

Characterisation of potential pollution sources in the quantitative assessment of risk to groundwater resources within the Birmingham aquifers, UK

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ABSTRACT: This work presents a methodological approach where distribution of potential pollution sources and historical frequency of pollution incidents are included in the assessment of risk to groundwater resources. Calibrated flow and transport models were setup, and integrated with a FORTRAN coded risk model. The risk model was run to generate synthetic contaminant source terms that were subsequently transported by the coupled flow and transport models. The ranges of calibrated values obtained for horizontal and vertical hydraulic conductivities are 5.787×10^{-6} - 2.315×10^{-5} m/s and 5.787×10^{-8} - 1.157×10^{-7} m/s, respectively. Layering within the aquifer is thought to account for the large vertical anisotropy. The corresponding values for the specific yield and specific storage are 0.10 - 0.12, and 1×10^{-4} - 5×10^{-4} , respectively. The estimated historical frequency of pollution occurrence per stress period of 91 days is 35, while the probability of pollution occurring at any of the sources over a period of stress period is calculated as 0.0014. The generated risk maps provide anticipatory capability for risk quantification and show that approximately 55% of the monitoring boreholes have high (i.e. 70 – 100 %) likelihood of having contaminant concentration being less than 0.06 mg/l throughout the simulation.

KEYWORDS: Quantitative risk, Groundwater modelling, Probability, Vulnerability, Risk model

I. INTRODUCTION

The statistics of groundwater use (Zektste and Everett, 2004) has shown that groundwater has become one of the most important global natural resources. In Denmark, Malta and Saudi Arabia, groundwater constitutes the only major source of water supply, while in Tunisia and Belgium, approximately 95 and 83 % respectively of the country's water resources is sourced from groundwater. This importance is underpinned by the inherent valuable properties of the resource compared to the surface water. These properties include higher quality, better protection from anthropogenic activities, less seasonal variation, large storage, relatively inexpensive developmental cost and wide spread occurrence, among others. However, occurrences of global pollution is increasingly becoming one of the major environmental concerns that pose threats to groundwater resources and can potentially cause depletion of these values. Cases of pollution occurrences have been reported in Beijing in China (Marilyn, 2001), Taejon area in Korea (Jeong, 2001), as well as in the developing countries (Egbu, 2004). The scale of impacted groundwater bodies is becoming more widespread and the persistence of groundwater pollutants is increasing, making the cost of aquifer restoration to be excessive in many cases. Therefore, pollution prevention rather than pollution management appears to proffer the basis for a truly sustainable approach to groundwater protection.

Generally, the extent of protection of groundwater resources is assessed based on the risk posed by anthropogenic activities, or the measure of ease with which an infiltrating pollutant reaches the groundwater resource. The contemporary techniques for the assessment of risk and vulnerability to groundwater can be broadly be categorized into three groups namely: ranking index methods, process-based computer simulation, and post-pollution assessment methods (Al-Adamat *et al.*, 2003; Aller *et al.*, 1985; Connell and Dale, 2003; Foster, 1987; Gustafson, 1989; Van Stempvoort *et al.*, 1992; Khan and Liang, 1989; Rao *et al.*, 1985; and USEPA, 1989). According to Haines (2006), risk is defined as the result of a threat with adverse effects to a vulnerable system. Following from this definition, it implies that the most vulnerable groundwater is not at risk without the presence of threats. This concept of risk therefore comprises of two-dimensional components. From the point of view of the water resources, the first component is the probability of contaminant source terms being generated from potential pollution sources at the ground surface while the second component is the assessment of impact of such occurrence. The ranking index methods are essentially qualitative and subjective in approach, and generally lacking good scientific judgement. Also, none of the existing methods incorporates quantifications of the probability of occurrence of polluting source terms from the potential sources.

In this work, potential pollution source is defined as a single, identifiable and localized source with risk of discharging pollutants that may infiltrate into the aquifer. Hence, the fact that potential sources often constitute threats to groundwater resources necessitates the need to include their occurrence and distribution in quantifying any risk posed to the underlying groundwater resources. Quantifying the probability of occurrence of pollution is generally the most uncertain part of the assessment of risk posed to groundwater system. Therefore, this work is set to demonstrate the field application of a novel two-dimensional risk assessment methodological approach, where assessment of risk to groundwater resource incorporates both the quantification of the probability of occurrence of source terms, as well as the impact of such pollution event. A more detailed discussion on the concept and structure of the method has already been presented in Oladeji and Elgy (2012).

II. METHODOLOGY

The algorithm of the methodology implemented in this work is presented in Figure 1. The risk model components of the Risk Assessment Method (RAM) structure are implemented by a computer program written in a standard FORTRAN 90. The risk model is run over the same period of time as the flow and transport models. Contaminant source terms are generated for each stress period of the simulation, which are then transported within the subsurface environment using the coupled flow and transport models. The effects of the generated source terms are assessed by observing the spatial and temporal concentrations of the contaminant at pre-determined monitoring boreholes within the aquifer, as well as by counting the number of times the contaminant concentration exceeds user defined ranges of concentration magnitude. Two grid systems namely a local system and a global system are implemented in the risk model. This is to allow the risk model to be run independently of the flow and transport models, as well as to increase the efficiency in the implementation of the risk model in terms of the time and memory requirements. The local grid may be equal to or smaller than the global grid system used in groundwater flow and contaminant transport models.

The purpose of the Risk Model Parametization module (see Figure 1) is to prepare the input data for the risk model. This involves obtaining locations of the potential pollution sources at the ground surface. The geographical locations of the potential sources are initially obtained using global positioning equipment, and subsequently transformed into the appropriate layer, row and column numbers of the model grid using GIS utilities.

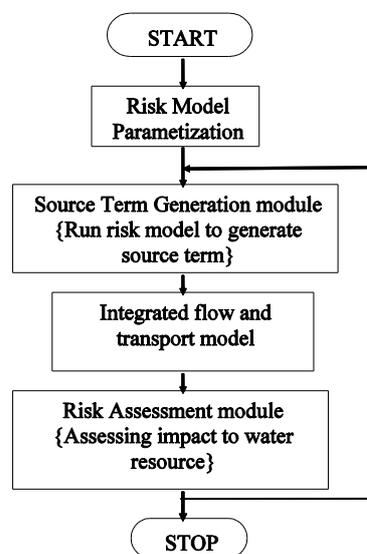


Figure 1: Conceptual algorithm of the risk assessment method

The process of the generation of synthetic source terms by the risk model involves determination of the condition for the generation of a synthetic source term, as well as the magnitude of the associated contaminant mass. In order to determine the condition for the generation of a synthetic source term in any stress period, the risk model computes a parameter called Probability of Pollution Occurrence (PPO) for each of the active model cells containing potential pollution source(s), using Equation 1:

$$PPO = \frac{\text{No of days of previously occurred pollution events} / \text{No of sources}}{\text{Total no. of days under consideration}} \quad (1)$$

Note that equation 1 is implemented when the PPO has to be evaluated during the execution of the risk model. If PPO is already known by priori knowledge, then the values can be entered appropriately.

Next, for each day in the current stress period and for each active node, the risk model generates a Random Number (RN) between 0.0 and 1.0, and compares the random generated number (RN) with the PPO value computed. If $PPO > RN$, then a pollution incident is assumed to occur. However, an array of integer values of between 0 and 5 is set for each model cell, and these dynamically control the actual proportion of infiltrating contaminant mass per each event. For example, a value of 0 indicates that all the synthetically generated probable mass loading rate of contaminant at a particular active node are transported from that source, while a value of 5 indicates that, although synthetic contaminant mass is generated at the source, no pollutant is assumed to be transported from that source. This utility is used to incorporate source control capability as mitigating measures based on the ground conditions. Also, in order to determine a contaminant mass associated with each of the synthetic pollution event, the risk model samples a random value from a range of the minimum and

maximum values of contaminant mass loading rates that have previously occurred based on historical records or other priori knowledge.

In this work, the probability distribution of the historical pollution events is represented by a Poisson distribution. A Poisson distribution expresses the probability of a number of events occurring in a fixed period of time if these events occur with a known average rate and independent of the time since the last event. If the expected number of occurrence in an interval of time is given as λ , then the probability that there are exactly k occurrences (where k being a non-negative integer) is given as:

$$f(k : \lambda) = \frac{\lambda^k e^{-\lambda}}{k!} \quad (2)$$

where e is the base of the natural logarithm, and $k!$ is the factorial of k .

Finally, the risk model extracts the spatial and temporal contaminant source terms generated for all the stress periods, and presents the source terms in a format that is compatible with the transport model input data file. In addition, the risk model transforms the row and column numbers from the local grid system into that of the global grid system used for flow/transport model.

The generated source terms serve as input into the transport model. After each run, the risk model counts the number of times at which the contaminant concentrations exceeds ranges of user defined concentration magnitudes, and express the result as a risk. These steps represents the first realisation of the risk assessment method, and subsequently iterated such that the frequency distribution of the observed contaminant concentration at points of interest in the aquifer is developed by observing the number of times that the user defined concentration magnitude is exceeded.

2.1 Description of the study area

The study area (Figure 2) extends 17 km from south to north, and 13 km from west to east, covering approximately 221 km², and forms part of the larger West Midlands conurbation. Birmingham has been a major manufacturing centre for over a century, and contains many industrial processes that may constitute risk to groundwater. According to Powell *et al.* (2000), the area is underlain by the Triassic sandstone, and consists of fluvioglacial thick successions of the sandstone deposit, commonly referred to as the Sherwood sandstone Group. The basal aquifer unit is the Kidderminster sandstone Formation, overlain by the Wildmoor and Bromsgrove sandstone Formations. These three sandstone aquifer horizons have distinct hydrogeological properties. The superficial geology consists of till, sand, gravel and alluvium, and overlies the Triassic geological successions. The soil types present within the study area are highly varied and complex, and their distribution and composition are influenced by factors such as climate, geology, geomorphology and hydrology. The landuse pattern is largely urban. The major rivers present within the study area are shown in Figure 2.

A major geological structure within the study area is the Birmingham Fault, which juxtaposes the Triassic mudstone to the east against the Triassic sandstone to the west. According to Allen *et al.*, (1997), transmissivity is generally reduced across the Birmingham Fault, and Knipe *et al.*, (1993) modelled the zone across the fault as a reduced aquifer thickness in order to represent the reduced transmissivity across the fault. The Triassic sandstone Group form the major aquifers in the study area, and their hydrogeological characteristics are dominantly controlled by lithological variations, vertical heterogeneity, anisotropy, fractures, scale of measurement, as well as uneven variations in the aquifer thickness (Allen *et al.*, 1997). The inorganic, organic contamination and the occurrence of pollution related acidification within the urban aquifer of Birmingham area have been respectively studied by Ford and Tellam, (1994), Rivett *et al.* (1990), and Ford *et al.* (1992).

2.2 Numerical groundwater flow and transport model

The U.S. Geological Survey numerical finite-difference groundwater flow model MODFLOW 2000 (Harbaugh *et al.* 2000) forms the basis for the model development and the subsequent calibration process. The initial conditions for the model setup are presented in Table 1. For the purpose of model calibration, the model was set up to run under transient conditions covering 20 years from January 1970 to December 1989, and validated using groundwater head data spanning from March 1985 to February 2015. The eastern and the southern boundaries of the aquifer geometry were defined using no flow cells because of the presence of Birmingham Fault which is assumed to inhibit flow across it. Also, the western boundary was defined as no flow because of the presence of the Westphalian Formations, which are older non permeable geological material. The northern boundary was delineated by the groundwater divide along an anticlinal axis on the base of Triassic sandstones (Knipe *et al.*, 1993), and therefore also represented as no flow boundary.

The initial groundwater heads within the aquifer horizons were interpolated from the available groundwater level observation data. Where the river path exists, the initial groundwater head was defined by the river stage. The rivers present within the model domain (see Figure 2) are contained within the first model layer. The Modflow head dependent river package allows the model to calculate the amount of streambed percolation and groundwater inflow to each river reach, using river bed conductance and the difference between the calculated model cell hydraulic head and the stage of the river.

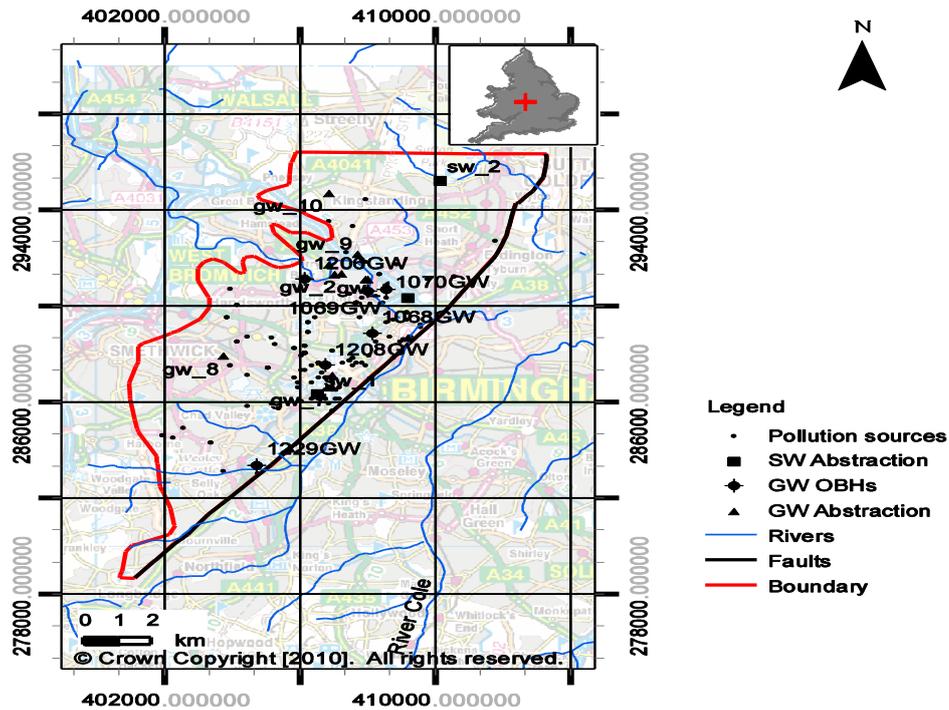


Figure 2: Location of the study area

Table 1: Summary of initial and final flow model data

Input parameter	Initial Conditions
Boundary Conditions	No flow conditions for the west, east, north and south boundaries.
Spatial discretization (m)	No of rows: 760; No of columns: 600; $\Delta x=25$; $\Delta y=25$
Horizontal hydraulic conductivity (m/s)	Bromsgrove Fm = 5.0×10^{-5} Wildmoor sst Fm = 2.0×10^{-4} Kidderminster Fm = 3.0×10^{-4}
Vertical hydraulic conductivity (m/s)	Bromsgrove Fm = 5.0×10^{-7} Wildmoor sst Fm = 1.0×10^{-6} Kidderminster Fm = 5.0×10^{-7}
Specific yield	Bromsgrove Fm = 0.10 Wildmoor sst Fm = 0.10 Kidderminster Fm = 0.10
Specific storage	Bromsgrove Fm = 1×10^{-3} Wildmoor sst Fm = 5×10^{-3} Kidderminster Fm = 1×10^{-3}
Effective Porosity (%)	Layer 1 = 26.8 %; Layer 2 = 23.8 %; Layer 3 = 26.4 %
α_L α_T ; α_{VT} / α_{VL} ; Mol. Diff. Coeff.	20 m ; 0.1 m; 0.01; 0.0 m ² /s

The river bed conductance controls the rate of flow to or from the river according to the difference between the river stage and the modelled groundwater head in the uppermost active cell. River bed conductance also defines the maximum leakage rate to the aquifer when heads fall below the bed of the river. The river paths contained within the model boundary were divided into reaches. The interaction with the underlying aquifer was simulated between each reach and the model cell that contains that reach. The river bed elevations were estimated from the digital elevation map (DEM), and the river stage was assumed to be 0.5 m above the estimated river bed.

The constant flux well package was used to simulate pumping from the 12 abstraction boreholes (gw_1 – gw_12) located within the model domain (Figure 2). The average abstraction rates used for each stress period are presented in

Figure 3a. The dearth of data for the abstraction rates restricts the use of the actual values of the historical abstraction rates in the transient model calibration. Also, the three locations (sw_1 - sw_3) where surface water abstraction is being abstracted within the study area (Figure 2) are lined and therefore no interaction with the underlying aquifer is assumed. The daily recharge values were estimated for the study area using a recharge calculator based on series of spreadsheet calculations underpinned by the Food and Agricultural Organisation (FAO) methodology. The average annual recharge values for the study area is 112 mm/yr, and represents the final recharge value distributed across each stress period (Figure 3b) in the flow model using the Modflow recharge package.

The model was calibrated with hydraulic head data spanning over 20 year period, from March 1970 and February 1989, by minimizing the residuals between the observed and the simulated groundwater head data. The convergence criterion for the hydraulic heads was set to 0.01 m within the Preconditioned Conjugate Gradient 2 (PCG2) solver package. The PCG2 solver package iteratively refines the initial estimates of the model until either an acceptable measure of residual is achieved or the difference between the results of successive iterations is less than a user specified convergence criteria.

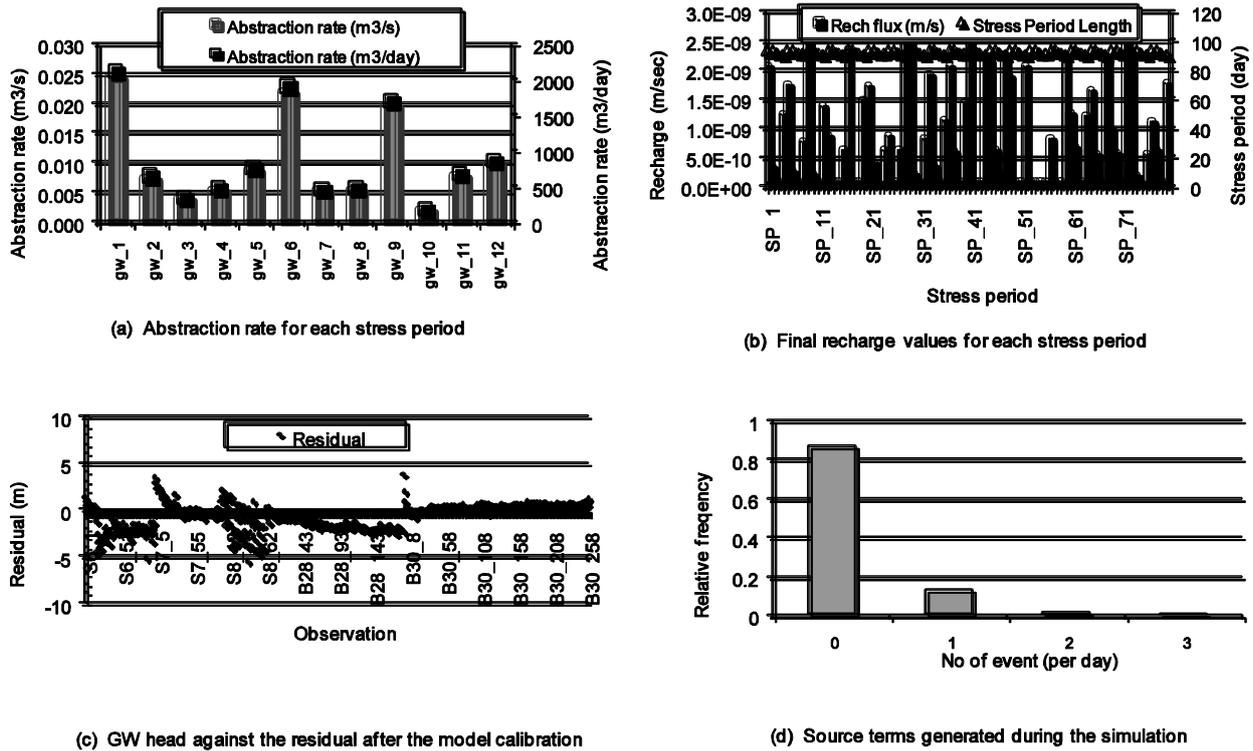


Figure 3: Abstraction and recharge as well as the residual and source terms

The groundwater level monitoring data obtained from the observation boreholes were used as targets for assessing the effectiveness of the calibration process. In order to make future predictions of the risk posed to the groundwater resource, the flow model was validated and further set up to run from March 1985 to February 2015. The corresponding groundwater head computed at the beginning of March 1985, which corresponds to the elapsed time of 15 years of the calibrated flow model, was set to be the initial groundwater heads for the model layers under the predictive transient simulation. Also, a predictive transport model (Zheng and Wang, 1999) was setup under transient conditions covering 30 years from March 1985 to February 2015.

2.3 Risk model

The records of the historical occurrence of chloride related pollution incidents within the study area spanning over January 2002 – December 2009 were used to determine the pattern of the historical occurrence of pollution incidents. This data is considered to be sufficient in the demonstration of the applicability of this risk assessment method, but thought that longer record length will be more representative for the study area. In order to keep the model simple, this work considered pollution sources from only five common industries within the Birmingham area, and these include food, chemical, garages, mining and mineral industries. The analysis of the historical pollution data shows that the average number of pollution incidents from the selected industries for the study area was 35 events per stress period of 91 days. These values were used to compute the PPO for the study area. The total number of pollution sources within the study area was 281. Using equation 1, the probability of pollution occurring at any of the sources over a given stress period of 91 days is computed as:

$$PPO = \frac{\text{No of days of previously occurred pollution events} / \text{No of sources}}{\text{Total no. of days under consideration}} = \frac{35 / 281}{91} = 0.0014$$

The calculated PPO was applied to each of the active cell of the risk model for each stress period. Although, the method as demonstrated in this work assumed that each type of the industry has the same probability of occurrence of pollution incidents in each of the stress period, this method can be adapted to assess the risk from the individual type of industry with varying probability of pollution occurrences per stress period for each of the industry.

III. PRESENTATION AND DISCUSSION OF THE RESULTS

The results of the applications of the risk assessment method are discussed under the following headings.

3.1 Flow model

The model was setup as a three-layer model, which represents (from top) the Bromsgrove, Wildmoor and the Kidderminster sandstone Formations. The respective final horizontal hydraulic conductivity values (K_h) are 5.787×10^{-6} , 2.315×10^{-5} , and 3.472×10^{-5} m/s. The corresponding values for vertical hydraulic conductivity (K_v) are 5.787×10^{-8} , 1.157×10^{-7} , and 5.787×10^{-8} m/s, respectively. Hydraulic layering within the Permo-Triassic sandstone aquifer is thought to account for the large vertical anisotropy in the final calibrated hydraulic conductivity values. The final horizontal conductivity values are within the same range compared to the values obtained by Allen *et al.* (1997) from field test data, for the respective aquifer horizons, as well as to those values obtained by Knipe *et al.* (1993). Furthermore, the final values for the specific yield are 0.12, 0.10 and 0.12, and for the specific storage are 1×10^{-4} , 5×10^{-4} , and 1×10^{-4} , respectively for Bromsgrove, Wildmoor and Kidderminster Formations. The value reported by Allen *et al.* (1997) for the specific yield of the undivided Sherwood sandstone Group is 0.12. Knipe *et al.* (1993) and Rushton and Salmon (1993) respectively reported specific yield value of 0.15, and 0.10 for the Bromsgrove sandstone Formation, and these values are similar to those obtained in this work.

The plot of the observations and the corresponding residual for the model calibration is presented in Figure 3c. The percentage numerical error associated with the volumetric balance is less than 0.1 % throughout the duration of the simulation, and this indicates that the model was converging without any significant numerical error. A sufficient degree of match was obtained between the measured head observations and the simulated equivalents (Figure 3c). The flow model was subsequently setup as a predictive model for a 30-year period spanning March 1985 – February 2015. The March 1985 groundwater head output of the calibrated model was used as the initial water level for the predictive model.

3.2 Risk model

The risk model was set up over the same period of 30 years, from March 1985 to February 2015. The global grid system for the risk model is the same as that of the flow and transport model. The number of potential sources of chloride pollution within the case study area was scoped for the food processing, garages, quarries, mineral and chemical industries, and 281 locations were identified as sources of chloride pollutant. The average occurrence of chloride pollution incidents over the eight-year period (2002 – 2009) was estimated as 35 incidents per stress period (91 days). Hence, the probability of pollution occurrence for each of the potential pollution source was computed to be 0.0014. The range of the contaminant mass loading rate of the historical pollution incidents within the study area is estimated based on the available information to be 250 – 5000 kg per incident. This represents the range of values within which the contaminant mass loading rate was sampled on each occasion when a synthetic pollution incident occurred.

The risk model was run to generate source terms for the transport model. The number of pollution events generated per each day is summarised in Figure 3d, and it indicates that zero incident occurred in 9,453 days out of the total 10,920 days. Single daily events occurred in 1363 days, two daily events in 98 days, while three daily events occurred in only 6 days. Given the generating mechanism used to create pollution events, the frequency of occurrence of 0, 1, 2... events per day should follow a Poisson distribution. The Chi (χ^2) test verifies this, as it showed that the probability that these are by chance from different distributions is very remote (1.02937×10^{-6}), and therefore confirms that the mechanism for generating random events is correct.

3.3 Transport model

The predictive transport model was setup over a 30-year period (March 1985 to February 2015). Chloride contaminant was used to demonstrate the applicability of this method because of its conservative and non reactive nature within the natural subsurface environment. The initial background chloride concentration was set to zero in order to prevent the background concentration from masking the effects of the generated source terms. The mass balance error is generally less than 0.1 %. The spatial distribution of the contaminant after 30 years of simulation is presented in Figure 4, and shows that the contaminant concentration within the study area varies between 0.0 – 0.1 mg/l. High correlation exists between the simulated contaminant concentration (see Figure 4) and the pattern of the distribution of the potential pollution sources (see Figure 2).

3.4 Risk assessment results

The risk to groundwater resources within the study area was determined as the number of times which chloride concentrations at the 12 observation boreholes exceeded the user defined concentration intervals. The two user defined

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