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GROUNDWATER CONTAMINATION PLUME DELINEATION USING LOCAL SINGULARITY MAPPING TECHNIQUE

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ABSTRACT: The evaluation and remediation of contaminated aquifers require accurate delineation of contamination plumes. Ideally a large number of observed concentration data are required to achieve an accurate delineation of the contamination plume. However, in practice due to the budgetary constraints, the contamination in groundwater resources is detected by limited number of arbitrary located or predesigned contamination monitoring wells. Therefore, a technique is required to estimate the boundaries of the plume using the available sparse observation data. In this work, Local Singularity Mapping Technique is used for plume delineation. The singularity mapping technique is based on the multifractal concept. In fractal geometry a local feature is similar to the whole in terms of shape and structure. Generalized self-similarity is characterized by a power-law relationship. Using this method, singularity indices are estimated for the entire study area using sampled concentration data. According to these indices the mapped area (study area) is classified into subsets including contaminated and clean areas. The boundaries between these two subset areas can be identified as the contamination plume edge. The performance of this method is evaluated in an illustrative contaminated study area to demonstrate the potential applicability of the proposed methodology. The singularity indices can be utilized to locate potential contamination sources as well as plume boundaries. These evaluation results demonstrated that the contamination plumes can be relatively accurately delineated using the fractal geometry.

Keywords: *Groundwater contamination, Fractal, Singularity mapping technique, Plume delineation, Monitoring.*

1. INTRODUCTION

Groundwater is the major potable, agricultural and industrial source of water. Due to industrial revolution together with the lack of appreciation of chemicals and their potential impact on the land and water bodies, groundwater is subjected to various sources of contamination. Often, effective groundwater pollution management and remediation relies on accurate delineation of the contamination plume. This paper focuses on a new method based on the fractal singularity mapping method to delineate the contaminant plume in the groundwater aquifers.

The contaminants move and spread into the groundwater aquifers primarily controlled by the hydraulic gradient. The size, shape and boundary conditions of the polluted area in addition to the geological, hydrogeological and geochemical properties, have substantial effect on the transport of contaminants. However, the investigation of contamination is complex and difficult as the result of the inherent uncertainty in definition of the groundwater systems in addition to lack of information and possible sources of error in available information. On the other hand, the groundwater flow and solute transport processes are very complex and generally are defined by partial differential equations [1]. Therefore, the delineation and the estimation of contaminant plume in the groundwater systems is a challenging task.

The presence of contamination in groundwater poses significant challenges to its delineation and quantification. Leakage from chemical and petrochemical distribution infrastructures, e.g. pipelines, as well as from waste water collection systems such as septic tanks and urban sewage channels and pipelines are a few sources of subsurface contamination. Further, products of mining activities and industrial complexes, which are stored on or underground without any provision to control the seepage into the ground, are two of the most common sources of groundwater contamination.

Various approaches were developed for delineation of contamination in the groundwater systems. The first approach is based on the identification of the contamination sources. The contamination sources should be identified in terms of location, activity duration and release fluxes. By knowing the characteristics of contamination sources, the plume can be delineated at any time by simulating the contaminant movement using flow and transport simulation models.

One of the effective contamination source identification methodologies is the linked simulation-optimization approach [2-4]. In this method the optimization models are linked with the flow and transport simulation models [4-10]. The optimal source characteristics are achieved when the difference between estimated and observed contaminant concentrations at monitoring locations is minimized. The effectiveness and accuracy of this method relies on the available observed contaminant concentrations collected at monitoring locations. Therefore, many researchers focused on optimally design monitoring networks which would result in better characterization of contamination sources. Some of the previous works using various methods for monitoring network design include integer programming [3, 11], Genetic Algorithm [12], Simulated Annealing [13, 14] , Mixed integer programming [15], Data interpolation techniques [12, 14], Plume detection [16], Redundancy reduction [17], Genetic Programming [14, 18], and Dynamic Time Wrapping Distance method [13]. The accuracy of identified contamination source characteristics can be improved by using optimally designed monitoring networks with appropriate objectives. The efficiency of using measurement data from such designed monitoring networks can be enhanced by utilizing sequential and feedback based monitoring network designs. In this method, the contamination source characteristics identified using available observed concentrations are utilized to design a new monitoring network. Then the new selected monitoring locations are used sequentially to improve the accuracy of identified source characteristics [3, 14, 19-21].

Accurate estimation of contaminant source characteristics are essential to delineate the contamination plume based on simulation of the flow and transport processes. The other approach involves directly delineating the contamination plume using available observed concentrations. The interpolation techniques such as Kriging [14, 16, 22], and Inverse Distance Weighting method [23, 24] are two of these methods. The accuracy of the interpolation methods depends on the values selected for the interpolation parameters. For instance, in the Kriging interpolation technique the effectiveness of the method depends on the accuracy of selected model variogram. As an alternative, in this study the Fractal Singularity Mapping technique is utilized to delineate the contamination plume using available observed contaminant concentrations. The accuracy and effectiveness of this method does not rely on the accuracy of parameter selection.

In environmental geochemistry, the term “baseline” often indicates the actual content of an element, irrespectively of its origin, in the environment at a given point in time as opposed to the term “background” that indicates the content depending on natural factors like lithology or climate [25]. Background, as represented in the environmental field, is the borderline between concentrations of a chemical element and component that naturally occurs in a media, compared to the concentrations present as a result of anthropogenic activities. In groundwater contamination problems, generally the background borderline represents the boundaries of the contamination plume in the groundwater aquifer. To evaluate the background values, there are two basic approaches: statistical frequency analysis and spatial analysis. Statistical frequency analysis uses techniques for characterizing the frequency distribution based on the assumption that point data from different locations may originate from different sources and present different populations [26]. The spatial analysis refers to methods dealing with spatial distribution of values on a 2-D map where geochemical point data are generally interpolated. Frequency based methods do not incorporate spatial variance of geochemical fields, which are important aspects of geochemical data. Methods of spatial data analysis such as geostatistics and fractal analysis are becoming more widely used frequency-space-based methods to quantify and model, spatial variances of geochemical data [27].

Fractals and multifractal are two important branches of nonlinear and complexity sciences. The analysis methods based on the fractal and multifractal concepts, have been used in many areas of natural sciences, including earthquake [28], flooding [29], rain and clouds [30], and geoscience [31]. Fractal models such as Number-Size model (N-S), Concentration-Area model (C-A) [32], Spectrum-Area model (S-A) [33, 34], Concentration-Distance model (C-D) [36], singularity index [37], and Concentration-Volume model (C-V) [35] have been developed for geochemical data analysis [27].

The Singularity theory was developed by Cheng [37] to quantify the geo-anomalies according to the invariant properties between fractal measure and scale. In this paper the local singularity mapping technique is used to characterize the groundwater contamination plume by specifying the “baseline” as the contamination plume boundaries. First, the methodology is explained. It is followed by the illustrative application of the singularity mapping technique in a contaminated study area. Then, the solution results representing the performance of the approach in terms of the efficiency of contaminant delineation are evaluated and discussed.

2. THE SINGULARITY MAPPING TECHNIQUE METHOLOGY

Generalized fractal self-similarity is often characterized by a power-law relationship in the spatial or frequency domain [31]. In the singularity mapping technique, the C-A model is used. In this context, the singularity in 2D map data is describe as a power-law relationship between area A in a sampled region, and the total amount of a certain physical quantity μ(A) as Eq. (1).

$$\langle \mu(A) \rangle = cA^{\alpha/2} \tag{1}$$

Here $\langle\rangle$ denotes the statistical expectation, α is the Holder exponent or singularity index, and c is a constant. The areal density value of μ(A) in the area A is defined by concentration ρ(A) as Eq. (2).

$$\langle \rho(A) \rangle = \mu(A) / A = cA^{\alpha/2-1} \quad (2)$$

2.1 The singularity mapping technique

Singularity is an index representation the scaling dependency from a multifractal point of view, and it characterizes how statistical behaviors change as the scale of geochemical values changes. In the singularity mapping technique the indices are estimated using the window-based procedure. The improved window-based procedure [31] is conducted as per the following steps.

1- Define a set of square windows $A(r_i)$ with variable window sizes $r_{min} = r_1 < r_2 < .... < r_i = r_{max}$ for a given sampling point on the map.

2- Calculate concentration $\rho\left[A(r_i)\right]$. In the improved method, the minimum vale (ρ_{min}) is subtracted from all concentration values in each window.

3- Eq. (3) is defined by taking logarithm of Eq. (2).

$$\rho\left[A(r_i)\right] = (\alpha - 2)\log(r_i) + C \quad (3)$$

Therefore the singularity index (α) can be calculated based on the slope of the log-log plot of Eq. (2). Based on the distribution of α, the 2D mapped area is classified into subsets of fractals and can be divided into following three cases.

1- If an anomaly [37] is convex, then ρ(A) is decreasing function of A and α<2 it indicates high density and positive singularity.

2- If an anomaly is concave, then ρ(A) is increasing function of A and α>2 it indicates high density and negative singularity.

3- If an anomaly is constant, then ρ(A) is a constant only and α=2 indicates a non-singular of linear behavior.

This idea can be used for detection of edges and boundaries of different bodies. In the groundwater contamination problems, this concept can be used to detect the edges of the contamination plume, as proposed here. For the purpose of boundary detection, the maximum horizontal gradient is located nearly over edges, which corresponds to the inflection point of the anomaly. Around the inflection point, the value of ρ(A) estimated by the window-based method, does not change with respect to the change of Area A. Therefore, near the plume edge, the third case is valid. This indicates that the singularity index $\alpha \approx 2$ detects the edges, and α<2 and α>2 specify the inside and outside of the boundary, respectively

3. APPLICATION AND PERFORMANCE EVALUATION

In this section, the local singularity mapping method is utilized to delineate the contamination plume in a polluted groundwater aquifer. In order to conduct a systematic performance evaluation of the proposed methodology, an illustrative study area is considered. It facilitates the evaluation of the methodology without having to consider the unknown reliability of field data. This is necessary only for evaluation purposes. Different scenarios regarding the shape and complexity of the contamination plume are defined and the accuracy of the proposed methodology is evaluated for the case of complex groundwater contamination scenarios.

3.1 Study Area

Figure 1 shows the plan view of the illustrative 3-dimentional study area measuring 2100m × 2500m × 50m and the top and bottom boundaries are specific head boundaries and the ones to the right and left are head dependent flux boundaries. The average recharge due to rainfall is applied to the whole study area. Eight water extraction wells are included in the model (shown by filled circles in Fig. 1). The natural gradient is from top to the bottom of the study area. A snap shot of the head contours are shown in Fig. 1. The study period is 8300 days. For the flow and transport simulation purposes, the area is discretized into 42×50 cells. MODFLOW-2000 [39] and MT3DMS [40] are utilized as the flow and contaminant transport simulation models, respectively. Both simulation models are computer programs that numerically solve the three-dimensional transient ground water flow and contaminant transport partial differential equation. The field hydro-geological parameter values are given in Table 1.

3.2 Groundwater Contamination Scenarios

The performance of the developed methodology is evaluated for two different scenarios. These scenarios represent various degrees of complexity in terms of location and number of pollution sources. The delineation of the contamination plume becomes more complex as the number and proximity of contaminant sources increase.

3.2.1 Scenario 1

In scenario 1, two actual sources of pollutants are present. In this case, the sources are relatively far from each other; therefore, very limited overlapping of pollutant plumes resulting from the individual sources occurs. In Fig. 1, numbers 1 and 2, show the location of these sources. The flow and transport simulation models are utilized to simulate the transport of pollutant released from these two sources. The resulting simulated concentrations corresponding to 2000 and 3000 days after the activation of sources

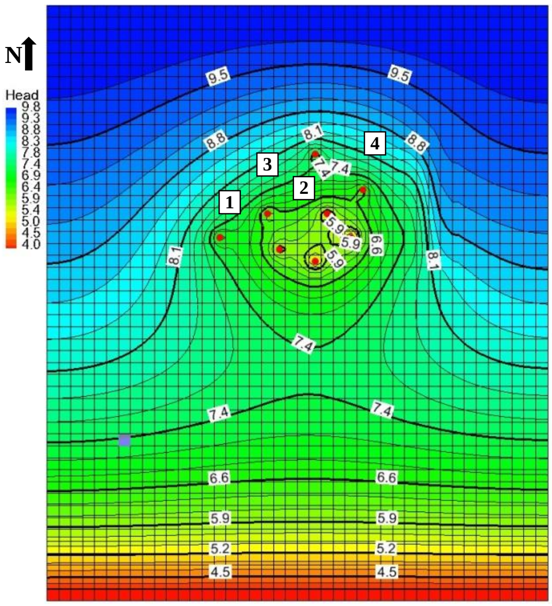


Fig. 1 The head contours in the study area, unit is m.

Table 1 Hydrogeologic parameters for the study area.

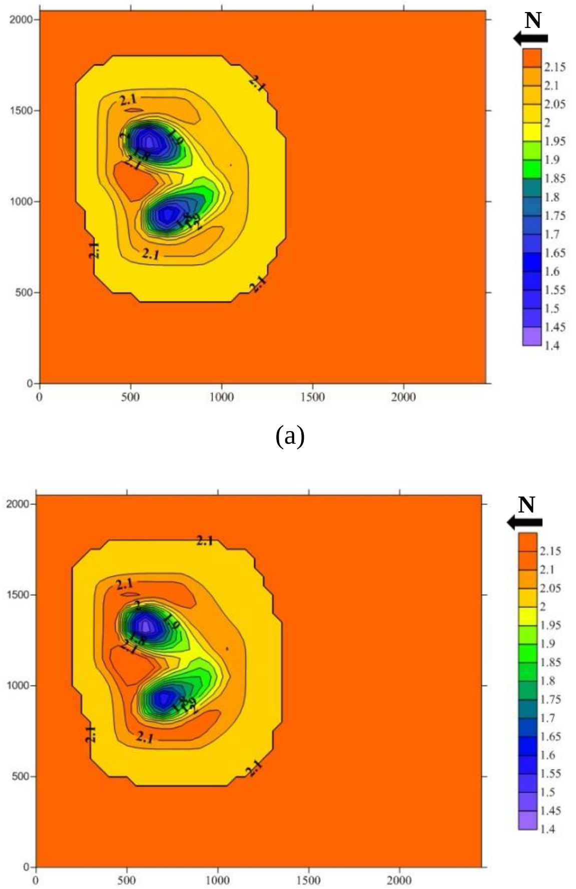
Parameter	Unit	Value
Number of Cells in x-direction	-	42
Number of Cells in y-direction	-	50
Number of Cells in z-direction	-	1
Horizontal Hydraulic Conductivity	m/d	15
Porosity	-	0.3
Longitudinal Dispersivity	m	20
Initial contaminant concentration	ppm	0
Diffusion Coefficient	-	0
Recharge	mm/day	0.5

are recorded. These two sets of concentrations are utilized to find the distribution of the singularity indices using the window based procedure. Figures 2-(a) and 2-(b) present the estimated singularity indices corresponding to 2000 and 3000 days after the release of contaminants, respectively.

3.2.2 Scenario 2

In this scenario, four actual sources of pollutants are present. In this case, the sources are relatively close to each other; therefore, substantial overlapping of pollutant plumes resulting from individual sources would happen.

In Fig. 1, numbers 1,2, 3, and 4, show the location of these sources. The flow and transport simulation models are utilized to simulate the transport of pollutant released from these four sources.



(a)

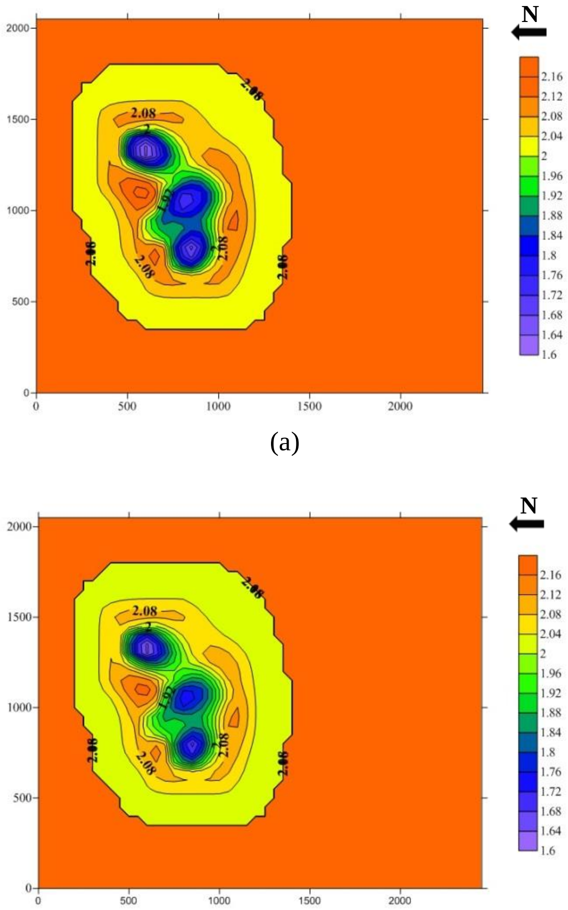
(b)

Fig. 2 The Singularity Index contours for scenario 1 after (a) 2000 days and (b) 3000 days of pollutant release activation.

The resulting simulated concentrations corresponding to 7300 and 8300 days after the activation of sources are recorded. These two sets of concentrations are utilized to find the distribution of the singularity indices using the window based procedure. Figures 3-(a) and 3-(b) present the estimated singularity indices corresponding to 7300 and 8300 days after the release of contaminants, respectively.

4. RESULTS AND DISCUSSION

The fractal singularity mapping method was used to delineate the contamination plume in two pollutant release scenarios. In the first scenario, two contaminant sources are active which are relatively far from each other. Therefore, the contamination plume is relatively simple, since there is very limited overlapping of the pollutant plumes. Figure 2-(a) and 2-(b) show the singularity index contours. Values more than 2, show the regions out of the plumes. The plume's inside regions are specified by values less than 2. Contour related to singularity index two is the representative of the plume boundaries. Since the sources are relatively far from each other in scenario 1, there are two distinct contamination plumes identified in each figures 2-(a) and 2-(b) related to each source.



(a)

(b)

Fig. 3 The Singularity Index contours for scenario 2 after (a) 7300 days and (b) 8300 days of pollutant release activation.

In scenario 2, four pollutant sources are active and since they are situated relatively close to each other, overlapping of the pollutant plumes released from individual sources is expected. Therefore, in scenario 2, the plume delineation is largely more complex than scenario 1. Figures 3-(a) and 3-(b) show the singularity index contours for 7300 and 8300 days after the start of contaminant release at sources. Similar to scenario 1, singularity indices more than two and less than two are associated with the areas outside and inside the pollutant plume, respectively. The plume boundaries are specified by singularity index two. As shown in Fig. 1, source 4 is relatively far from other three sources. Therefore, in Figs. 3-(a) and 3-(b), a separated contour related to singularity index 2 shows the contaminant plume release from this source. However, the other three sources are relatively close. As a result of overlapping, in Figs. 3-(a) and 3-(b), one contour related to singularity index 2 shows the contaminant plume boundary resulting from these three sources. In Figs 2 and 3, the singularity index contours depict approximate location of pollutant sources. Therefore the singularity indices using the window based procedure has the potential to be used for identifying the unknown location of contamination sources using available observed concentrations.

5. CONCLUSION

The fractal Singularity Index Mapping Technique gained substantial attention in many areas of science especially geology, however, the contamination plume delineation is a new application for this method. In this study, the window based singularity mapping technique is utilized in an illustrative contaminated site. The singularity indices is used to divide the study area into contaminated and clean characterization by assigning singularity indices smaller and larger than 2, respectively. Therefore, contours corresponding to singularity index two are used to delineate the contamination plume boundaries. The performance of the proposed methodology is evaluated for two scenarios with different degrees of contamination plume complexity. The contamination plume delineation becomes complex when the contamination sources are located relatively close to each other and overlapping of plumes resulting from individual sources is expected. The illustrative application of the proposed methodology demonstrates potential applicability of this methodology for fairly accurate delineation of contamination plumes for different contamination scenarios. These illustrative applications show that this methodology performs satisfactorily for both simple and complex groundwater contamination scenarios. The potential for utilizing fractal analysis of contaminant plumes for effective management of contaminated aquifers is demonstrated through this exploratory study.

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