Etrace Express: software for risk analysis of trace elements in inorganic fertilizers post application

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Abstract
Trace Elements are generally present in inorganic fertilizers as by-products or contaminants. There are however some trace elements that are plant nutrients and are intentionally included in fertilizer formulations. It is acknowledged that exposure to high levels of trace elements (nutrient or not) could pose a health risk to humans. This risk may be estimated by evaluation models. Thus, this work presents a tool, the software Etrace Express, for easy calculation of Risk Based Concentrations of trace elements in inorganic fertilizers post application, which suggest safe limits for agricultural use. The main purpose of this version was to calculate values of trace element concentrations in inorganic fertilizers that may, flexibly, be used by regulators aiming to protect the human health. Etrace Express was based on a model developed for a document prepared by The Fertilizer Institute (TFI, United States) for the US scenario of fertilizer use, entitled "Health Risk Evaluation of Selected Metals in Inorganic Fertilizers Post Application". RBCs calculated by Etrace Express for the US scenario matched those values presented in TFI's document. We thus used Etrace Express to obtain RBCs for the Brazilian scenario. The advantage of using such software is the easiness of customizing parameters for specific scenarios very rapidly.

Key Words
Heavy metals, soil contamination, food safety, Delphi platform.

Introduction

An estimate of risk-based concentrations (RBCs) of trace elements (TE) provided by an industry-commissioned study (TFI 2000) has shown that TE levels in commercial inorganic fertilizers are safe for consumers of farm products in the United States. A RBC is the amount of a TE in a fertilizer that is considered safe or protective of health. RBC calculation involves several parameters for many trace elements. To simplify RBCs calculation we produced the software Etrace Express. The software uses the same methodology proposed to develop the risk based concentration in the TFI study. The methodology is a back-calculation of health risks and is standard for a screening level risk evaluation. The software helped us to assess health risks of TEs in the current scenario of fertilizers use in Brazil (Guilherme and Marchi 2007). Parameters such as application rates, soil accumulation factors, body weight, ingestion rates (crops), and plant uptake factors were adopted from the scientific literature. Data on inorganic fertilizers were taken from industry as well as literature studies. Other parameters, considered non-specific for the Brazilian population, were derived from the USEPA, according to TFI. The results obtained indicate that trace elements do not cause harm to human health when considering post application of inorganic fertilizers in Brazil (based on information for phosphate as well as Zn-carrying fertilizers). This study also suggests that the limits currently established by the Brazilian legislation are safe in terms of health risk assessment. Etrace Express is the second generation among the versions of a package that is still being developed. Delphi 2007 platform was used for programming. The aim of this work was to present the software Etrace Express, a tool for RBCs calculation of trace elements in inorganic fertilizers that can be used as an initial guidance for regulators seeking the protection of human health in the current scenario of fertilizers use in Brazil.

Methods

Risk based concentrations (RBCs) for Brazilian fertilizers
Unit RBCs (normalized RBCs representing 1 percent fraction of nutrient content) were calculated by Etrace Express software to represent Brazilian fertilizers. RBCs were calculated according to the equation 1 (Shown in the last page).

Screening health evaluation
The lowest RBC for TE were compared to the maximum concentration of metals of potential concern

(MOPCs; e.g. As, Cd, Hg, and Zn). This comparison provided the most health protective estimate of health risk. If the concentration of the MOPC in the fertilizer is below the RBC, there is no health risk. If the concentration of the MOPC in the fertilizer is above the RBC, further evaluation is warranted.

Results

Etrace express

Data input are presented in two tabs. In the "Configuration" tab, the user may define parameters about fertilizers and main scenarios. The "Input" tab allows definition of parameters such as those related to exposition pathways. After data were provided for these two tabs, RBC calculations are presented in the "Results" tab. Etrace Express calculated RBCs for the data provided in the TFI report (TFI 2000), presenting identical results to those of the original document. For the Brazilian scenario, the software calculated RBCs (Tables 1 and 2) according to data presented in Guilherme and Marchi (2007).

Equation 1.

$$RBC = \frac{\text{TR or THI}}{SACF * \{AR * 1/FON * [(\frac{ED * EF * IRs * RAFs * CF}{BW * AT} * TOX) + (\frac{ED * EF * SA * AF * ABS}{BW * AT} * TOX) + (\frac{ED * EF * IRc * RAFc}{AT} * PUF * TOX)]\}}$$

Where:

RBC = Risk Based Concentration (mg MOPC/kg product);
TR/THI = Acceptable Target Risk or Hazard Index (Unitless);
AR = Application Rate (g/m^2-year);
FON = Fraction of Nutrient (unitless);
SACF = Soil Accumulation Factor (m^2-year/g);
ED = Exposure Duration (years);
EF = Exposure Frequency (days/year);
BW = Body Weight (kg);
AT = Averaging Time (days);
CF = Conversion Factor (1X 10^{-6} kg/mg);
IRs = Ingestion Rate Soil (mg/day);
SA = Surface Area (cm^2/event-day);
AF = Adherence Factor (mg/cm^2);
IRc = Ingestion Rate Crops (kg/day);
RAF = Relative Absorption Factor (RAF) (unitless);
ABS = Dermal Absorption Factor (unitless);
PUF = Plant Uptake Factor (unitless); and
TOX = Toxicity Values (mg/kg-day or mg/kg-day $^{-1}$).

Table 1. Unitary RBCs for phosphate fertilizer (mg trace elements/kg product for each 1% of P2O5 in the fertilizer product).

Scenario	As Adult	Cd Child	Cr Child	Co Child	Cu Child	Pb Child	Hg Child	Mo Child	Ni Child	Se Child	V Child	Zn Child
Brazil	2.9	5.8	81470	6389	165	85	0.6	216	435	582	10064	388
TFI	4.5	23	34000	3100	280	73	0.9	42	350	120	2200	1200

Table 2. Unitary RBCs for Zn containing micronutrient fertilizers (mg trace elements/kg product for each 1% of Zn in the fertilizers product).

Scenario	As Adult	Cd Child	Cr Child	Co Child	Cu Child	Pb Child	Hg Child	Mo Child	Ni Child	Se Child	V Child	Zn Child
Brazil	128	351	3195903	277481	6531	3818	31	8575	19556	23919	483249	14418
TFI	38	210	220000	23000	1800	500	6.5	300	2600	800	17000	8600

Conclusion

The software Etrace Express calculated risk based concentrations using data from the TFI report and from Guilherme and Marchi (2007). RBC results calculated by the software matched those of both works. This means that the software is reliable, and may be used in order to simplify RBC calculations.

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