Science of the Total Environment 651 (2019) 561–569

Contents lists available at ScienceDirect

Science of the Total Environment

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

A deeper look at plant uptake of environmental contaminants using intelligent approaches

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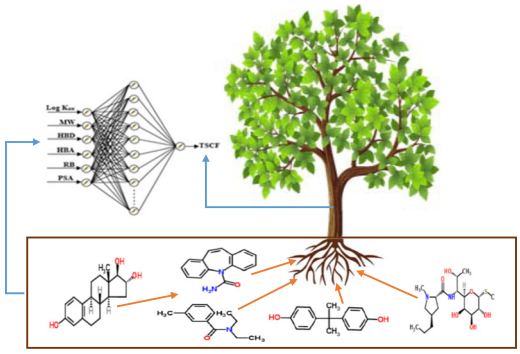
HIGHLIGHTS

- Uptake and translocation of emerging and fugitive contaminants
- Application of artificial neural network to predict uptake and translocation
- Fuzzy logic was used to examine the interaction between chemical properties.
- New physicochemical cutoffs for uptake and translocation of contaminants

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 28 May 2018
Received in revised form 29 August 2018
Accepted 4 September 2018
Available online 05 September 2018

Editor: Jay Gan

Keywords:
Emerging contaminants
Physiochemical properties
Plant uptake
Neural network
Fuzzy logic

ABSTRACT

Uptake of contaminants from the groundwater is one pathway of interest, and efforts have been made to relate root exposure to transloation throughout the plant, termed the transpiration stream concentration factor (TSCF). This work utilized machine learning techniques and statistcal analysis to improve the understanding of plant uptake and translocation of emerging contaminants. Neural network (NN) was used to develop a reliable model for predicting TSCF using physicochemical properties of compounds. Fuzzy logic was as a technique to examine the simultaneous impact of properties on TSCF, and interactions between compound properties. The significant and effective compound properties were determined using stepwise and forward regression as two widely used statiscal techniques. Clustering was used for detecting the hidden structures in the plant uptake data set. The NN predicted the TSCF with improved accuracy compared to mechanistic models. We also delivered new insight to compound properteis and their importance in transmembrane migration. The sensitivity analysis indicated that log K_{ow}, molecular weight, hydrogen bond donor, and rotatable bonds are the most important properties. The results of fuzzy logic demonstrated that the relationship between molecular weight and log K_{ow} with TSCF are both bell-shape and sigmoidal. The employed clustering algorithms all discovered two major distinct clusters in the data set.

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1. Introduction

While many contaminant-containing waters undergo advanced treatment to destroy recalcitrant organic pollutants, many other municipal wastewaters, fugitive contaminant plumes and agricultural run-off

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https://doi.org/10.1016/j.scitotenv.2018.09.048
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Nomenclature

TSCF	transpiration stream concentration factor
log K_{ow}	octanol/water partition coefficient
NN	neural network
MW	molecular weight
HBD	hydrogen bond donor
HBA	hydrogen bond acceptor
RB	rotatable bonds
PSA	polar surface area
R	correlation coefficient
MSE	mean squared error
PCA	principal component analysis

contain considerable synthetic organic molecules (Hayashi et al., 2010; Hong et al., 2001; Tanoue et al., 2012). Crop irrigation with reclaimed wastewater and application of agricultural chemicals have in part ameliorated water shortage problems and also enhanced agricultural productivity (Paraíba et al., 2010). With the irrigation of reclaimed wastewater and application of agricultural chemicals the exposure of plants to these compounds has increased by design (Aitchison et al., 2000; Dettenmaier and Doucette, 2007; Yoon et al., 2002).

The chemical contaminants in the soil have the potential of being transported to foliage through plant transpiration (Ciucani et al., 2002; Doucette et al., 2005a; Doucette et al., 2005b; Hsu et al., 1990; Orchard et al., 2000). Thus, quantification and prediction of transmembrane migration and transport from soil to foliage has direct linkage to potential human health impacts. (Russell and Shorrocks, 1959) introduced transpiration stream concentration factor (TSCF) to show the possibility of transporting a given chemical to foliage. TSCF is the ratio of a chemical concentration in the xylem sap to the concentration of that chemical in the solution passively transferred to leaves (Crowdy and Jones, 1956; Davis et al., 1998; Geissbühler et al., 1963; Su and Liang, 2011).

The high cost of experimental studies and inconsistent data collection have resulted in generating few number of experimental TSCF values for a limited number of chemicals and plant species (Fantke et al., 2016). The variability of the reported TSCF values for a given chemical and plant species is large due to the lack of consistent testing guidelines and difficulty in measuring metabolism and volatilization losses during the experiments (Edwards et al., 1982; Garvin et al., 2015; Yifru and Nzengung, 2006). The estimation of TSCF values for new contaminants not only helps to have predictive tools on efficiency of a specific molecule to be translocated by plants but also helps researchers focus efforts on contaminants with likely translocation capacity. Since 1974 several studies have been conducted to introduce a relationship between the physical properties of organic chemicals and their translocation in plants (Briggs et al., 1982; Briggs et al., 1987; Dettenmaier et al., 2008; Shone et al., 1974). These studies introduced single-parameter relationships relating the TSCF to octanol/water partition coefficient (log K_{ow}) which is as a term to describe hydrophobicity.

Due to the lacking precision of single-parameter relationships and the limitation of these relationships for applying to a wide variety of contaminants and plants species (Pussemier, 1991), more complicated prediction models for plant uptake and translocation have been proposed. The single-parameter relationships were outperformed with the advent of recent models correlating multiple compound properties to TSCF (Limmer and Burken, 2014; Miller et al., 2016). More complex approaches are compartmental models (Collins and Finnegan, 2010; Manzoni et al., 2011; Undeman et al., 2009), which consider more chemical and environmental properties, and also incorporate the complexity of uptake and translocation processes into their mechanistic relationships. These modeling approaches still have limited accuracy in many cases in spite of improving our understanding of plant uptake and translocation of contaminants. However, in the majority of these modeling efforts, the models are calibrated or verified with specific plant species and chemicals tested in the laboratory portion. Plant selection and experimental design can certainly impact findings and modeling efforts. Plant species variability and physiological differences certainly play a role, but are more consistent than the vast disparity in chemical properties of organic molecules that persist in the environment. Species variability has not been adequately addressed in developing the current data pools, and further research in this area is recommended with the increased understanding of chemical properties impacting uptake. The current field of contaminant uptake has developed a large data pool (Felizeter et al., 2014; Limmer and Burken, 2014; Miller et al., 2016) that can be used to investigate the comprehensive data sets for uptake of a wide array of compounds, by a range of plants, and in multiple laboratory arrangements, thereby limiting impacts of any one arrangement or data set. The assessment of these large data agglomerations can be challenging given the complexity of the data, and thus needing advanced data assessment methods and tools.

Simulation has been a useful approach to deal with various problems in different fields of science and engineering (Sofizadeh et al., 2016; Trapp et al., 1994). In this work, a neural network (NN) predicts the plant uptake and translocation of environmental contaminants. The NN uses physicochemical properties of compounds to assess past data collections and predict TSCF. The physicochemical properties of compounds are analyzed using statistical analysis to determine the importance of each property to the TSCF values. Fuzzy logic was used to examine the interactions between important physicochemical properties as predictors of experimentally-determined TSCF values. Furthermore, clustering techniques were utilized to determine any distinct groups and hidden data structures in the comprehensive data set.

2. Material and methods

2.1. Plant uptake data set

There are considerable number of published studies, which have investigated the uptake of various compounds (Crowdy and Pramer, 1955; Farlane et al., 1990; Kim et al., 2004; Qiu et al., 2016a; Qiu et al., 2016b; San Miguel et al., 2013; Sheets, 1961; Thompson et al., 1999). In order to build the NN model, a comprehensive selection of TSCF data was compiled from published literature (Supporting information). The selected TSCF data set to build general model includes 300 measurements of 155 compounds measured using 34 plant genera under various experimental approaches from 41 studies. The measurements for TSCF were not included when there was no evidence of reaching the steady state, measurements included metabolites, there was metabolism of the parent compound in planta, or the TSCF calculation was not reliable. Moreover, we did not include the measurements when depletion of the dosing solution was higher than 50%, roots were damaged prior to dosing, or other modes of exposure such as particle deposition were included in the measurements (Limmer and Burken, 2014). To build a general model that is not plant specific, the compound properties including log K_{ow}, molecular weight (MW), hydrogen bond donor (HBD), hydrogen bond acceptor (HBA), rotatable bonds (RB) and polar surface area (PSA), were obtained from chemical structure databases such as US EPA Chemistry Dashboard, and ChemSpider. For the properties like log K_{ow} that both predicted and experimental values are available, by considering the range of variation for the properties, the experimental values were considered in the analysis. Table 1 shows the compound properties used as input parameters in this study for the neural network modeling and other analyses.

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