Oxygen-18 sampling is recommended in southern and southwestern parts of Essex County.

5) The stable carbon isotopes from the bedrock need to be analyzed. This will help distinguish whether the dilution of $\delta^{13}$C in groundwater is caused by mineral dissolution or by methanogenesis.

6) Installation of monitoring wells in Malden, Anderdon and Colchester South Townships including Windsor and its suburbs will facilitate water level recording stations and sampling points for isotopic studies. The data obtained from these wells would improve the accuracy of results.
REFERENCES


APPENDIX 1


Bedrock Geology of Essex County (after Freeman, 1979).
Paleozoic Geology of southwestern Ontario
(after Hewitt, 1972)

<table>
<thead>
<tr>
<th>System</th>
<th>Subsystem</th>
<th>Formation or Group</th>
<th>Lithology</th>
</tr>
</thead>
<tbody>
<tr>
<td>Devonian</td>
<td>Middle Devonian</td>
<td>Hamilton Formation</td>
<td>Grey Shale interbedded with argillaceous Limestone</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Dundee Formation</td>
<td>Buff coloured Limestone and Chert</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Detroit River Group</td>
<td>Brown Limestone Buff to Brown Dolomite and black carbonaceous Limestone</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Bois Blanc Formation</td>
<td>Dolomitic limestone Calcereous dolomite Chert and Sandstone</td>
</tr>
<tr>
<td>Silurian</td>
<td>Upper Silurian</td>
<td>Bass Islands Formation</td>
<td>Buff coloured Dolomite</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Salina A1,A2,B,C D,E,F,G</td>
<td>Evaporite deposits of salt and gypsum</td>
</tr>
</tbody>
</table>
The Paleozoic geology of southwestern Ontario is composed of Silurian and Devonian age and, in Essex county the bedrock belongs to the Middle Devonian age (Hewitt, 1972). The bedrock is comprised of the Detroit River group, overlain by glacial till and, there are no reported out crops (Vagners, et al., 1973 a,b).

Sylvania Sandstone is the basal member of the Detroit River group directly overlying the Bois Blanc formations, is discontinuous and is often used as an index to separate the Detroit River group from the under lying Bois Blanc. The Detroit River group is overlain by the Dundee formation, except in the southwestern part of the study area where it is overlain by the till. The Dundee formation is overlain by glacial till in most parts of the study area except near Maidstone where it overlain by the Hamilton formation. The Hamilton formation, composed of grey shales and limestones, occurs only around Maidstone area otherwise it is chiefly confined to Kent and Lambton Counties (Telford and Russell, 1981).

The Salina formation has eight members, A-1, A-2, B, C, D, E, F, G, and is comprised of evaporite beds of salt and gypsum. The Salina formation and its associated brines are exploited at various locations for salt production. In Essex county, salt is commercially produced near Windsor and Amherstburg areas. The Salina formation is overlain by Bass Island formation, which is composed of massive dolomitic members ranging from 60-395 ft. in thickness (Sanford and Brady, 1955).

The Bois Blanc formations rests unconformably on the Bass Island formation and thins down in the southern direction. Although Bois Blanc lies between the Bass Island and Detroit river group, it does not subcrop in the Essex county region The Detroit river group is brought very close to the surface on the western side of the Chatham syncline, near Amherstburg. The excavations due to mining and other activities expose the bedrock near the surface and provide small areas for direct observation (Telford and Russell, 1981).
Bedrock Geology of Essex County (after Freeman, 1972).
Appendix 2

Flow chart of the MOC main program (after Konikow and Bredehoeft, 1979).

Flow chart of the updated version of MOC (after Konikow and Goode, 1989).

List of parameters varied during MOC simulations

Order of Magnitude Analysis
Flow chart of the MOC main program (after Konikow and Bredehoeft, 1979).
Flow chart of the updated version of MOC (after Konikow and Goode, 1989).
List of parameters varied during MOC simulations

<table>
<thead>
<tr>
<th>Hydraulic Conductivity in $10^3$ m/s</th>
<th>Longitudinal Dispersivity (m)</th>
<th>Porosity</th>
<th>Ratio of Number correct to Total (%)</th>
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<tbody>
<tr>
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<td>5000</td>
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<td>0.30</td>
<td>14/24</td>
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<td>10/24</td>
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<td>8/24</td>
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<td>8500</td>
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</tr>
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<td>7500</td>
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<td>10/24</td>
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<td>7500</td>
<td>0.35</td>
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<td>7.5</td>
<td>7500</td>
<td>0.40</td>
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</tr>
</tbody>
</table>
Order of Magnitude Analysis

The equation describing the transportation of non-reactive solutes in saturated homogeneous medium, when the length of a flow path and time are large, is (Ogata, 1970 quoted in Freeze and Cherry, 1979):

\[
\frac{C}{C_0} = \frac{1}{2} \left[ \text{erfc} \left( \frac{l - \frac{v}{D}}{2\sqrt{D_t t}} \right) \right]
\]

where,

\( C \) = initial concentration;

\( C_0 \) = concentration after a certain time;

\( t \) = time;

\( l \) = distance along a flow path;

\( v \) = average groundwater velocity;

\( D_t \) = coefficient of hydrodynamic dispersion.

\( D_t = \alpha_L \cdot v + D^* \)

where,

\( \alpha_L \) = dispersivity of the medium;

\( D^* \) = coefficient of molecular diffusion (negligible when \( v \) is large).
The values plugged into the equation are as follows:

\( v = 2.0 \text{ m/year} \) is an assumed value of average ground water velocity;

\( l = 20000 \text{ m} \) is the advance of -15% from recharge area to the observation point;

\( \alpha_L = 7500 \text{ m} \) is the value estimated from MOC simulations;

\[
\frac{C}{C_0} = \frac{1}{2} \left[ \text{erfc}(0.09) \right]
\]

\[
\frac{C}{C_0} = 0.45
\]

The dispersive and advective fronts remain 2400 m apart after a time span of 11200 years.
APPENDIX 3

Well log details of $^{18}$O sampling sites
(after Ontario Ministry of Environment, 1974)
Well log details of $^{18}$O sampling sites
(after Ontario Ministry of Environment, 1974)

<table>
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<tr>
<th>Cell#</th>
<th>Township</th>
<th>MOE well#</th>
<th>Easting</th>
<th>Northing</th>
<th>Static water level (m)</th>
<th>$\delta^{18}$O in %o</th>
<th>Source</th>
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<td>4658125</td>
<td>177.1</td>
<td>-8.7</td>
<td>R.M.</td>
</tr>
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<td>4496</td>
<td>362680</td>
<td>4655480</td>
<td>185.5</td>
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<td>R.M.</td>
</tr>
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<td></td>
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<td>4661020</td>
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<td>4669510</td>
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APPENDIX 4

Well log details of the sampling points
(after Ontario Ministry of Environment, 1974)

Results of the chemical analyses
Well log description of domestic wells used for carbon-14 sampling.

(after Ontario Ministry of Environment, 1974)

<table>
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<tr>
<th>Cell #</th>
<th>Township</th>
<th>Well# OMOE</th>
<th>Northing</th>
<th>Easting</th>
<th>Static water level in feet</th>
<th>$\delta^{13}$C in % units</th>
</tr>
</thead>
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Results of the chemical analyses

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<th>SO$_4$</th>
<th>Cl</th>
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The major ions are reported in ppm.

Ca, Mg, Na, K were analysed by atomic absorption, HCO$_3$ by wet chemical method, and Cl was analysed by using an electrode.
APPENDIX 5

Input files of MOC and DSC simulation
### DSC Input Data

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VITA AUCTORIS

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Education:

1978-1981 Pre-University Education
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