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Application of a combined sensitivity analysis approach on a pesticide environmental risk indicator

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ABSTRACT

Sensitivity analysis aims to characterize factors (i.e., model inputs) accounting for the amount of uncertainty in model output. Input factors are usually assumed to be independent, which may lead to incorrect conclusions. In this study, a combined sensitivity analysis approach, composed of the Sobol' and Importance Measurement (IM) methods, is applied on a pesticide environmental risk indicator (called PURE), where main, interaction, and correlation effects (i.e., the effects of factor correlations on sensitivity indices) are all addressed. PURE calculates pesticide risk scores for air, soil, groundwater, and surface water based on pesticide properties and surrounding environmental conditions. The Sobol' method calculates the first-order sensitivity index (S_i) and the total-effect sensitivity index (S_{Ti}) in noncorrelated-factor setting to address the main and interaction effects; while the IM method calculates S_i in both noncorrelated-factor and correlated-factor settings to show the correlation effects. In the tested case, the S_i estimations in noncorrelated-factor setting by the Sobol' and IM methods are very similar, which not only cross-validates the main effect estimations by the two different methods, but also provides the common ground for combining the two methods to address both interaction and correlation effects. In addition, the S_i estimations in correlated-factor setting are relatively different from the ones in noncorrelated-factor setting, which demonstrates that it is cautious to assume all factors are independent in sensitivity analysis. Take the soil risk evaluation as an example, the positive correlation between the chronic no-observed-effect concentration and acute 50%-lethal concentration to earthworms largely increases the S_i of the latter factor. The results of S_i estimations show that the risk scores for air, soil, groundwater, and surface water are most sensitive to the application rate of pesticide product, the application rate of pesticide active ingredient, the organic carbon sorption constant, and the monthly maximum daily water input, respectively. In summary, while this study enhances the understanding of PURE, it also provides an option for investigating both interaction and correlation effects, and hence promotes sensitivity analysis with factor-correlation structures in environmental modeling.

1. Introduction

Pesticide use, along with fertilizer, newly bred crop cultivars, and machinery, assures that agricultural production keeps pace with global population growth. However, many pesticides are toxic, persistent, and mobile. A large portion of the pesticides don't reach their targets but were transported or emitted to the environment, posing risks to ecosystems and human health (Bolognesi, 2003). Stakeholders seek available tools for assessing pesticide risk and choosing appropriate low risk pest management practices. Pesticide risk is determined by pesticide exposure to nontargeted organisms and the caused effects, but the risk value is difficult to measure. Therefore, an indicator approach, providing information on variables that are difficult to access (Bockstaller et al., 2008), is appropriate for pesticide risk assessment. In a broad sense, pesticide environmental risk indicators are also a group of environmental models. Numerous pesticide risk indicators have been developed around the world (Bockstaller et al., 2009), such as the Environmental Impact Quotient (EIQ) based on simple combinations of important variables (Kovach et al., 1992) and the Environmental Potential Risk Indicator for Pesticides (EPRIP) derived from simple simulation models for predicting pesticide concentrations (Trevisan et al., 2009). Whether employing complex (*e.g.*, Šimůnek et al., 2003) or simple simulation models in developing pesticide risk indicators depends on data availability and temporal–spatial scales of assessment. While various types of pesticide

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environmental risk indicators exist, only one of 20 reviewed indicators since year 2000 has been evaluated with sensitivity analysis. Nevertheless, sensitivity analysis is an essential step in environmental model development (Jakeman et al., 2006) and one of the important methods for analyzing uncertainty in the environmental modelling process (Refsgaard et al., 2007).

Sensitivity analysis serves to characterize factors (*i.e.*, model input variables) accounting for the amount of uncertainty in model output (Saltelli and Annoni, 2010), and the sensitivity analysis results are valuable to model diagnosis, interpretation, and parameterization, and prioritizing data collection (Berthiaume et al., 2010; Confalonieri et al., 2010; Nossent et al., 2011; Pannell, 1997). Sensitivity analysis methods can be classified into local and global sensitivity analyses based on the techniques for exploring the input factor space. Local sensitivity analysis exploits the factor space around a specific point to study the effect of small variations of factors on model output, and the result can be highly biased for nonlinear models (Yang, 2011). On the contrary, global sensitivity analysis exploits the entire factor space by simultaneously varying all factors (Jacques et al., 2006; Lilburne and Tarantola, 2009). Global sensitivity analysis techniques include (1) regression or correlation based techniques, such as standardized regression coefficients and Spearman rank correlation coefficients; (2) elementary effect methods, including Morris (Campolongo et al., 2007; Morris, 1991; Pujol, 2009), Latin Hypercube-OAT (van Griensven et al., 2006), and winding stairs (Jansen, 1999), etc.; (3) metamodeling (emulation-based), such as high dimensional model representation (HDMR) (Li et al., 2006, 2002; Rabitz et al., 1999) and Gaussian emulators (Oakley and O'Hagan, 2004); and (4) variance-based techniques, such as the Sobol' method (Saltelli, 2002; Sobol', 1993; Tarantola et al., 2006), Fourier amplitude sensitivity test (FAST) (Cukier et al., 1973, 1975; McRae et al., 1982; Saltelli et al., 1999), and the importance measurement (IM) method (McKay, 1995). Variance-based sensitivity analysis techniques are popular in environmental modeling (*e.g.*, Nossent et al., 2011; Yang, 2011). In spite of the high computational expenses, variance-based techniques are model independent, provide easy-interpretable sensitivity indices, can capture interaction effects among factors, and can handle qualitative and quantitative factors. Saltelli and Annoni (2010) suggested using the Sobol' method when input factors are noncorrelated. Nevertheless, pesticide environmental fate models, which are usually computational expensive, tended to employ one-at-a-time sensitivity analysis methods (*e.g.*, Dubus et al., 2003; Ma et al., 2004).

Both interaction and correlation among input factors can affect sensitivity analysis results. Interaction is a property of the model while correlation is a property of input factors (Saltelli and Tarantola, 2002). Interaction, or nonlinear effect, means that a factor would act nonlinearly on the model output when its interacted factors are at different values. In a case when factors are correlated, fixing a factor would restrict the distributions of its correlated factors, and hence the effect of the studied factor would be carried over, which is referred to as the correlation effect hereafter. While interaction effects are usually studied, correlation effects are often ignored due to expensive computation cost (*e.g.*, Nossent et al., 2011; Vezzaro and Mikkelsen, 2012). Nevertheless, correlation commonly exists in real cases and may considerably impact sensitivity analysis results (Saltelli and Tarantola, 2002). Specifically in pesticide risk assessment, ignoring the existence of correlation between input factors may have a significant effect on the results of exposure assessments. Yet, to the authors' knowledge, none of the sensitivity analysis studies on pesticide risk assessment or fate modelling have taken factor correlations into account, except the regression-based sensitivity analysis study on three pesticide leaching models (Soutter and Musy, 1999). A few methods were developed for sensitivity analysis on correlated factors, such as the IM method mentioned above (McKay, 1995), which was employed by Saltelli and Tarantola (2002) and recommended by Saltelli and Annoni (2010). In addition, sensitivity analysis with correlated input factors may also be analyzed by emulation-based methods, such as the local polynomial technique (Da Veiga et al., 2009), the State Dependent Parameter (SDP) method (Ratto et al., 2007), and the Bayesian approach (Oakley and O'Hagan, 2004); nevertheless, they are more difficult to implement.

This study aims to enhance the understanding of the PURE (Pesticide Use Risk Evaluation) indicator (Zhan and Zhang, 2012) and to draw more attention to correlated factors in sensitivity analysis of environmental models by applying a combined variance-based sensitivity analysis approach. PURE is able to evaluate site-specific risk to air, soil, groundwater, and surface water from agricultural pesticide use. It employs the risk ratio approach (*i.e.*, the ratio of the predicted environmental concentration to the toxicity) under worst case scenarios, which is also applied by the European Union System for the Evaluation of Substances (EUSES) suited for initial and refined risk assessments on industrial chemicals and pesticides (Vermeire et al., 2005). PURE considers the short- and long-term exposure levels, rather than the environmental fate at equilibrium status that for example is evaluated by the Equilibrium Concentration (EQC) model (Mackay et al., 1996a, b, c).

The combined sensitivity analysis approach is composed of two parts. The first part uses the Sobol' method (Saltelli, 2002; Sobol', 1993) to estimate the first-order sensitivity index or main effect (S_i) and the total sensitivity index or total effect (S_{Ti}) in noncorrelated-factor setting. The second part uses the IM method (McKay, 1995) to estimate S_i in both noncorrelated-factor and correlated-factor settings. The specific objectives of this study are (1) to identify sensitive factors in PURE, with associated interaction or correlation effects; (2) to compare S_i estimations and convergence between the Sobol' and the IM methods in noncorrelated-factor setting; and (3) to investigate the applicability of the combined approach to evaluating interaction and the correlation effects. The results and conclusions of this study are anticipated to improve the confidence in the PURE risk scores and to promote sensitivity analysis with correlated input factors in environmental modeling.

2. Materials and methods

2.1. Model description

The PURE indicator (Zhan and Zhang, 2012) is composed of four submodels, including air, soil, groundwater, and surface water, with outputs of risk scores R_A, R_S, R_G, and R_W, respectively. A stepwise procedure is employed for each submodel except for the air (Fig. A.1). First, R_A is based on the multiplication of the pesticide application rate (*RATE*), the emission potential (*EP*) that is a pesticide product property for estimating potential volatile organic compound (VOC) emissions by the California Department of Pesticide Regulation (CEPA, 2007), and the application method adjustment factor (*AMAF*). Second, R_S is the maximum of the short-term and long-term risk scores for soil, which are derived from the ratios of the predicted short-term (PEC_{SS}) and long-term (PEC_{SL}) pesticide concentrations in topsoil to the acute and chronic pesticide toxicities to earthworms, respectively. PEC_{SS} is contributed by the amount of the pesticide reaching ground right after the pesticide application, while PEC_{SL} is the average concentration in topsoil considering the decay of PEC_{SS} during 21 days (the typical period for measuring the chronic toxicity) after the application. Third, R_G is based on the ratio of the predicted pesticide concentration leaching to groundwater (PEC_G) to the acceptable daily intake (*ADI*). PEC_G is calculated by using an adapted version of the attenuation factor