Mapping Groundwater Pollution Risk within an Agricultural Watershed Using Modeling, Geostatistics and GIS

Sidney R. Vieira[1], W.D. Reynolds[2], R. de Jong[2], G.C. Topp[2] & R. Clemente[2]

[1]Instituto Agronomico, Caixa Postal 28, CEP 13001-970, Campinas, SP, Brazil,
EMail:SIDNEY@AGR.UNICAMP.BR, [2]Agriculture Canada, Central Experimental Farm, Ottawa, K1A 0C6, Canada

1. Abstract

With the objective of studying the atrazine transport using all the available soil attributes as input for a model and to predict the risk of groundwater pollution within a region which contributes to the Great Lakes, two study areas were selected for Southern Ontario: the Grand River Watershed at 1:1,000,000. The polygon information was obtained from the National Soil Data Base (NSDB). Using the soil codes and modifiers as a key, the soil attributes needed were extracted from the Soil Layer Files (SLF), for three layers. From the 119 polygons within the window, many attributes were missing, for which values were estimated using pedotransfer functions available from the literature. The pedotransfer functions were tested against field measured data and their performance was evaluated through the value of the linear correlation coefficient. The assessment of groundwater contamination with atrazine was done through the calculation of the annual mass loading and the time necessary for it to reach 3 ppb at 90 cm depth, through a water and solute transport model called LEACHM. The input data for the LEACHM model requires that for each soil profile data set a corresponding set of climatological attributes should be provided. For that purpose, the climatological data corresponding to the station closest to each soil profile was extracted and used for that soil unit. The expansion from point data to regions was done through geostatistical analysis, under the assumption that there is a continuous variation in soil properties from one point to its neighbour, as indicated by spatial autocorrelation between neighbouring observations. This assumption was verified through examination of the semivariograms for the attributes under investigation. Kriging was then used to estimate 1467 values on a fine regular grid of 2km by 2km for the watershed. The contour maps generated with the values estimated by kriging were input in the GIS and the rasterized maps were reclassified and colour printed with respective legends. The loadings of atrazine to the groundwater were limited by the soil attributes where there are heavy textured soils, whereas the climate attributes showed more influence on the loadings for the soils with higher hydraulic conductivities. Maize crop cultivation and the use of agrochemicals on high hydraulic conductivity soils should be restricted because virtually all of the unused chemical passes through in less than one year.

2. Introduction

The use of pesticides in Ontario has increased substantially in recent years. In the Great Lakes basin, between 1978 and 1983, the total amount of pesticides used for agricultural purposes increased from 6,123,680 kilograms to 8,391,010 kilograms, which represents a 35 percent increase in 5 years (McGee, 1983).

As the use of pesticide in agriculture increased in time, so did the concern over its presence in surface and ground water systems. Agriculture appears to be a major source of pesticides in the Great Lakes basin. Research to understand better the pathways and processes involving pesticides is needed to minimize their adverse impact on the biota.

This study is concerned with developing the capability to use the available data from soil databases for modeling water and solute transport through soil profiles. By extending the modeling from a profile to landscapes it is possible to assess the soil potential for preventing or contributing to pollution of ground water resources by the downward percolation of agrochemicals (e.g. nutrients, pesticides). Such a capability would be of great assistance to scientists, planners and policy makers in the development of soil quality inventories of "pollution potential", and in the development of agricultural land use practices and guidelines that maintain agrochemical inputs to the ground water at acceptable and sustainable levels.

An increasing awareness of the need for careful management of land use and land development has grown over the last decade, in particular, with respect to environmentally related sensitivity. Agriculture has especially received a considerable attention in this respect. Although, in general, pesticide residues above minimum detection limits in ground water are found in fewer cases than are nitrate and coliform bacteria (Agriculture Canada, 1992), it is still an important problem. Many studies related to ground water quality have been conducted in southern Ontario. Millette and Torreiter (1992), on a review of ground water contamination for the Great Lakes basin report levels of residues, primarily atrazine and metolachlor, ranging from 0.2 to 34 mg/L. Frank et al. (1987) report that between 1969 and 1984, in 596 wells examined in Ontario, 293 (49.2%) had pesticide concentrations above the minimum detection limit, constituted mostly by atrazine and 2,4-D. In order to prevent soil erosion, the use of no-tillage or minimum tillage systems has increased drastically in the last years, and it is estimated, for instance, that, by the year 2000, 60 to 70% of all cropland in the United States will be farmed according to some conservation tillage system (USDA-ARS, 1988). Most of the conservation tillage systems require the use of herbicides in their weed control programs because, often, no mechanical control is used to avoid mixing and revolving the soil. Sadeghi and Isensee (1992) found higher atrazine residues on conventional tillage than in no tillage plots. Therefore, it is expected that, if the pesticide could infiltrate into the soil immediately after it was applied, i.e., high soil infiltration rate, and the longest it could persist within the soil the better for its degradation. Temperature, soil moisture and soil characteristics play an important role on the persistence of pesticides. Walker et al. (1992) found the degradation rate of alachlor to be positively correlated with microbial biomass and microbial respiration, and adsorption positively correlated with soil organic matter content. They also found the persistence of alachlor in the field plots to be weather dependent.

The variability in pesticide concentration and fluxes within large fields is dependent both on the variability of the soil properties and on soil management practices (Trangmar et al. 1985). Millette et al. (1992) found the surface topography to have a major effect on the spatial distribution of atrazine, cyanazine and metolachlor even three to four years after their last application.

Spatial prediction precision depends greatly on the amount of information available and on the correlation between neighbouring observations and it has been quit extensively reported (Vieira et al. 1983, Trangmar et al., 1985, Beek et al. 1992, McBratney et al. 1992, Heuvelink and Bierkens, 1992)

Within this study methodologies have been adopted for characterizing and predicting the downward migration of the widely used herbicide, atrazine. Spatial and temporal variability in the atrazine migration is being accounted for via the combined use of a solute transport model, pedotransfer functions, geostatistical analyses, and a geographical information system.

3. Background

Although most pesticide contamination of ground water is below current Canadian drinking water guidelines, there are growing public concerns over potential health hazards related to long - term exposure to low levels of pesticides and their metabolites. Pesticide residues, especially atrazine, have been detected in surface, ground and tile drainage waters of many agricultural watersheds, particularly where there is some combination of high pesticide usage, intensive agriculture, high rainfall, irrigation, coarse and other highly permeable soils, high water tables, and sloping topography.

Pesticide contamination of ground water has traditionally been considered to be due primarily to spills, and to improper practices for storage, disposal and application. There is increasing evidence, however, that normal agricultural practices can also result in low - level, non - point source contamination of ground water via the downward migration of pesticides through the soil profile. There is consequently a need to determine how important and widespread this type of contamination might be, what the controlling soil quality, land use and environmental factors are, and what agricultural practices are required to limit this type of pollution to acceptable levels.

Essential steps in obtaining the above information include, identification of the primary mechanisms controlling pesticide movement through the soil profile, and development of the capability to characterize and predict the pesticide movement in space and time with acceptable accuracy. The approach being taken to achieve these steps is to employ a sophisticated solute transport simulation model in combination with pedotransfer functions, geostatistical analyses and a geographical information system (GIS). The solute transport model, which is an in house modification of a well established and tested modeling package called LEACHM (Hutson and Wagenet, 1989), integrates the major processes that occur in the soil profile, including: soil horizonation; saturated, unsaturated, steady and transient water flow; crop growth and transpiration; solute (e.g. atrazine) sorption, degradation, advection and dispersion; precipitation and evaporation; soil heat flow; and water table elevation. The pedotransfer functions are used to estimate, from available soil data, the soil attributes that are required as input to the solute transport model (e.g. hydraulic conductivity function, soil water characteristic). The geostatistical analyses are used to extend the model predictions of solute percolation behaviour from a point basis (the model is one -dimensional) to an aerial basis (e.g. farmer's field, watershed, landscape), using procedures that take into account the inherent spatial variability of the area. The GIS is used to create maps of the geostatistically extended solute percolation behaviour, and to overlay these maps with those of soil attributes, land management practices, cropping practices, weather, etc. Such maps and overlays are the "end product" which can be used to show the importance and distribution of ground water contamination by downward percolating pesticides; to determine the major soil, land use and environmental factors controlling the contamination; and to estimate the potential environmental impact of changes in land management practices.

Specifically, the objectives of this study are:
i) To develop an appropriate numerical estimation procedure for deriving from the Canadian National Soil Data Base (NSDB) and Archived Weather Data Base (AWDB) the soil, hydrologic and climatic parameters that control the water and solute movement in soil, and which can meet the requirements for modeling these processes;
ii) To incorporate the derived parameters of objective 1, the adopted modeling approaches, and other related data available from the NSDB into a geographic information system (GIS) to assess the risk of ground water contamination in selected Canadian agricultural landscapes;
iii) To assess and quantify the level of uncertainty associated with the risk assessments developed under objective 2.

4. Material and Methods

4.1 Criteria for Selection of the Study Areas and Working Scales

The basic criteria for choosing the study area required that:

- the basic land use had to be agricultural;
- there should be a reasonable range of soil texture;
- the region should use pesticides in their crops;
- there should be data available.

All of the first three conditions above are well documented in the literature for the Grand River watershed (Shelton at al., 1988). As far as the availability of data, the possible sources where the detailed soil survey for small areas or the Soil Landscapes of Canada database, and the Soil Carbon database for larger areas.

Throughout this study, the depth of the water table was considered constant at 90cm based on the depth of tile drains for southern Ontario.

4.2 Grand River Watershed

The Grand River is located in Southern Ontario and runs mostly southward towards Lake Erie. An arbitrary window encompassing the entire watershed was marked on a Southern Ontario map to eliminate border effects on the statistical calculations. A total of 119 polygons from the Soil Landscapes of Canada exist within the window. These polygons are identified with a unique number which is associated with its Soil Landscape unit through the soil code and modifier as a key to relate with other databases, such as the Soil Layer File (SLF), in order to extract soil attributes. Some polygon numbers are repeated within the window because they are pieces of a big unique polygon which was split in smaller pieces by the arbitrary line used as the limit of the window.. A total of 3 layers of data, corresponding approximately to the horizons A, B and C of the dominant soils, were obtained. Because the data base does not have any information as to where the subdominant soils are located within the polygon, only the dominant soils were used, as if they covered the entire polygon. For a few polygons, it was possible to obtain a fourth layer of data. However, because these layers corresponded to depths beyond the interest of this study, and because it was available only for a few soils, they were not used. From the 119 polygons within the window, there were 77 with textural components data, 46 with bulk density and soil desorption data, and 11 with saturated hydraulic conductivity. The missing values for soil texture and for soil organic carbon data in the Soil Layer File were obtained from the Soil Carbon of Canada (SCC) database, and the remaining attributes were estimated using pedotransfer functions. Most of the pedotransfer functions need the textural components and the organic carbon content as input to estimate soil attributes. For this reason, it was important to obtain these attributes for all polygons. A data set containing soil attributes for 119 polygons was passed on to other collaborators in this study to run LEACHM. The soil attributes were: Upper and Lower depths (cm), Sand (%), Silt (%), Clay (%), Bulk Density ($g.cm^{-3}$), Organic Carbon (%), Saturated Hydraulic Conductivity - Ksat ($cm.d^{-1}$), and the Soil Desorption curve parameters.

In the Archived Weather Data Base (AWDB) there are 510 stations for southern Ontario, from which, 82 are inside the window. These data were extracted with respective latitude and longitude co-ordinates, which were used to obtain the X-Y co-ordinates in kilometers on the same projection as the soil polygons. The data extracted include the monthly normals (1950-1980) of maximum and minimum temperatures, the daily precipitation and days with precipitation. Using the X-Y co-ordinates of the centroid of the 119 polygons, the nearest weather station was selected to be used as the source of climatic attributes to run LEACHM, and a list containing their names and respective numbers was given our collaborators to run the model. Using these normals as a source, a standard computing procedure was follow to obtain daily climatic attributes.

The LEACHM model was run for 10 consecutive years, assuming that, for every year, corn was planted over the entire area in early may, and the recommended amount of atrazine was applied at the recommended time. The annual mass loading of atrazine ($mg.m^{-2}$) and the elapsed time for it to reach 3 parts per billion at 90 cm depth, were the parameters chosen to measure groundwater contamination. The 90 cm depth value was chosen based on the average tile drain depth. The threshold value of 3 ppb for atrazine is the recommended drinking water level by the United States Environmental Protection Agency (USEPA, 1989).

The mean elevation above the sea level of the watershed region ranges from 50 to 120 meters. An earlier study on the use of pesticides in agriculture shows high pesticide application rates over the area chosen (Shelton et al., 1988). This same study shows that around 75% of the land is used for field crops over the watershed region.

4.3 Pedotransfer functions

Indirect estimation of soil hydraulic properties from basic soil properties has received considerable attention in the literature (van Genuchten et al., 1992). In order to better monitor and manage the migration of agricultural chemicals in the subsurface, scientists have developed increasingly complex computer models describing how water and solutes move in the unsaturated zone. Application of computer models to field scale transport problems requires a large number of model parameters, especially soil hydraulic properties. Thus, there is a growing need for more efficient and accurate methods to estimate the relevant model parameters, especially in situations in which, only basic soil properties such as textural components and soil organic carbon are available. Pedotransfer functions are essentially empirical relationships that estimate required, but unavailable (i.e. not measured), soil properties from the soil properties that are available. These functions, the forms of which have been established in the scientific literature, are calibrated for a particular study area by least squares fitting to a subset of "available" (i.e. directly measured) soil data. The functions are then used to estimate the required data where these data have not been measured. Extensive testing of pedotransfer functions for estimation of soil hydraulic properties can be found elsewhere in the literature (Vereecken et al., 1992, Vereecken, 1992, Wosten and Bouma, 1992). The goodness of fit of pedotransfer functions are usually evaluated using the coefficient of determination (Vereecken et al., 1992), and the higher its value, the better the predictive capacity of the equations.

Another important factor in testing pedotransfer functions is the availability of a reliable set of measured values. In this study, the measured data sets used contains a large variety of soils from southern Ontario provided by Topp (1993) (Topp, G.C. 1993. Personal communication), with some of it described in De Jong et al., (1992). Table 3 shows some general descriptive information about the measured data set.

Throughout this study, the pedotransfer functions were used only for the missing points, i.e., whenever there was a value in the data base it was used, regardless whether it was measured or estimated by an expert.

Potential evapotranspiration is an important parameter for any soil water balance and also for the processes involved in the LEACHM simulation model. Because these measurements are not available, estimation was made using Baier & Robertson (1965). Although this is a widely accepted model, unfortunately there was no measured data to verify its goodness. The model equation is:

$$
\begin{aligned}
&L.E. = -87.03 + 0.928\,T_{\max} + 0.933(T_{\max} - T_{\min}) + 0.0486\,Q_o \\
&P.E. = 0.094(L.E.)
\end{aligned}
\qquad (1)
$$

where L.E. is the latent evaporation, P.E. is the potential evapotranspiration (mm), T_{max} and T_{min} are the daily maximum and minimum air temperatures, respectively, and Q_o is the daily solar energy at the top of the atmosphere obtained from tables based on latitude and longitude values. The values of T_{max} and T_{min} used were the 30 year normals (1950-1980) for every month, which were then submitted to simple computing routine to generate daily values.

The soil bulk density was only available in the data base for 46 out of 119 polygons. Therefore, for 73 polygons this property had to be estimated somehow. Three pedotransfer functions were used and compared, namely, Gupta and Larson (1979a), Rawls (1983) and a stepwise multiple regression method. The method suggested by Gupta and Larson (1979a) showed the highest correlation coefficient with the measured values and for this reason it was used for the estimation of the missing 73 values. This method does not have one simple equation and it simulates 30 random packings of the particle size fractions given as input, and the average of these 30 packings is used. The program inputs are: the number of fractions of particle size with respective bulk densities, the percentual amount of each fraction, and the percent organic carbon content. The number 30 is the program default, but if desired, the user can specify other number.

From the 119 polygons, only 11 had values for the saturated hydraulic conductivity in the data base. The pedotransfer functions tested for the estimation of this attribute were: Saxton et al. (1986), Rawls et al. (1982), Cosby et al. (1984) and Jabro (1992). None of these methods were exceptionally good. Keeping the same criteria of the best correlation coefficient the model by Jabro (1992) was chosen for the estimations through the equation

$$\log(K_s) = 9.56 - 0.81 \log(\%silt) - 1.09 \log(\%clay) - 4.64(Bd) \qquad (2)$$

Where K_s is the saturated hydraulic conductivity (cm h^{-1}), and Bd is the soil bulk density (g cm^3).

As it was discussed earlier, the data base has only 4 soil desorption curve points (KP0, KP10, KP33, and KP1500), for which there were 46 out of 119 available. First of all, this number of points in the curve is far too few for a good estimation of the desorption curve equation, which is required for the LEACHM model. A reasonable number of points in the curve is 10-12, which were estimated using the pedotransfer functions described by: Saxton et al. (1986), Cosby et al. (1984), McBride and Macintosh (1984), Rawls and Brakensiek (1982) and Gupta and Larson (1979b). The results showed that the McBride & Macintosh (1984) is clearly much better than the others.

$$\log_{10}\theta_m = [\log_{10}\theta_{mi} - (\alpha \log_{10}\psi_i)] + (\alpha \log_{10}\psi) \qquad (3)$$

The basic equation for computing soil water content at specified pressure values is
where $-\psi_i$ is the pressure potential at the primary inflection (kPa), $-\psi$ is the pressure potential for which θ_m is to be predicted (kPa), θ_{mi} is the gravimetric moisture content at the primary inflection (% g g^{-1}), $\theta_{m1.5}$ is the gravimetric moisture content at the pressure potential of -1.5 MPa (% g g^{-1}), θ_m is the predicted gravimetric moisture content at a pressure potential of $-\psi$ (% g g^{-1}) and a is the slope = $(\log_{10}\theta_{m1.5} - \log_{10}\theta_{mi})/(3.176-\log_{10}\psi_i)$. For all the polygons, values of θ_m were calculated using equation (3) for 5, 10, 20, 40, 60, 80, 100, 150, 225, 300 and 500 kPa, $\theta_{m1.5}$ were calculated

$$\theta_{m1.5} = 1.338(\%clay)^{0.7}$$

and θ_{ms} were calculated from the bulk density.

With the soil desorption curve points estimated, it is necessary to fit an equation to it. Because the van Genuchten's model is widely accepted and its parameters are required to run the LEACHM model, it was used to obtain the parameters for each of 119 polygons. Details about the model can be found in van Genuchten (1980). The functional equation is

$$\Theta = \Theta_r + \frac{\Theta_s}{[1+(ah)^n]^m} \qquad (4)$$

where θ_r, θ_r, a, n and m are parameters determined by non linear least squares method. The goodness of fit of the van Genuchten's model fitted to the 13 soil desorption curve points of each of the 119 polygons, as measured by the correlation coefficients were very good, with the R^2 values above 0.96 in all instances.

1.4 Statistical analysis

Examination of the classical statistical moments of a data set usually reveals preliminary information that can be very important, such as the extreme values, the coefficient of variation, or the indicators of frequency distribution type. The classical statistical moments used within this study are: the mean,

$$\overline{Z} = \sum_{i=1}^{N} \frac{Z_i}{N} \qquad \textbf{(5)}$$

the variance,

$$s_Z^2 = \sum_{i=1}^{N} \frac{[Z_i - \overline{Z}]^2}{N-1} \qquad (6)$$

the coefficient of variation (C.V.),

$$C.V. = 100 \frac{\sqrt{s_Z^2}}{\overline{Z}} \qquad (7)$$

the coefficient of skewness,

$$g_1 = \frac{AM_3}{(s_Z^2)^{1.5}} \qquad (8)$$

where,

$$AM_3 = \sum_{i=1}^{N} \frac{(Z_i)^3}{N} - 3\overline{Z} \sum_{i=1}^{N} \frac{(Z_i)^2}{N} + 2(\overline{Z})^3$$

the coefficient of kurtosis,

$$g_2 = \frac{AM_4}{(s_Z^2)^2} \qquad (9)$$

where,

$$AM_4 = \sum_{i=1}^{N} \frac{(Z_i)^4}{N} - 4\overline{Z} \sum_{i=1}^{N} \frac{(Z_i)^3}{N} + 6(\overline{Z})^2 \sum_{i=1}^{N} \frac{(Z_i)^2}{N} - 3(\overline{Z})^4$$

where N is the number of measurements for each variable, Z.

The correlation matrix can be calculated for all combinations of any two attributes using the equation,

$$r(Z_i, Z_j) = \frac{COV(Z_i, Z_j)}{\sqrt{s_{Z_i} s_{Z_j}}} \qquad (10)$$

where,

$$COV(Z_i, Z_j) = \sum_{i=1}^{N} \frac{Z_i Z_j}{N} - \overline{Z_i}\,\overline{Z_j}$$

The expansion from point data to regions can be done through geostatistical analysis, under the assumption that there is a continuous variation in soil properties from one point to its neighbour, as indicated by spatial autocorrelation between neighbouring observations. The continuity of the spatial distribution of the measurements has been evaluated using geostatistics (Vieira et al., 1981, Vieira et al.,1983, Vieira et al. 1991). All geostatistical analysis are based on the assumption that measurements separated by small distances are more likely to be similar to each other than those farther apart, i.e, spatial autocorrelation exists. This assumption can be verified through examination of the semivariograms for the attributes under investigation, i.e., the semivariogram is a statistical tool to measure the autocorrelation. For a set of values $Z(x_i)$, measured at every one of the N locations x_i, which, in turn is defined by a pair of co-ordinates *x,y* the semivariogram can be calculated using the equation

$$g(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} [Z_i - Z_{(i+h)}]^2 \qquad (11)$$

where N(h) is the number of neighbours separated by a distance, h. For autocorrelated data, the semivariogram computed with equation (11) is an increasing function, because the neighbours close together are more similar to each other than those which are further apart. A graph of g(h) versus values of distance, h, is called the semivariogram and will represent the average similarity between neighbours, which can, in turn, be used to interpret the spatial variation of the data and to densify the grid with values estimated by the kriging interpolation method (Vieira et al., 1983), to be described below. The assumption of spatial autocorrelation is accepted as valid if the semivariogram increases as a function of the separation distance between neighbouring values up to a certain distance, where it equals the value of the sample variance. This distance is known as the range of correlation and defines the radius over which the values can affect the estimation of an unknown value. The Y-axis intercept of the semivariogram graph is called the nugget variance and represents the degree of discontinuity that exists at small distances, i.e., the smaller the nugget variance, the more similar neighbouring values are. The proportion of the nugget variance to the value the sample variance is a measure of the degree of randomness of the data at small distances. The magnitude of the nugget variance value is inversely related to the precision of any estimation made using the semivariograms. All semivariograms used in this paper were scaled according to the procedure established by Vieira et al. (1991), by dividing each of them by the value of their respective variances. This way, the value to which the resulting semivariograms stabilise is approximately one and comparison between them can be easily made. To the graph of g(h) versus values of distance, a model equation must be fit in order to be used during kriging interpolation. Within this study, the spherical, the exponential and the power models were used and their equations will be described below. The curve fitting technique used to adjust models to the calculated values of the semivariograms should not involve least squares methods because of the difficulties in judging the influence of local variation at small distances in the final model as suggested by Journel and Huijbregts (1978). The step by step procedures for the curve fitting are described in Vieira et al. (1983).

The spherical model adjusted to the experimental values follows the equation

$$g(h) = C_0 + C_1 [1.5(\frac{h}{a}) - 0.5(\frac{h}{a})^3] \qquad (12)$$

denoted in the referred figures as Sph(C_0,C_1,a) where the value C_0 (called nugget effect) represents the variability at scales smaller than the sampling distance, C_0+C_1 is the value at which semivariances stabilise, and **a** is the range, whose value indicate the distance up to which the samples have spatial autocorrelation.

The exponential model follows the equation

$$g(h) = C_0 + C_1 [1 - \mathrm{Exp}(\frac{-3h}{a})] \qquad (13)$$

denoted in the referred figures as Exp(C_0,C_1,a).

As long the assumption of autocorrelation can be proven to exist, then the kriging interpolation method can be used. The kriging estimation follows the equation

$$Z^*(x_0) = \sum_{i=1}^{N} l_i Z(x_i) \qquad (14)$$

where N is the number of neighbours measured involved in each estimation, and l_i are the weights attached to each measured value. Kriging method requires the estimation to unbiased, i.e.,

$$E[Z^*(x_0) - Z(x_0)] = 0 \qquad (15)$$

and that the variance of the estimation be minimum, i.e.,

$$E[Z^*(x_0) - Z(x_0)]^2 = minimum \qquad (16)$$

Using the estimator proposed in equation (14) subjected to the conditions (15) and (16), and applying Lagrangian techniques of minimization, the kriging system is derived. The kriging equations are

$$\sum_{j=1}^{N} l_j g(x_i, x_j) + m = g(x_i, x_0), i = 1,N$$

$$\sum_{j=1}^{N} l_j = 1 \tag{17}$$

Therefore, kriging is an interpolation method that takes the similarity between neighbouring measurements, i.e, autocorrelation, into account for each estimation made through the values of the weights, l, used in each estimation. That means, if measurements are taken on a 10 kilometre grid in the field, and autocorrelation between neighbouring measurements exists as calculated by equation [11], then kriging interpolation can be made using this autocorrelation to obtain values for any desirable spacing, such as 1 kilometre, 2 kilometres, etc. For each kriging estimation, the uncertainty involved on the interpolation process can be assessed through the estimation variance,

$$s^2(x_0) = m + \sum_{i=1}^{N} l_i g(x_i, x_0) \tag{18}$$

A detailed development of the kriging equations can be found in Vieira et al. (1983). The kriging grid had 1657 values at the separation distance of 2 kilometers. All the kriging estimation for the Grand River watershed was made on this grid, from which it can be seen that whatever software is used for the construction of contour maps, it will be very precise because of the high density of information. Once the attribute of interest is estimated on a fine grid through kriging, contour maps can be easily made in commercially available software, and subsequently transported to the GIS.

1.5 Map analysis through a Geographical Information System (GIS).

Throughout this report, whenever there is a reference to a GIS, it should be understood that it refers to a particular GIS software called ILWIS (Integrated Land and Water Information System), used within this study. ILWIS is both a raster and vector based GIS, which works on DOS environment, and has converting capabilities to both import to and from many other known GIS.

There are two fundamental approaches to the representation of the spatial component of geographic information: the vector model and the raster model (Aronoff, 1989). In the vector mode, objects and conditions in the real world are represented by the points and lines that define their boundaries, much as if they were being drawn on a map. In the raster model, the space is regularly subdivided into cells (usually square in shape). The location of geographic objects or conditions is defined by the row and column position of the cells they occupy.

The basic sequence of map analysis for the contour maps resulting from the kriging interpolation done through the GIS involves: digitising the contour maps of the attributes for which kriging was done; rasterizing the segment (contour map), in vector mode, creating an attribute map with the values of each contour; interpolating from isolines, in the spatial modeling mode of the raster analysis; erasing the interpolated region located outside of the map boundaries, in map calculation of the spatial modeling, by multiplying the interpolated map by a rasterized map with the value of 1 for the inside and 0 for the outside region; reclassifying the resulting map, with the appropriate classification table in map calculation; manually making the appropriate look up table, in raster visualization; making the appropriate map legend, in the annotation mode of output; and finally printing the map with corresponding legend.

Because of their nature, some attributes such as soils map and soil surface texture could not be interpolated and thus, the procedure to produce these maps is different from the above. For the soils map, the sequence is: digitizing of the map with the soil polygons with segment codes different for each item, such as boundary, river, soils, etc.; checking segments for dead ends and nodes; making polygons; naming the polygons according to the soil codes, modifiers and polygon numbers. All of these are done in the digitizing mode. Subsequently, the map is rasterized in vector mode without attribute values; the appropriate look up table is selected in raster visualization; the map legend is created in the annotation mode of output; and then the final map is printed. For the maps of the attributes which were not possible to be interpolated by kriging such as surface texture, rooting depth, coarse fragments, etc., the procedure to follow is: load the INF file (a file produced during rasterizing of the soils map, which is a table with the polygon names, number of polygons, area, area and perimeter), in table calculation mode; add a column with the desired appropriate name; edit the table entering the desired values; produce the resulting map in map calculation, using the syntax OUTMAP:=TABLE.COLUMN[INMAP] producing a byte map; make appropriate colour look up, in raster visualization; make appropriate legend, in annotation mode of output; and print map.

The basic difference between the two above categories of maps is that the one produced via kriging interpolation, contouring, etc., assume the attribute is continuously changing across the field, while the maps produced with attribute table calculation assume that the entire polygon has one single value of that attribute and is uniform for it. While for some qualitative attributes this is the only possibility at this point, it may not be statistically correct to assume that one entire polygon has one single and pure value of that attribute (Topp et al., 1980). Overlaying of raster maps can be done between the two categories without any problem. The overlaying of maps is done within map calculation using the IF statement with the syntax: OUTMAP:=IF(CONDITION,THEN,ELSE), with the appropriate output map type.

5. Results and Discussion

A working scale had to be chosen right at the beginning, since there were basically two choices: a 1:1,000,000 scale or a detailed scale of 1:45,000. It is important to emphasize that the detailed scale is not really available as a whole for Southern Ontario, but rather, the soil survey was done on a county-by-county basis. The integrated map covering regions not related to counties has not been put together yet. Had it been done, a generalization for whatever larger scale could have been easily made. In order to accomplish the objectives i) and ii) of this work, it was necessary to use a large area for which, neither of the two scales were ideal, because one is too small and the other is too big. A scale of 1:250,000 for the watershed would be ideal for it would provide enough variety of soils to allow for a good evaluation of the performance of the LEACHM model, and enough detail to allow for very high precision geostatistical estimation of soil attributes.

Table 1. Estatistical moments for atrazine loading, time and soil physical attributes Grand River, Ontario, Canadá

Name	Unit	N	Mean	Variance	C.V.	Minimum	Maximum	Skewness	Kurtosis
Horizon 1									
Depth	Cm	119	15.130	37.270	40.36	5.000	33.000	0.548	2.833
Coarse sand	%	85	2.259	21.420	204.90	0.000	25.000	3.236	14.680
Very fine sand	%	59	12.510	118.900	87.16	0.000	40.000	0.873	3.070
Total sand	%	119	43.110	546.000	54.20	10.000	86.000	0.389	1.801
Silt	%	119	39.450	245.600	39.73	9.000	64.000	-0.545	1.976
Clay	%	119	18.960	113.000	56.06	5.000	49.000	0.593	2.547
Bulk density	g/cm^3	119	1.366	0.023	11.03	0.900	1.590	-0.820	3.111
Organic Carbon	%	119	1.733	0.533	42.11	0.500	3.900	0.550	2.982
Alpha	1/cm	119	0.022	1.675E-05	18.24	0.007	0.028	-2.168	7.457
M coefficient	dml	119	0.324	0.003	16.54	0.260	0.442	0.790	2.588
Residual moistute	% vol	119	14.270	30.490	38.68	6.000	26.600	0.168	1.846
Saturation moisture	% vol	119	48.810	36.790	12.43	40.000	66.000	0.751	2.783
Hydraulic conductivity	cm/s	119	6.652E-04	1.016E-06	151.50	2.100E-06	4.090E-03	2.282	7.099
Loading	mg/m^2	119	0.840	1.890	163.70	0.000	8.290	2.486	10.560
Time	year	119	16.580	162.000	76.78	0.770	27.390	-0.333	1.122
Horizon 2									
Depth	cm	119	40.550	553.800	58.03	10.000	102.000	1.348	4.167
Coarse sand	%	88	1.807	12.660	196.90	0.000	25.000	3.769	21.850
Very fine sand	%	61	11.000	113.700	96.92	0.000	39.000	0.980	3.039
Total sand	%	119	40.950	693.900	64.33	4.000	94.000	0.496	2.029
Silt	%	119	39.130	262.400	41.39	5.000	64.000	-0.537	2.363
Clay	%	119	19.920	186.700	68.60	1.000	63.000	0.850	3.364
Bulk density	g/cm^3	119	1.513	0.022	9.87	1.000	1.700	-1.051	4.459
Organic Carbon	%	119	0.965	0.588	79.45	0.170	5.160	2.812	15.620
Alpha	1/cm	119	0.020	6.634E-05	39.95	0.006	0.036	-0.665	2.318
M coefficient	dml	119	0.342	0.005	20.19	0.244	0.526	0.732	2.980
Residual moistute	% vol	119	17.220	75.340	50.41	2.000	34.100	-0.011	1.844
Saturation moisture	% vol	119	44.450	41.030	14.41	35.900	66.000	1.144	4.977
Hidraulic conductivity	cm/s	119	1.425E-04	6.953E-08	185.00	0.000E+00	1.980E-03	5.799	39.880
Loading	mg/m^2	119	0.840	1.890	163.70	0.000	8.290	2.486	10.560
Time	year	119	16.580	162.000	76.78	0.770	27.390	-0.333	1.122

Horizon 3									
Depth	cm	119	122.400	895.500	24.44	43.000	190.000	0.327	4.034
Coarse sand	%	90	3.222	38.640	192.90	0.000	25.000	2.156	6.454
Very fine sand	%	62	10.390	155.000	119.90	0.000	46.000	1.288	3.721
Total sand	%	119	40.390	795.900	69.85	3.000	93.000	0.513	1.946
Silt	%	119	34.670	235.400	44.25	6.000	56.000	-0.381	2.175
Clay	%	119	24.940	310.700	70.67	1.000	65.000	0.477	2.169
Bulk density	g/cm^3	119	1.549	0.014	7.57	1.200	1.700	-0.859	3.685
Organic Carbon	%	119	0.465	0.182	91.76	0.100	3.000	3.613	21.450
Alpha	1/cm	119	0.024	9.271E-05	40.35	0.006	0.055	-0.067	3.826
M coefficient	dml	119	0.331	0.005	21.11	0.249	0.516	0.885	2.976
Residual moistute	% vol	119	19.740	100.500	50.76	2.100	36.700	-0.174	1.781
Saturation moisture	% vol	119	41.450	20.020	10.79	35.500	63.000	2.092	10.340
Hidraulic conductivity	cm/s	119	1.450E-04	1.020E-07	220.20	1.160E-07	1.780E-03	4.205	19.970
Loading	mg/m^2	119	0.840	1.890	163.70	0.000	8.290	2.486	10.560
Time	year	119	16.580	162.000	76.78	0.770	27.390	-0.333	1.122

Because the ideal situation was not available, and because it was impossible to work with the detailed scale for a large area, the 1:1,000,000 scale was chosen. Two other good reasons for choosing this scale are that the Soil Landscapes of Canada and the Soil Carbon of Canada databases are both on this scale, and were ready to be used. Moreover, good or bad, adequate or not, for large areas such as the watershed, the Soil Landscapes of Canada is the only option available.

From the classical statistical moments shown in table 1, it can be seen the high variability in soil properties. Even bulk density, which usually does vary excessively over large areas, has coefficients of variation of significant magnitude. As it is commonly found in field data, the saturated hydraulic conductivity is highly variable and has a very skewed distribution, most probably lognormal. Another important point here is the decrease in hydraulic conductivity from the top horizon (Horizon 1) to the subsurface. This condition may favour the persistency of pesticides within the soil profile for longer times, giving them the opportunity for degradation, adsorption, and other processes. Moreover, it seems like the change in hydraulic conductivity is likely due to change in soil structure, since the texture components do not change much with depth. The high value for the coefficient of variation for the annual loadings of atrazine to the groundwater, indicates that a high soil variability over the watershed. From the 119 polygons, there are many soil profiles that did not have any loading at all after 10 years, but also, there are soils with 8.29 mg/m^2.

The semivariogram for the saturated hydraulic conductivity for the 3 horizons together and for the atrazine loadings and treshold times are shown in figure 1. The exponential model showed a reasonable fit to the experimental values of the semivariogram for loadings, time and Ksat for horizon 1, with a range of 30 km. Since these semivariograms have been scaled by dividing the original semivariance values by the corresponding variance (Vieira et al. 1991), their closeness indicates similarity in the variability of the corresponding variables. It follows then, that the atrazine loadings and threshold times have a very similar spatial behavior to Ksat 1, but quite different of the hydraulic conductivity for the other horizons. For this reason, it is possible that the hydraulic conductivity of the horizon 1 is the one controlling the atrazine flow to deeper layers. The semivariograms for Ksat for horizons 2 and 3 show a very clear periodical behavior. Because of the nature of this attribute with many factors affecting it in different proportions across the landscape, it is so variable from place to place, that the random component of the variation almost surpasses the correlation. This is verified by the large nugget variance values, and by the ups and downs of calculated semivariogram values. Remembering that the semivariogram is a result of the mean squared differences between the neighbouring values, it can be seen that values close together have more similar Ksat and atrazine attributes than those farther apart. That means, the elevations are very well behaved and mathematically continuous from point to point.

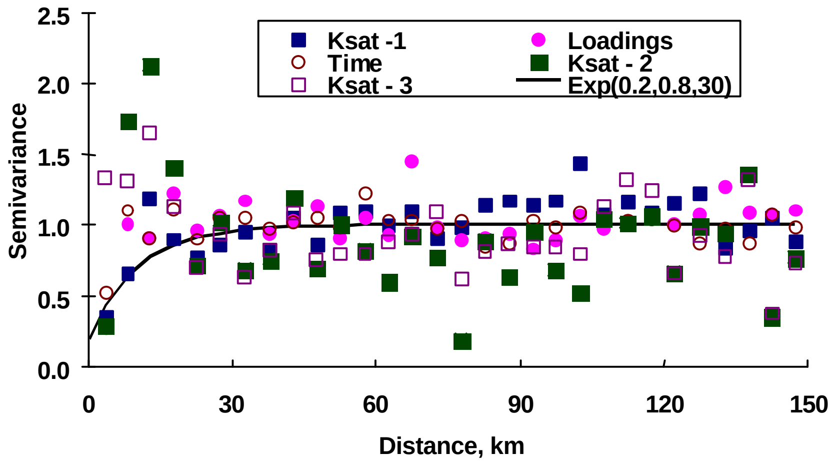

Figure 1. Semivariograms for saturated conductivity, atrazine loadings and time,Grand River watershed, Ontario,

The continuity between neighbouring observations of the textural components expressed through the semivariograms shown in figure 2 for horizons 1, 2 and 3, with one single exponential model adjusted to all of them, with a correlation range of 50 kilometres. This guarantees that these attributes have continuity from place to place, and also supports the geostatistical expansion from point information to the watershed region. Since the semivariograms for the textural components are very well scaled to one single model, it can be said that the change in hydraulic conductivity with depth is probably due to structure.

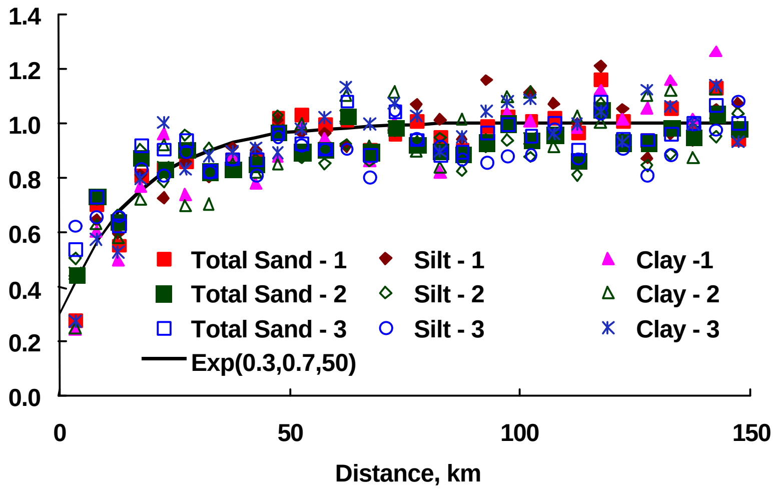

Figure 2. **Semivariograms for particle size attributes. Grand River watershed, Ontario, Canada.**

Virtually the same can be said about the semivariograms for the van Genuchten's parameters shown in figure 3. The correlation ranges are almost the same and so are the models. That means that the soil desorption curves over the watershed are closely related to the textural components. The high variability of the saturated hydraulic conductivity discussed above, is also reflected on the semivariograms shown in figure 3.

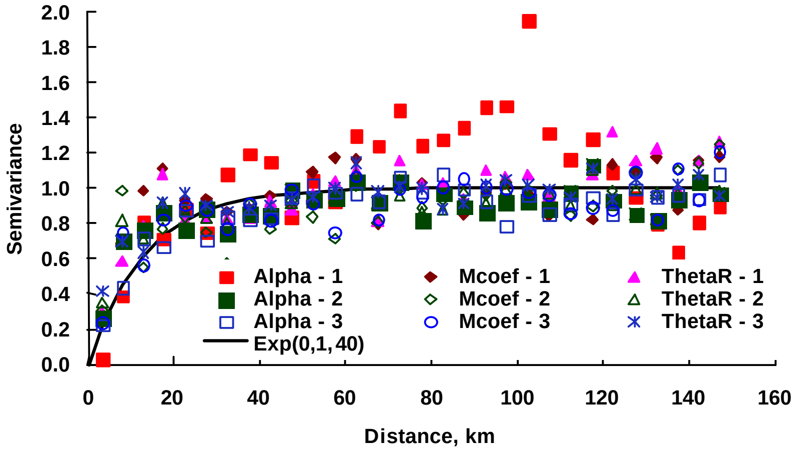

Figure 3. **Semivariograms for van Genuchten's parameters. Grand River watershed, Ontario, Canada.**

The maps obtained through kriging, digitising, etc., for the atrazine loadings and treshold times are shown in figures 4 and 5, respectively. The comparison of these maps may be useful in the interpretation of the results. The surface texture of the soils of the watershed, as it can be seen in figure 31, is predominately from loam to heavier soils, a fact that may favour the persistence of agrochemical within the soil profile for longer times. The lower part of the watershed is constituted of soils having predominantly heavy clay texture. The amount of coarse fragments, although it is not a input parameter for the LEACHM model, had the highest correlation with the annual atrazine loadings. It should be emphasised that one large soil unit in the central part of the watershed which is loamy sand has also the highest amount of coarse fragments. The slope gradient for most of the watershed is flat or has small slopes. For this reason, it is expected that small amounts of agrochemicals is lost by surface erosion. However, there is one portion at the top of the watershed that shows shallow water table and is a silt loam soil, which could contribute to faster leaching of pesticides to the water table.

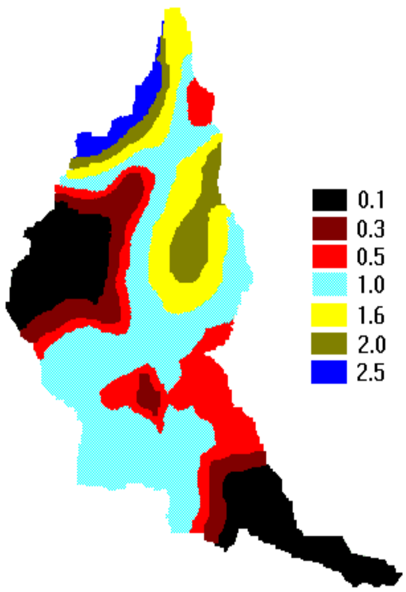

Figure 4. Atrazine loadings (mg/m^2).

Figure 4 shows the annual atrazine loadings to a constant depth water table at 90 cm, from which it can be seen that the regions where there is low atrazine loadings are more likely to be controlled by the soil factors, in particular at the lower portion of the watershed. The portion with the highest loadings at the top left of the watershed seems to be more affected by the total precipitation, which is also high in that region, in particular for winter and fall. There is one region on the half left of the map that shows low atrazine loadings, in spite of very high total precipitation in all four seasons. Since the surface texture is silt loam to clay loam it is possible than low hydraulic conductivity is the factor controlling the flow. The remaining portion of the map seems to be affected by both climate and soil factors. Another fact noticeable on the annual atrazine loadings shown in figure 4 is their high variability over the watershed. Considering that the map on figure 4 was obtained by classifying the original values into the arbitrarily chosen classes, fact that tends to smooth some of the extreme values, the variability is very high. Just from the classification legend it can be seen that a change from 0.1 to 2.5 mg/m^2 corresponds to 25 times. The reason for this extreme variability seems to be much more related to the soil properties than to the climate attributes. The textural components: minima and maxima shown in table 1 indicate a very extreme textural change for any of the three depths. In fact, the deeper layers have a higher variability than the surface layer, which is probably caused by the mode of deposition of the soils of the majority of this region. Moreover, the saturated hydraulic conductivity values for the deeper layers are 5 times smaller than that for the surface layer, and the coefficients of variation increase with depth. This fact also contributes for the variability of the annual atrazine loadings.

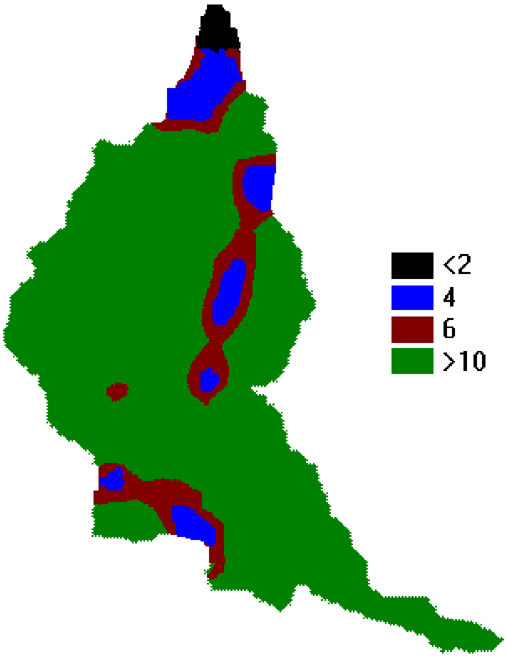

Figure 5. Time (years) to reach threshold concentration

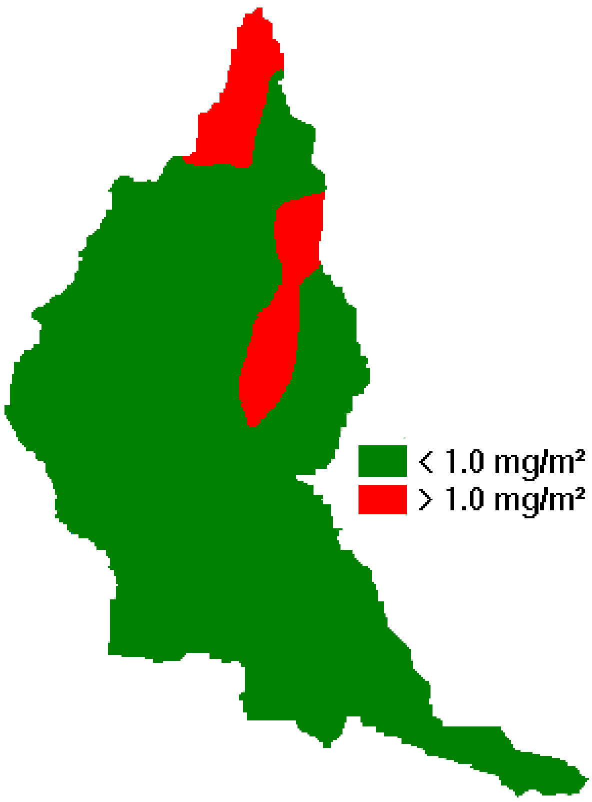

Figure 6. Pollution risk

The map on figure 5 shows the time in years to reach the concentration of 3 ppb at the 90 cm depth. The threshold value of 3 ppb was chosen according to the USEPA standards for drinking water (USEPA, 1989). For the majority of the watershed, it takes more than 10 years for the concentration to reach the threshold level. It is interesting to note that the places where it takes less time to reach 3 ppb at 90cm are not the same where the highest loadings occur. The soil properties may be of high importance for this fact.

Using the resources of map calculation within ILWIS, the two previous maps were overlaid to produce what is referred to, here, as contamination potential map, shown in figure 38. This map produced using the map calculation:
"OUTMAP:=IF(LOAD>1.0,IF(YEARS<3,1,0),0)"
which means that, if the loadings are greater than 1.0 mg/m^2 and if it takes less than 3 years to reach this level then paint the map red, else paint it green. Therefore, the red portions of the map are not only where the loadings are greater than 1.0 mg/m^2 but also where it takes less than 3 years for this to happen.

Because of the complexity of the processes involved within the calculations made to generate the maps for this study, the assessment of the uncertainty level for the maps is not an easy task. Many components with different contributions can be responsible for some degree of uncertainty of the results, amongst which, the pedotransfer functions, the expansion from point information to landscapes through Geostatistics, and the map handling within ILWIS, will be addressed below.

The pedotransfer functions used to estimate soil properties for the polygons which did not have them in the data base is one of the sources of uncertainty which present the most difficulty to evaluate. First of all, because it is an estimation technique, it involves an error which is expected to increase as the correlation coefficient, R^2, decreases. The number of points in the regression was 834 which is a result of 13 points in the desorption curve, for 68 different soils. Therefore, all the points from the saturation to 15000 kPa were used for the calculation of the regression of Estimated = a + b Measured. The only two slope factor significantly different from the others are the ones for McBride and Macintosh (1984) and the ones fro Gupta and Larson (1979), which are the two extremes best and worst, respectively. The correlation coefficients are also, respectively, the best and worst for the above two models. Therefore, these parameters seem to be reasonably good indicators of the goodness of fit for the pedotransfer function model. However, the degree of uncertainty for each individual soil is no easily assessed.

The error involved on the expansion of the information from point to landscapes through kriging estimation at very fine grid can be assessed through the estimation variance. The variation of the estimation variances values within any area is directly proportional to the distance between the closest measured value and the estimated (Vieira et al., 1981), being zero at the exact location of the measured value, and maximum at the maximum distance. Therefore the uncertainty will be greater where there are fewer or sparse values which is an obvious information since it is much easier to trust an estimation if the neighbours used for the estimation are close. The magnitude of the estimation variance with respect to the sample variance depends upon the proportion of the nugget variance value of the semivariogram to the sample variance, being the highest for a pure nugget variance semivariogram (a semivariogram for which the nugget variance equals the sample variance, i.e., does not have any spatial correlation).

The map handling through ILWIS has a much smaller contribution to the final uncertainty of the results, because, up to a certain degree, it is somewhat operator dependent and decreases with the experience acquired. For this study, most of the map handling was done at the final phase of the project and this source of error was minimized.

6. CONCLUSIONS

Although the simulation model - transfer function - geostatistics - GIS methodology is still under development, the preliminary results are very encouraging. The calculated pedotransfer functions and semivariograms are, for the most part, well behaved; and the kriged distributions seem plausible for the regions in question. Consequently, it is felt that this methodology is very useful for assessing the risk of agrochemical pollution of ground water resources, as well as for the development of land use practices and guidelines leading to acceptable levels of agrochemicals in the environment.

The analysis of the results of this study allow to conclude that:

- The loadings of atrazine to the groundwater are controlled by soil hydraulic properties at the regions where the loadings are low, and more likely to be controlled by the weather conditions at places where the hydraulic conductivity of the soils is not limiting. For the most part of the watershed, the loadings of atrazine are below 1.0 mg/m^2 but at some places they are both greater than 1.0 mg/m^2 and they reach this level in less than 3 years.

- The methodology used to expand information from point to landscapes with the geostatistical techniques has proved itself very useful, with the assumptions easily verified through the semivariograms.

As a recommendation for future research, it can be said that improvements in the techniques adopted within this study would be achieved if more dependable data could be made available, and if better pedotransfer functions could be developed for the estimation of values for soils for which they had not been measured. Field measured soil properties for different environmental conditions is essential for adequately testing the pedotransfer functions.

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