Environmental Pollution 211 (2016) 98–110

Contents lists available at ScienceDirect

Environmental Pollution

journal homepage: www.elsevier.com/locate/envpol

A decision-making approach for delineating sites which are potentially contaminated by heavy metals via joint simulation[☆]

Wei-Chih Lin [a], Yu-Pin Lin [a,*], Yung-Chieh Wang [b]

[a] Department of Bioenvironmental Systems Engineering, National Taiwan University, Taipei 10617, Taiwan
[b] Department of Soil and Water Conservation, National Chun-Hisn University, Taiwan

A R T I C L E I N F O

Article history:
Received 12 September 2015
Received in revised form
16 December 2015
Accepted 16 December 2015
Available online xxx

Keywords:
Decision-making
Robustness
Contaminated sites
Conditional simulation
Uncertainty
Heavy metals
Soil
GIS

A B S T R A C T

This work develops a new approach for delineating sites that are contaminated by multiple soil heavy metals and applies it to a case study. First a number of contaminant sample data are transformed into multiple spatially un-correlated factors using Uniformly Weighted Exhaustive Diagonalization with Gauss iterations (U-WEDGE). Sequential Gaussian simulation (sGs) is then used to generate sets of realizations of each resultant factor. These are then transformed into sets of sGs contaminant distribution realizations, which are then used to analyze the local and spatial (global) uncertainties in the distribution and concentration of contaminants via joint simulation. Finally, Info-Gap Decision Theory (IGDT) is used to consider different monitoring and or remediation regimes based on the analysis of contaminant realization spatial uncertainty. In our case study each heavy metal contaminant was considered individually and together with all other heavy metals; as the number of heavy metals considered increased, higher critical proportion values of local probability were chosen to obtain a low global uncertainty (to provide high reliability). Info-Gap Decision Theory (IGDT) yielded the most appropriate critical proportion values which minimized information loss in terms of specific goals. When the false negative rate is set to zero, meaning that it is necessary to monitor all potentially polluted areas, the corresponding false positive rates are at least 63%, 65%, 66%, 68%, 70%, and 78% to yield robustness levels of 0.50, 0.60, 0.70, 0.80, 0.90, and 1.00 respectively. However, when the false negative rate tolerance threshold is raised to 50%, the false positive rate tolerance which yields robustness levels of 0.50, 0.60, 0.70, 0.80, 0.90 and 1.00 drop to 12%, 14%, 15%, 18%, 20%, and 39%. The case study demonstrates the effectiveness of the developed approach at making robust decisions concerning the delineation of sites contaminated by multiple heavy metals.

1. Introduction

While the adverse effects of soil heavy metal pollutants are well known, estimating their distribution accurately has proven to be a difficult task. Although heavy metals found in soil can arise naturally from parent materials, anthropogenic sources, such as those originating from industrial and or agricultural activities, are of greatest concern since they are complex and are primarily responsible for dangerous concentrations of soil metalloids (Lin et al., 2010; Escarré et al., 2011; Guillén et al., 2012; Mmolawa et al., 2011; Nanos and Martín, 2012; Petrotou et al., 2012; Lv et al., 2013; Massas et al., 2013; Martín et al., 2013; Werkenthin et al., 2014), particularly in urbanized and industrialized regions globally. Due to the complicated nature of soil heavy metal contaminants and the risks they pose to ecosystems, agricultural pursuits and or human health, robust decision-making procedures for the delineation of contaminated sites, or the execution of competent monitoring programs based on previously sampled data is a concern among bodies responsible for the monitoring and remediation of heavy metal pollutants all around the world. Accurately mapping heavy metal soil contaminants while considering the relative level of uncertainty intrinsic to different projections or areas is essential to assessing potential environmental pollution, designating future sampling sites and prioritizing remediation sites (Huo et al., 2012). Uncertainty arises from technical limitations of available sampling instruments, limitations of the analytical methods (Stewart and Purucker, 2011) and the natural

[☆] This paper has been recommended for acceptance by Klaus Kummerer.

* Corresponding author. Department of Bioenvironmental Systems Engineering, National Taiwan University, No. 1, Sec. 4, Roosevelt Road, Taipei 10617, Taiwan.
E-mail address: yplin@ntu.edu.tw (Y.-P. Lin).

http://dx.doi.org/10.1016/j.envpol.2015.12.030
0269-7491/

heterogeneity of parent materials (Lin et al., 2010). In addition, collected sample data may exhibit significant uncertainty owing to extremely complex spatial patterns or errors in measurement of pollution sources (Lin et al., 2011). Spatial uncertainty should therefore be considered while making robust decisions concerning the delineation of soil contamination. Robust decision analysis tools are widely considered necessary in the assessment of estimated uncertainty (Lin et al., 2010), and to manage environmental contamination (O'Malley and Vesselinov, 2014). A structured approach, such as Information-Gap Decision Theory (IGDT) can be used to make a robust decision which takes multiple sources of uncertainty into consideration, such as those associated with varying projection procedures. IGDT can reveal the uncertainty associated with different decisions, and can yield an acceptable outcome even when decisions are made under the worst-case scenario (Harp and Vesselinov, 2013; Korteling et al., 2013; Matrosov et al., 2013; O'Malley and Vesselinov, 2014).

Geostatistical methods are widely used to estimate or simulate the distributions of heavy metal soil contaminants and to estimate its spatial patterns; these include indicator kriging (Cressie, 1993; Goovaerts, 1997; Lin et al., 2011) and the kriging interpolation procedure to locate pollution and hotpots of heavy metals in soil (Goovaerts, 1997; Li and Feng, 2012; Li et al., 2013; Lin et al., 2014a, 2011). Recently, geostatistical conditional simulation methods, such as sequential Gaussian simulation (sGs) (Sánchez-Vila et al., 2004; Jagat et al., 2008) and Sequential Indicator Simulation (SIS) were used to simulate the spatial distribution of heavy metals in soil and to explore spatial uncertainty in their concentrations (Atkinson and Lloyd, 2009; Gómez-Hernández et al., 1999). However, in soil science, methods for simulating a single variable of interest may be unsuitable for generating spatial distributions due to their failure at reproducing correlations between variables (Rondon, 2012; Tajvidi et al., 2013). Moreover, as the number of variables increases, decorrelation methods are preferred owing to their better computational efficiency (Rondon, 2012). Accordingly, multivariate geostatistical methods, such as Sequential Gaussian Co-simulation (joint simulation) and Sequential Indicator Co-simulation, have been used to map multiple heavy metals in soils (Franco et al., 2006; Yao et al., 2013; Zhao et al., 2008). However, before performing such sequential co-simulation, it is necessary to fit variograms and cross-variograms with a linear model of coregionalisation in order to satisfy the positive definiteness condition for solving the kriging equation. Unfortunately, for a larger set of variables, it is difficult to fit the model in such a way.

Due to the difficulties involved in co-simulation, preliminary decorrelation methods such as principal component analysis (PCA), the method of minimum/maximum autocorrelation factors (MAF), and Uniformly Weighted Exhaustive Diagonalization with Gauss iterations (U-WEDGE) have been developed (Mueller and Ferreira, 2012; Lin et al., 2015). The Principle Component Analysis (PCA) method that incorporates geostatistical methods has been widely used to map multiple heavy metals in soil (Li and Feng, 2012; Lin, 2002; Nanos and Martín, 2012; Petrotou et al., 2012; Lv et al., 2013; Martín et al., 2013). In the PCA method, the original data are rotated to orthogonal factors using PCA, but these factors may remain correlated at distances greater than zero (Wackernagel, 2003). The method of MAF assumes that the semivariogram function of the attributes can be modeled by a two-structured linear model of coregionalisation, following the transformation of the original data into a space where they are uncorrelated (da Silva and Costa, 2014). Based on the above assumption, MAF transforms the original data into non-orthogonal factors with weak spatial correlation by diagonalizing a pair of symmetric coregionalisation matrices (Mueller and Ferreira, 2012; Lin et al., 2015). Sohrabian and Tercan (2014) also used Minimum Spatial Cross-correlated (MSC) factors in the simulation process of some attributes of an andesite quarry and compared the results to those of MAF simulations. They showed that MSC-simulations have some advantages over MAF-simulations. Tajvidi et al. (2013) integrated MAF and sGs conditional simulation to classify mineral resources and to assess uncertainty in grade–tonnage curves. Barnett et al. (2014) found that MAF and its related spatial decorrelation are unlikely to make variables independent of one another when complex multivariate data are considered. To efficiently perform spatial decorrelation in multivariate geostatistical simulations, Tichavsky and Yeredor (2009) presented a more general approach to Approximate Joint Diagonalization (AJD), called the U-WEDGE method. U-WEDGE makes no assumption regarding the semivariogram function structure of the attributes. The resultant realizations of multivariate attributes that are simulated via AJD are similar to those generated by a full co-simulation (Bandarian et al., 2010; Barnett et al., 2014; Lin et al., 2015).

Decision analysis is based on an axiomatic decision theory which utilizes findings from decision making studies (Parnell et al., 2013), i.e. Information-Gap Decision Theory (IGDT) and multi-criteria decision analysis (MCDA). Although realizations obtained by geostatistical simulations such as sGs and SIS can yield possible distributions of heavy metals in soils and can even quantify spatial uncertainty in their concentrations, the tools are unable to provide a structured means of assessing the uncertainty intrinsic to different remediation or pollution monitoring decisions. Fortunately, IGDT may provide just such a structured approach (Harp and Vesselinov, 2013; Korteling et al., 2013; Matrosov et al., 2013; O'Malley and Vesselinov, 2014). The Information-Gap decision theory is a decision analysis approach which provides a general framework for decision analyses that seeks to maximize the robustness of a decision given a minimum performance requirement under severe uncertainty. An Information-Gap Decision Analysis has the following three components (Harp and Vesselinov, 2013): (1) an appropriate system model, (2) an uncertainty model, which influences the decision making, and (3) decision performance goals. These components are used to derive immunity functions that characterize the robustness of a decision, given a minimum performance requirement. In the context of environmental management, this method maximizes the robustness of a decision against uncertainty given a minimum performance requirement. Korteling et al. (2013) quantified the uncertainty of the projected demand for water resources and used IGDT to quantify the robustness of each water resources management option. IGDT provided a comprehensive analysis of water resource systems, supporting the development of an adaptive management approach to meet future demands under severe uncertainty. In another example, IGDT was used to evaluate different water resource plans based on various reliable simulation models in the Thames basin, UK (Matrosov et al., 2013). Harp and Vesselinov (2013) used IGDT to characterize the uncertainty, due to the incompleteness of available information, intrinsic to different hydrogeological contaminant remediation decisions. O'Malley and Vesselinov (2014) compared two remedial scenarios with the same cost to demonstrate the applicability of IGDT to decision-making in the field of groundwater remediation; their results suggested that IGDT is a practical tool for decision makers, allowing them to take uncertainties and implementation costs into account while planning remediation efforts.

In this work, the concentrations of eight soil heavy metals found in Changhua county of Taiwan, including arsenic (As), cadmium (Cd), chromium (Cr), copper (Cu), mercury (Hg), nickel (Ni), lead (Pb), and zinc (Zn), were transformed into eight spatially uncorrelated factors, using the U-WEDGE method. Next, sGs was used to generate 1000 sets of realizations of each resultant factor, which