

Etrace Express: software for risk analysis of trace elements in inorganic fertilizers – User's manual and reference guide



Etrace Express

© 2010. All rights reserved.

*Brazilian Agricultural Research Corporation
Embrapa Cerrados
Ministry of Agriculture, Livestock and Food Supply*

Documentos 300

Etrace Express: software for risk analysis of trace elements in inorganic fertilizers – user’s manual and reference guide

*Giuliano Marchi
Luiz Roberto Guimarães Guilherme
Alexandre Beserra da Silva
Veridiana Cardozo Gonçalves
Paulo Jorge de Pinho
Maria Aparecida Pereira Pierangeli
Ozanival Dario Dantas*

Embrapa Cerrados
Planaltina, DF
2010

Copies of this publication can be obtained from:

Embrapa Cerrados

BR 020, Km 18, Rod. Brasília/Fortaleza

P. O. Box 08223

CEP 73310-970 Planaltina, DF

Phone: (61) 3388-9898

Fax: (61) 3388-9879

<http://www.cpac.embrapa.br>

sac@cpac.embrapa.br

Embrapa Cerrados Publication Committee

President: *Fernando Antônio Macena da Silva*

Executive Secretary: *Marina de Fátima Vilela*

Secretary: *Maria Edilva Nogueira*

Editorial supervision: *Jussara Flores de Oliveira Arbués*

Revision assistant: *Eder de Souza Martins*

Bibliographical norms: *Paloma Guimarães Correa de Oliveira*

Electronic editing: *Wellington Cavalcanti*

Cover: *Wellington Cavalcanti*

Cover photos: *Embrapa Cerrados Archives*

Printing and finishing: *Divino Batista de Sousa*

Alexandre Moreira Veloso

1st edition

1st printing (2010): 100 copies

Online edition (2010)

All rights reserved

Non-authorized complete or partial reproduction of this publication is a violation of copyrights (Law no. 9610).

Library of Congress Cataloging-in-Publication Data

Embrapa Cerrados

E85 Etrace Express: software for risk analysis of trace elements in inorganic fertilizers – user’s manual and reference guide / Giuliano Marchi... [et al]. – Planaltina, DF : Embrapa Cerrados, 2010.

29 p.— (Documentos / Embrapa Cerrados, ISSN 1517-5111, ISSN online 2176-5081 ; 300).

1. Soil - contamination. 2. Heavy metals. 3. Agriculture. I. Marchi, Giuliano. II. Series.

631.4 - CDD 21

© Embrapa 2010

Authors

Giuliano Marchi

Research and Development at Embrapa Cerrados,
D.Sc. Soils and Plant Nutrition
giuliano.marchi@cpac.embrapa.br

Luiz Roberto Guimarães Guilherme

Associate Professor at Soil Science Department
(DCS) from Federal University of Lavras (Ufla),
Ph.D. Soil Chemistry and Environmental
Toxicology
Campus da UFLA, Caixa Postal 3037,
37200-000, Lavras, MG
guilherm@dcs.ufla.br

Alexandre Beserra da Silva

CNPq Scholar at Embrapa Cerrados,
União Pioneira de Integração Social – Upis
ale.beserra@gmail.com

Veridiana Cardozo Gonçalves

D.Sc. Soils and Plant Nutrition
Fapemig Scholar at DCS/Ufla
vericg79@yahoo.com.br

Paulo Jorge de Pinho

D.Sc. Soils and Plant Nutrition
Fapemig Scholar at DCS/UFLA
pinhopj@yahoo.com.br

Maria Aparecida Pereira Pierangeli

D.Sc. Soils and Plant Nutrition.
Associate Professor at Universidade do Estado
de Mato Grosso (Unemat)
BR 174, KM 209, Pontes e Lacerda-MT
mappierangeli@gmail.com

Ozanival Dario Dantas

M.Sc. Electric Engineering and Computer Science,
Database Specialist
Analyst at Embrapa Cerrados
dario@cpac.embrapa.br

Presentation

Trace elements are present in soils, sediments, and aquatic systems normally in low concentrations. Some fertilizer products used to add nutrients to the soil or balance soil pH represent a source of trace elements, and may, in the long term, increase trace element concentrations in the environment. Even if the levels of these elements in soils do not reach alarming values, they may remain in bioavailable forms for many years. Thus, food produced in fields with high levels of trace elements may contain cadmium, chromium, zinc, among others, a way up the recommended for human intake. Toxicological effects from the intake of food containing trace elements are known. Consequently, to avoid contamination of food producing soils by adding successive doses of fertilizer products with high levels of trace elements, it is necessary to follow strict norms ruling acceptable limits of contaminant levels in fertilizers.

Guilherme and Marchi (2007) methodology to develop risk based concentrations was used in this document and rely on a back-calculation of health risks that is standard for a screening level risk evaluation. The purpose of a back-calculation of health risks is to estimate a concentration of trace elements in a fertilizer, in which its health risks are acceptable. The software Etrace Express, developed by Embrapa Cerrados and Federal University of Lavras staff calculates risk-

based concentrations for twelve trace elements in phosphate and zinc micronutrients fertilizer products post application in several exposition scenarios. The quick calculation and easy customization makes this tool of great utility to be used by regulators aiming to protect the human health.

José Robson Bezerra Sereno
Director General Embrapa Cerrados

Summary

Introduction.....	9
Health Risk Evaluation	10
Data input	13
Risk Based Concentration (RBC) Equation (TFI, 2000)	22
Etrace Express	23
References	27
Resumo	28
Abstract.....	29

Etrace Express: software for risk analysis of trace elements in inorganic fertilizers – user’s manual and reference guide¹

*Giuliano Marchi; Luiz Roberto Guimarães
Guilherme; Alexandre Beserra da Silva; Veridiana
Cardozo Gonçalves; Paulo Jorge de Pinho; Maria
Aparecida Pereira Pierangeli; Ozanival Dario
Dantas*

Introduction

Trace elements (TEs) are present in inorganic fertilizer products as contaminants. However, some trace elements (e.g., Zn, Cu, Fe, and Mn) are plant nutrients and are included intentionally in the fertilizer formulation. Exposition to high levels of trace elements (nutrients or not) may pose a risk to human health. This risk can be estimated by assessment models. The present work presents the software Etrace Express, which is a tool that may be used to calculate Risk Based Concentrations (RBCs) of trace elements in fertilizer products.

The software was prepared using the same model presented in the document *Health Risk Evaluation of Selected Metals in Inorganic Fertilizers Post Application*, prepared by *The Fertilizer Institute* (TFI) for the North American scenario.

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 main purpose of this program is to suggest safe concentrations of trace elements in inorganic fertilizer products that may, flexibly, be used by regulators.

¹ Projects results: 578674/2008-4 and 578647/2008-7, CNPq.

Validation of Etrace Express was performed comparing its results with the original data published by TFI (2000). Etrace Express calculated RBCs with data compiled by Guilherme and Marchi (2007). Results of this work showed that trace elements present in inorganic fertilizer products do not pose a health risk in the current Brazilian scenario. The present manual brings information about use, and organized data, aiming to facilitate user operation. Data from a new compilation (updated in 2010), regarding Plant Uptake Factors (PUF), and soil-water partition coefficients (Kd), is also included in this manual. The present manual do not intend to bring detailed information about fundamentals or meaning of variables of risk analysis. Thus, the user may look for another source of information ((GUILHERME; MARCHI, 2007; TFI, 2000) about risk analysis to understand each variable.

Health Risk Evaluation

The present human health risk assessment focused on the latter part of the life cycle, i.e., post application (Figure 1). Therefore, this work comprises the human exposition to fertilized soil (skin absorption, and unintentional ingestion), and ingestion of food produced in fertilized soils. In the other hand, it does not comprise human exposition by fertilizer handling (ingestion, skin absorption and inhalation; Figure 2). The scope of the risk evaluation is focused in fertilizer products, TEs, and an exposure scenario of highest concern (Figure 3). The resident farmer is the population with the highest exposure potential (more exposition pathways: non intentional ingestion, dermal contact with contaminated soil, and ingestion of food produced with use of fertilizers), rather than the public consumer (only ingestion of food produced with use of fertilizers).

The lowest RBC for TEs provides the most health protective estimate of health risk, and may be compared to the concentration of TEs in fertilizer products. If the concentration of the TE in a fertilizer is below the RBC, there is no health risk. If the concentration of TE in the fertilizer is above the RBC, further evaluation is warranted (TFI, 2000).

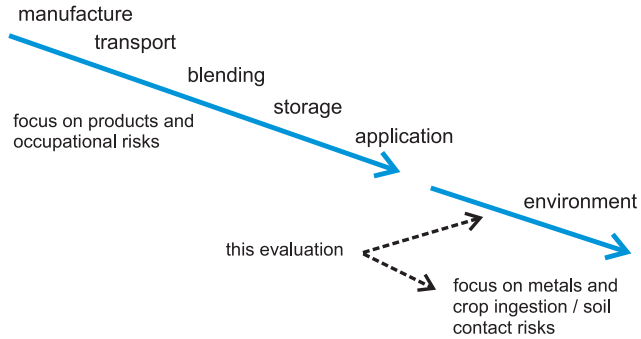


Figure 1. Risk evaluation for the life cycle of inorganic fertilizers. Source: TFI (2000).

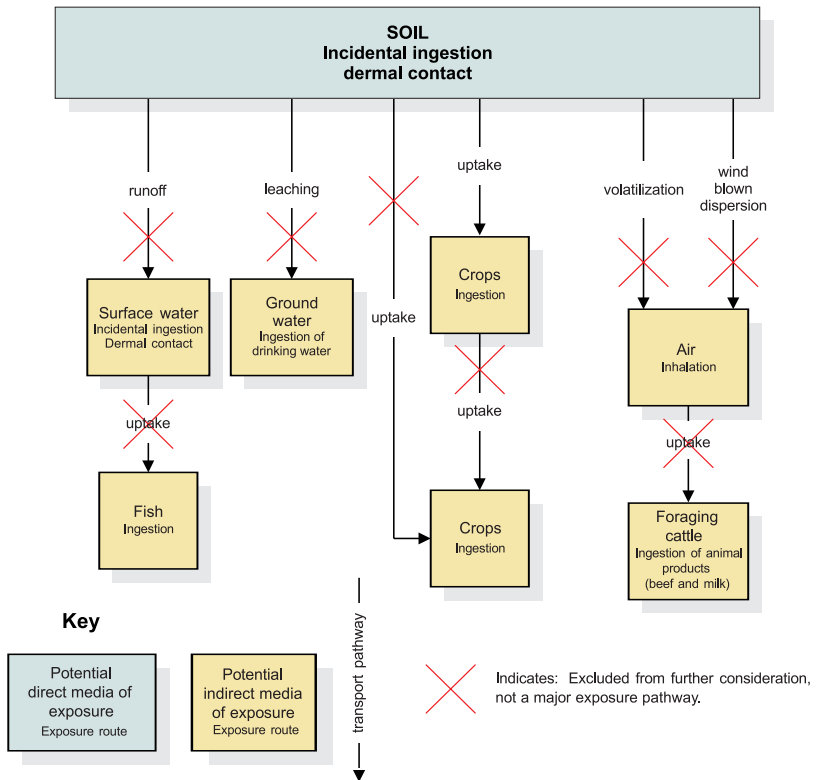


Figure 2. Potential exposure pathways of trace elements in inorganic fertilizer post application includes: transport pathways, media of potential concern, and associated exposure routes (TFI, 2000).

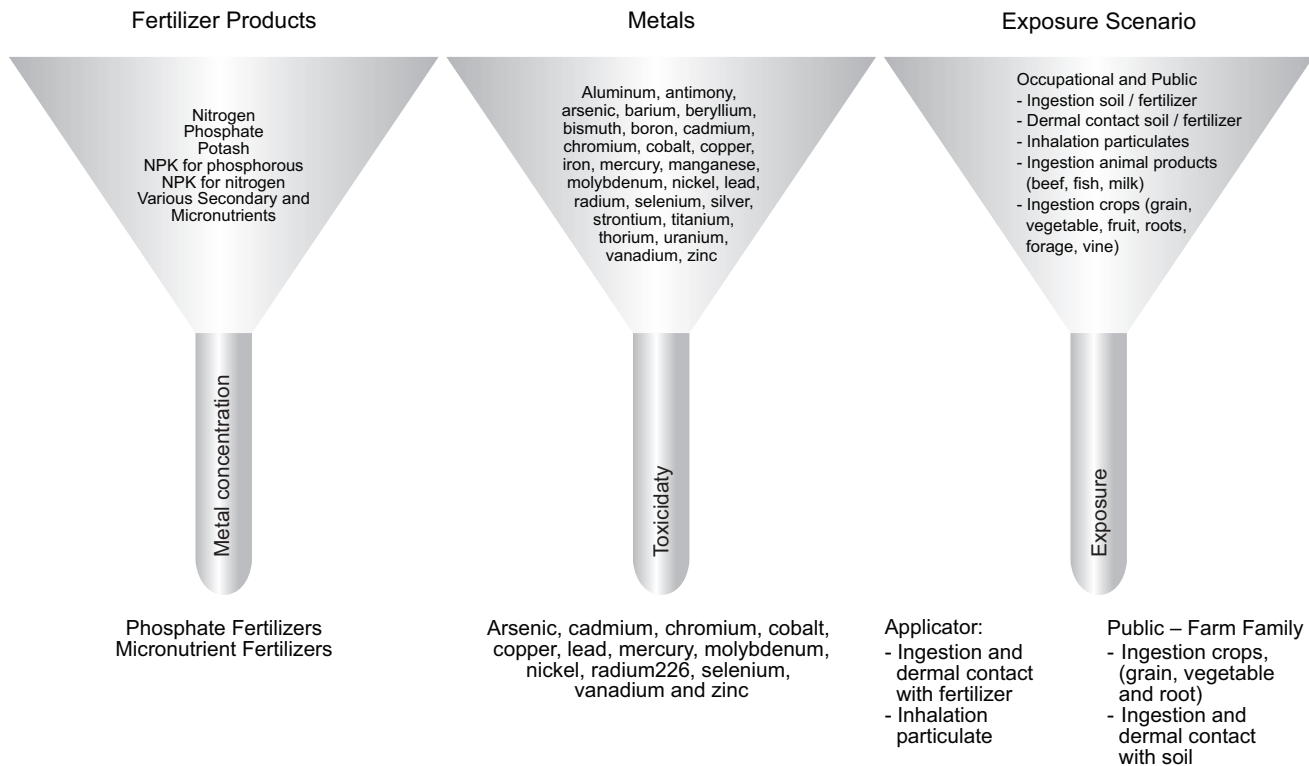


Figure 3. Narrowing the scope of this screening level evaluation – focusing on the fertilizer products, trace elements, and exposure scenario of highest concern (TFI, 2000).

Data input

To enter data correctly in the software, the user needs to understand the meaning of all parameters and its acronyms that appear in the software tabs, including its units, and how to add scattered data (Table 1). Scattered data denotes the data of body weight, soil ingestion rate, plant uptake factor, and soil-water partition coefficient, which has its data inputs as means, medians, or 95% upper confidence limits.

Table 1. Parameters, acronyms, units, and input of scattered data.

Parameter	Acron.	Unit	Entry
Application Rate - Crops	AR	$\text{g m}^2 \text{ year}^{-1}$	UCL 95%*
Fraction of Nutrient	FON	unitless	-
Exposure Duration	ED	year	-
Exposure Frequency	EF	days year^{-1}	-
Body Weight	BW	kg	Mean
Ingestion Rate Soil	IRs	mg day^{-1}	Mean
Relative Absorption Factor - Soil	RAFs	unitless	-
Surface Area	AS	$\text{cm}^2 \text{ event}^{-1} \text{ day}^{-1}$	-
Adherence Factor	AF	$\text{mg cm}^{-2} \text{ event}^{-1}$	-
Ingestion Rate Crops	IR	kg day^{-1}	-
Relative Absorption Factor	RAF	unitless	-
Dermal Absorption Factor	ABS	unitless	-
Plant Uptake Factor	PUF	unitless	UCL 95%*
Toxicity Value Oral	TOXo	$\text{mg kg}^{-1} \text{ day}^{-1}$ or mg day kg^{-1}	-
Toxicity Value dermal	TOXd	$\text{mg kg}^{-1} \text{ day}^{-1}$ or mg day kg^{-1}	-
Fraction of Land	FOL	unitless	-
Time period of Application	T	years	-
Soil Mixing Depth	Z	cm	-
Soil Bulk Density	BD	g cm^{-3}	-
Average Annual Precipitation	P	cm year^{-1}	-
Average Annual Irrigation	I	cm year^{-1}	-
Average Annual Evapotranspiration	EV	cm year^{-1}	-
Soil-water Partitioning Coefficient	Kd	mL g^{-1}	Median

* UCL 95%: 95% upper confidence limit of the geometric mean, which is considered a high-end estimate.

Non-specific data for all trace elements

The presentation of data that are common to all trace elements, according to TFI (2000) and Guilherme and Marchi (2007), aim to simplify data entry (Tables 2 and 3). Some of these data are considered non specific for the Brazilian population or for the Brazilian scenario, or for other population in the world, such as: Acceptable Target Risk or Hazard Index; Exposure Duration; Exposure Frequency; Relative Absorption Factor; Dermal Absorption Factor; Average Time; Soil Ingestion Rate; Relative Absorption Factor - Soil; Surface Area, and Adherence Factor, and were derived from USEPA (GUILHERME; MARCHI, 2007). Inasmuch as the data entry is not fixed, the user may change values according to its necessities.

Table 2. Non-specific data entry for all trace elements, according to TFI (2000) and Guilherme and Marchi (2007).

Parameter	Adult	Child
ED (years)	30	6
IRs (mg day ⁻¹)	50	200
AS (cm ² event ⁻¹ day ⁻¹)	5700	2900
AF (mg cm ⁻² event ⁻¹)	0.08	0.3
FON	0.01	0.01
EF (days year ⁻¹)	350	350
RAFs ⁽¹⁾	1	1
RAF ⁽²⁾	1	1
ABS ⁽³⁾	0.01	0.01
FOLg ⁽⁴⁾	0.5	0.5
FOLv	0.4	0.4
FOLr	0.1	0.1
T (years)	50	50
Z (cm)	20	20
BD (g cm ⁻³)	1.5	1.5
I (cm year ⁻¹)	0	0
EV (cm year ⁻¹)	0	0

⁽¹⁾ RAFs for arsenic, consider 0.42 for adult and child; for lead, consider 0.41 for adult and child.

⁽²⁾ RAF for lead, consider 0.5 for adult and child.

⁽³⁾ ABS for arsenic, consider 0.03 for adult and child; for lead, consider 1 for adult and child.

⁽⁴⁾ Letters, "g", "v", and "r", following FOL, mean grains, vegetables, and roots, respectively.

Table 3. Non-specific data entry of all trace elements according to TFI (2000), and Guilherme and Marchi (2007) for phosphate, and micronutrients fertilizer products.

Parameter ⁽¹⁾	Fertilizers			
	Phosphate		Zinc Micronutrients	
	TFI (2000)	Guilherme and Marchi (2007)	TFI (2000)	Guilherme and Marchi (2007)
ARg (kg ha ⁻¹ year ⁻¹)	69	72	11	2
ARv (kg ha ⁻¹ year ⁻¹)	130	133	11	2
ARr (kg ha ⁻¹ year ⁻¹)	170	429	11	2
BW adult (kg)	71.8	66.6	71.8	66.6
BW child (kg)	15.5	15.4	15.5	15.4
IRg (kg day ⁻¹)	0.244	0.149	0.244	0.149
IRv (kg day ⁻¹)	0.122	0.012	0.122	0.012
IRr (kg day ⁻¹)	0.079	0.025	0.079	0.025
P (cm year ⁻¹)	28	150	28	150

⁽¹⁾ Letters, "g", "v", and "r", following AR, and IR, mean grains, vegetables, and roots, respectively.

Specific Data for Each Trace Element

The presentation of specific data for each trace element also aims to simplify data entry (Tables 4 to 15). For each of the parameters were attributed specific values according with existing information or information compiled from national and international publications, according to TFI (2000), and Guilherme and Marchi (2007). Additional details about how each of these parameters was obtained may be found at <http://aapfco.org/tfiRiskStd.pdf>; and at <http://www.anda.org.br/publicacoes.aspx>.

Table 4. Parameters for data entry in the Etrace Express software for phosphate fertilizers and zinc micronutrient fertilizers for the risk based concentration calculation for arsenic.

As	Fertilizers			
	Phosphate Fertilizers		Zinc Micronutrient Fertilizers	
Parameters	TFI (2000)	Guilherme and Marchi (2007)	TFI (2000)	Guilherme and Marchi (2007)
PUFg	0.03	0.03	0.03	0.03
PUFv	0.03	0.03	0.03	0.03
PUFr	0.0061	0.0061	0.0061	0.0061
TOXo (mg kg ⁻¹ day)	1.5	1.5	1.5	1.5
TOXd (mg kg ⁻¹ day)	1.5	1.5	1.5	1.5
Kd (mL g ⁻¹)	6.7	158	6.7	158
Kd (mL g ⁻¹) ⁽¹⁾		158.5		158.5

⁽¹⁾Updated Partition coefficients (Kd) values.

Table 5. Parameters for data entry in the Etrace Express software for phosphate fertilizers and zinc micronutrient fertilizers for the risk based concentration calculation for cadmium.

Cd	Fertilizers			
	Phosphate Fertilizers		Zinc Micronutrient Fertilizers	
Parameters	TFI (2000)	Guilherme and Marchi (2007)	TFI (2000)	Guilherme and Marchi (2007)
PUFg	0.12	0.12	0.12	0.12
PUFg ⁽¹⁾		0.942		0.942
PUFv	0.17	0.17	0.17	0.17
PUFr	0.11	0.11	0.11	0.11
TOXo (mg kg ⁻¹ day ⁻¹)	0.001	0.001	0.001	0.001
TOXd (mg/kg-day ⁻¹)	0.001	0.001	0.001	0.001
Kd (mL/g)	6.7	221	6.7	221
Kd (mL/g) ⁽¹⁾		142.5		142.5

⁽¹⁾Updated Plant Uptake Factor (PUF), and Partition coefficients (Kd) values.

Table 6. Parameters for data entry in the Etrace Express software for phosphate fertilizers and zinc micronutrient fertilizers for the risk based concentration calculation for chromium.

Cr	Fertilizers			
	Phosphate Fertilizers		Zinc Micronutrient Fertilizers	
Parameters	TFI (2000)	Guilherme and Marchi (2007)	TFI (2000)	Guilherme and Marchi (2007)
PUFg	0.037	0.037	0.037	0.037
PUFv	0.00018	0.00018	0.00018	0.00018
PUFr	0.00014	0.00014	0.00014	0.00014
TOXo (mg kg ⁻¹ day ⁻¹)	1.5	1.5	1.5	1.5
TOXd (mg kg ⁻¹ day ⁻¹)	0.03	0.03	0.03	0.03
Kd (mL g ⁻¹)	2200	100	2200	100
Kd (mL g ⁻¹) ⁽¹⁾		86		86

⁽¹⁾Updated Partition coefficients (Kd) values.

Table 7. Parameters for data entry in the Etrace Express software for phosphate fertilizers and zinc micronutrient fertilizers for the risk based concentration calculation for cobalt.

Co	Fertilizers			
	Phosphate Fertilizers		Zinc Micronutrient Fertilizers	
Parameters	TFI (2000)	Guilherme and Marchi (2007)	TFI (2000)	Guilherme and Marchi (2007)
PUFg	0.002	0.002	0.002	0.002
PUFv	0.005	0.005	0.005	0.005
PUFr	0.00037	0.00037	0.00037	0.00037
TOXo (mg kg ⁻¹ day ⁻¹)	0.06	0.06	0.06	0.06
TOXd (mg kg ⁻¹ day ⁻¹)	0.026	0.026	0.026	0.026
Kd (mL g ⁻¹)	55	81	55	81
Kd (mL g ⁻¹) ⁽¹⁾		85.5		85.5

⁽¹⁾Updated Partition coefficients (Kd) values.

Table 8. Parameters for data entry in the Etrace Express software for phosphate fertilizers and zinc micronutrient fertilizers for the risk based concentration calculation for copper.

Cu	Fertilizers			
	Phosphate Fertilizers		Zinc Micronutrient Fertilizers	
Parameters	TFI (2000)	Guilherme and Marchi (2007)	TFI (2000)	Guilherme and Marchi (2007)
PUF _g	0.31	0.226	0.31	0.226
PUF _g ⁽¹⁾		0.314		0.314
PUF _v	0.0034	0.0043	0.0034	0.0043
PUF _v ⁽¹⁾		0.0429		0.0429
PUF _r	0.027	0.027	0.027	0.027
TOX _o (mg kg ⁻¹ day ⁻¹)	0.04	0.04	0.04	0.04
TOX _d (mg kg ⁻¹ day ⁻¹)	0.039	0.039	0.039	0.039
K _d (mL g ⁻¹)	22	744	22	744
K _d (mL g ⁻¹) ⁽¹⁾		471.5		471.5

⁽¹⁾ Updated Plant Uptake Factor (PUF), and Partition coefficients (K_d) values.

Table 9. Parameters for data entry in the Etrace Express software for phosphate fertilizers and zinc micronutrient fertilizers for the risk based concentration calculation for lead.

Pb	Fertilizers			
	Phosphate Fertilizers		Zinc Micronutrient Fertilizers	
Parameters	TFI (2000)	Guilherme and Marchi (2007)	TFI (2000)	Guilherme and Marchi (2007)
PUF _g	0.05	0.05	0.05	0.05
PUF _g ⁽¹⁾		0.0357		0.0357
PUF _v	0.008	0.00053	0.008	0.00053
PUF _v ⁽¹⁾		0.0054		0.0054
PUF _r	0.0061	0.0061	0.0061	0.0061
TOX _o (mg kg ⁻¹ day ⁻¹)	0.0036	0.0036	0.0036	0.0036
TOX _d (mg kg ⁻¹ day ⁻¹)	0.0036	0.0036	0.0036	0.0036
K _d (mL/g)	99	2520	99	2520
K _d (mL/g) ⁽¹⁾		1190		1190

⁽¹⁾ Updated Plant Uptake Factor (PUF), and Partition coefficients (K_d) values.

Table 10. Parameters for data entry in the Etrace Express software for phosphate fertilizers and zinc micronutrient fertilizers for the risk based concentration calculation for mercury.

Hg	Fertilizers			
	Phosphate Fertilizers		Zinc Micronutrient Fertilizers	
Parameters	TFI (2000)	Guilherme and Marchi (2007)	TFI (2000)	Guilherme and Marchi (2007)
PUFg	0.26	0.26	0.26	0.26
PUFv	0.061	0.3946	0.061	0.3946
PUFv ⁽¹⁾		3.946		3.946
PUFr	0.082	0.1573	0.082	0.1573
PUFr ⁽¹⁾		1.291		1.291
TOXo (mg kg ⁻¹ day ⁻¹)	0.0003	0.0003	0.0003	0.0003
TOXd (mg kg ⁻¹ day ⁻¹)	0.000021	0.000021	0.000021	0.000021
Kd (mL g ⁻¹)	330	3300	330	3300
Kd (mL g ⁻¹) ⁽¹⁾		118515		118515

⁽¹⁾ Updated Plant Uptake Factor (PUF), and Partition coefficients (Kd) values.

Table 11. Parameters for data entry in the Etrace Express software for phosphate fertilizers and zinc micronutrient fertilizers for the risk based concentration calculation for molybdenum.

Mo	Fertilizers			
	Phosphate Fertilizers		Zinc Micronutrient Fertilizers	
Parameters	TFI (2000)	Guilherme and Marchi (2007)	TFI (2000)	Guilherme and Marchi (2007)
PUFg	0.22	0.22	0.22	0.22
PUFr	0.018	0.018	0.018	0.018
PUFv	0.11	0.11	0.11	0.11
TOXo (mg kg ⁻¹ day ⁻¹)	0.005	0.005	0.005	0.005
TOXd (mg kg ⁻¹ day ⁻¹)	0.005	0.005	0.005	0.005
Kd (mL g ⁻¹)	20	20	20	20

Table 12. Parameters for data entry in the Etrace Express software for phosphate fertilizers and zinc micronutrient fertilizers for the risk based concentration calculation for nickel.

Ni	Fertilizers			
	Phosphate Fertilizers		Zinc Micronutrient Fertilizers	
Parameters	TFI (2000)	Guilherme and Marchi (2007)	TFI (2000)	Guilherme and Marchi (2007)
PUFg	0.05	0.05	0.05	0.05
PUFv	0.015	0.00134	0.015	0.00134
PUFv ⁽¹⁾		0.0135		0.0135
PUFr	0.0086	0.0086	0.0086	0.0086
TOXo (mg kg ⁻¹ day ⁻¹)	0.02	0.02	0.02	0.02
TOXd (mg kg ⁻¹ day ⁻¹)	0.00014	0.00014	0.00014	0.00014
Kd (mL g ⁻¹)	63	179	63	179
Kd (mL g ⁻¹) ⁽¹⁾		110		110

⁽¹⁾ Updated Plant Uptake Factor (PUF), and Partition coefficients (Kd) values.

Table 13. Parameters for data entry in the Etrace Express software for phosphate fertilizers and zinc micronutrient fertilizers for the risk based concentration calculation for selenium.

Se	Fertilizers			
	Phosphate Fertilizers		Zinc Micronutrient Fertilizers	
Parameters	TFI (2000)	Guilherme and Marchi (2007)	TFI (2000)	Guilherme and Marchi (2007)
PUFg	0.57	0.57	0.57	0.57
PUFr	0.093	0.093	0.093	0.093
PUFv	0.088	0.088	0.088	0.088
TOXo (mg kg ⁻¹ day ⁻¹)	0.005	0.005	0.005	0.005
TOXd (mg kg ⁻¹ day ⁻¹)	0.005	0.005	0.005	0.005
Kd (mL g ⁻¹)	2.7	2.7	2.7	2.7
Kd (mL g ⁻¹) ⁽¹⁾		54.35		54.35

⁽¹⁾ Updated Partition coefficients (Kd) values.

Table 14. Parameters for data entry in the Etrace Express software for phosphate fertilizers and zinc micronutrient fertilizers for the risk based concentration calculation for vanadium.

V	Fertilizers			
	Phosphate Fertilizers		Zinc Micronutrient Fertilizers	
Parameters	TFI (2000)	Guilherme and Marchi (2007)	TFI (2000)	Guilherme and Marchi (2007)
PUFg	0.007	0.007	0.007	0.007
PUFv	0.0007	0.0007	0.0007	0.0007
PUFr	0.00086	0.00086	0.00086	0.00086
TOXo (mg/kg-dia)	0.007	0.007	0.007	0.007
TOXd (mg/kg-dia)	0.00021	0.00021	0.00021	0.00021
Kd (mL/g)	11	11	11	11

Table 15. Parameters for data entry in the Etrace Express software for phosphate fertilizers and zinc micronutrient fertilizers for the risk based concentration calculation for zinc.

Zn	Fertilizers			
	Phosphate Fertilizers		Zinc Micronutrient Fertilizers	
Parameters	TFI (2000)	Guilherme and Marchi (2007)	TFI (2000)	Guilherme and Marchi (2007)
PUFg	0.58	1.503	0.58	1.503
PUFg ⁽¹⁾		1.91		1.91
PUFv	0.17	0.028	0.17	0.028
PUFv ⁽¹⁾		0.281		0.281
PUFr	0.056	0.056	0.056	0.056
TOXo (mg kg ⁻¹ day ⁻¹)	0.3	0.3	0.3	0.3
TOXd (mg kg ⁻¹ day ⁻¹)	0.24	0.24	0.24	0.24
Kd (mL g ⁻¹)	16	129	16	129
Kd (mL g ⁻¹) ⁽¹⁾		105.2		105.2

⁽¹⁾ Updated Plant Uptake Factor (PUF), and Partition coefficients (Kd) values.

Risk Based Concentration (RBC) Equation (TFI, 2000)

The RBC equation is developed using standard USEPA risk practices and exposure parameters (USEPA, 1989). The standard equation to calculate risk combines 3 factors: estimated intake from exposure, toxicity of the element of interest, and concentration of the trace element in the media of concern (i.e., fertilizer or product). In a back-calculation risk based approach, the equation is arranged to solve the RBC using an estimate of exposure potential, toxicity, and an acceptable risk level.

The back calculation allow to estimate safe limits for ET concentration in the fertilizer product for acceptable health risk levels. An acceptable risk is, in this case, relative to a TE concentration with minimum potential to cause adverse effects. The equation may be adjusted for the single crop farm (equation 1) or multiple crop (equation 2) scenarios.

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

Where:

$$\frac{ED * EF * SA * AF * ABS * CF}{BW * AT} = \text{Summary intake factor (SIFd) dermal contact soil/fertilizer}$$

$$\frac{ED * EF * IRs * RAFs * CF}{BW * AT} = \text{Summary intake factor (SIFsi) incidental ingestion soil/fertilizer}$$

$$\frac{ED * EF * IRc * RAFC}{AT} = \text{Summary intake factor (SIFc) ingestion crop}$$

TR or THI is Acceptable Target Risk or Hazard Index (Unitless). Other parameters were defined in Table 1.

Equation 1. RBC for the single crop farm.

The RBC equation for the multi-crop farm scenario is more complicated than the RBC equation for the single crop farm, because all three-crop groups are integrated into one equation (Equation 2). Yet, each crop group has a different AR and PUF. Note the addition of a new factor, Fraction of Land (FOL), in the equation. FOL is used to fractionate the addition of trace element to soil by the different application rates for the different crop groups. Also note the use of SIFs in the equation. SIFs are summary intake factors that are derived for the single crop farm in equation 1.

$$RBC = \frac{TR \text{ or } THI}{SACF * \{AR_v * 1 / FON * [(SIF_s * TOX + SIF_d * TOXd) * FOL_v] + PUF_v * SIF_v * TOX\} + \frac{TR \text{ or } THI}{\{AR_r * 1 / FON * [(SIF_s * TOX + SIF_d * TOXd) * FOL_r] + PUF_r * SIF_r * TOX\} + \frac{TR \text{ or } THI}{\{AR_g * 1 / FON * [(SIF_s * TOX + SIF_d * TOXd) * FOL_g] + PUF_g * SIF_g * TOX\}}$$

Equation 2. RBC for the Multi-crop farm.

Etrace Express

The software presents four tabs, in which the two first are for data entry, the third is to show RBC results, and the last one to show credits, and how to contact software developers (Figures 4 to 6). In the first tab, entitled configuration, parameters defining scenarios are chosen. The main fertilizers, crops, and one among 12 trace elements may be chosen.

Etrace Express

Cálculo da Concentração Baseada em Risco

Configuração | Entrada de Dados | Resultado | Créditos

Fertilizante:

- Fosfatados
- Com micronutrientes contendo Zinco

Cenário de propriedades agrícolas:

- Um grupo de cultura
- Vários grupos de culturas

Categoria:

- Adulto
- Criança

Culturas:

- Grãos
- Vegetais
- Raízes

Metais:

- Arsênio
- Mercúrio
- Cádmio
- Molibdênio
- Cromo
- Níquel
- Cobalto
- Selênio
- Cobre
- Vanádio
- Chumbo
- Zinco

Figure 4. Configuration tab.

In the second tab, data presented in the tables 2 to 15 are added, according to the metal of interest.

Etrace Express

Cálculo da Concentração Baseada em Risco

Configuração | Entrada de Dados | Resultado | Créditos

Taxa de Aplicação (kg/ha-ano):
 Fração do Nutriente no Fertilizante (Adimensional):
 Duração da Exposição (anos):
 Frequência da Exposição (dias/ano):
 Massa Corporal (kg):
 Taxa de Ingestão do Solo (mg/dia):
 Área da Pele Exposta (cm²/evento-dia):
 Fator de Aderência (mg/cm²):
 Fator de Absorção Relativa Via Solo (Adimensional):
 Fator de Absorção Relativa (Adimensional):
 Ingestão de Produtos Agrícolas (kg/dia):

Fator de Absorção Dermal (Adimensional):
 Fator de Absorção pela Planta (Adimensional):
 Toxicidade Oral (mg/kg-dia):
 Toxicidade Dermal (mg/kg-dia ou mg/kg-dia⁻¹):
 Profundidade de Cultivo do Solo (cm):
 Densidade Global do Solo (g/cm³):
 Irrigação Média Anual (cm/ano):
 Precipitação (cm/ano):
 Evapotranspiração Média Anual (cm/ano):
 Tempo de Aplicação (anos):
 Coeficiente de Partição solo-água (mL/g):

Calcular

Figure 5. Data Entry tab.

The third tab presents the results of the RBC calculations, as well as some user´s entered information.

Figure 6. Results tab.

After adding data in the tabs, if the information presented at the tables 2 to 14 were followed (data from TFI, 2000, or GUILHERME; MARCHI, 2007), unit RBCs must be equal to those presented at the tables 15 (for phosphate fertilizers) or 16 (zinc micronutrient fertilizers).

Table 16. Unit risk based concentrations⁽¹⁾ for phosphate fertilizers.

Scenario	Arsenic, carcinogenic	Cadmium	Chromium	Cobalt	Copper	Lead	Mercury	Molybdenum	Nickel	Selenium	Vanadium	Zinc
	Adult	Child										
Brazil ⁽²⁾	2,9	5,8	81470	6389	165	85	0,6	216	435	582	10064	388
Brazil ⁽³⁾	2,9	1,8	91602	6105	132	110	0,1	216	579	31	10064	350
TFI	4,5	23	34000	3100	280	73	0,9	42	350	120	2200	1200

⁽¹⁾ Unit RBCs (mg kg⁻¹).

⁽²⁾ Data from Guilherme and Marchi (2007).

⁽³⁾ Updated data.

Table 17. Unit risk based concentrations ⁽¹⁾ for zinc micronutrient fertilizers.

Scenario	Arsenic, carcinogenic	Cadmium	Chromium	Cobalt	Copper	Lead	Mercury	Molybdenum	Nickel	Selenium	Vanadium	Zinc
	Adult	Child										
Brazil ⁽²⁾	128	351	3195903	277481	6531	3818	31	8575	19556	23919	483249	14418
Brazil ⁽³⁾	128	70	3593365	265141	5133	5194	12	8575	26231	1257	483249	13013
TFI	38	210	220000	23000	1800	500	6,5	300	2600	800	17000	8600

⁽¹⁾ Unit RBCs (mg kg⁻¹).

⁽²⁾ Data from Guilherme and Marchi (2007);

⁽³⁾ Updated data.

RBCs are normalized to represent a 1 percent fraction of nutrient (FON) content. These RBCs are called unit RBCs. Unit RBCs can easily be adjusted to represent a particular product with a certain percent nutrient content. The concentrations of the MOPC in products must be in the same units as the RBCs to make a direct comparison. RBCs, and the TE in fertilizer products database are reported in mg TE kg⁻¹ of product (i.e., part per million or PPM). However, before proceed the comparison, TE concentrations in fertilizers must be adjusted to the same fraction of nutrients (FON) used in the RBCs (1%). TE concentrations in fertilizer products are adjusted by dividing its value by the P₂O₅ percent concentration, for phosphate fertilizers, or Zn, for Zn sources.

System requirements

Windows 98 or later version of Microsoft Windows operating system.

Where do I find the software

www.cpac.embrapa.br/publico/usuarios/uploads/Downloads/Softwares/Etrace/Etrace.zip

References

GUILHERME, L. R. G.; MARCHI, G. Metais em fertilizantes inorgânicos: avaliação de risco à saúde após a aplicação. 1. ed. São Paulo, SP: ANDA, 2007. 154 p. Disponível em: <<http://www.anda.org.br/publicacoes.aspx>.>

THE FERTILIZER INSTITUTE – TFI. Health risk evaluation of select metals in inorganic fertilizers post application. [S.l.]: prepared for the Fertilizer Institute, The Weinberg Group, January 16, 2000. Disponível em: < <http://aapfco.org/tfiRiskStd.pdf>.>

UNITED States Protection Agency (USA EPA). Risk assessment guidance for superfund.: human health evaluation manual (part A): Interim Final. Washington, D.C.: Office of Emergency and Remedial Response. EPA/540/1-89/002. 1989. v. 1. Disponível em: <http://www.epa.gov/oswer/riskassessment/ragsa/pdf/rags-vol1-pta_complete.pdf.>

Etrace Express: programa para análise de risco de elementos-traço em fertilizantes inorgânicos – manual e guia de referência

Resumo

Elementos-traço estão presentes geralmente em fertilizantes inorgânicos como produtos secundários ou contaminantes. Há, entretanto, alguns elementos-traço que são nutrientes de plantas e são incluídos em formulações de fertilizantes intencionalmente. Sabe-se que a exposição a altos níveis de elementos-traço (nutrientes ou não) podem causar risco à saúde para humanos. Este risco pode ser estimado por modelos de avaliação. Desta forma, este trabalho apresenta uma ferramenta, o programa Etrace Express, para fácil cálculo de Concentrações Baseadas em Risco de elementos-traço em fertilizantes inorgânicos, os quais sugerem limites seguros para uso agrícola. A principal proposta desta versão é a de calcular valores de concentrações de elementos-traço em fertilizantes inorgânicos que possam, com flexibilidade, ser usadas por órgãos reguladores com objetivo de proteger a saúde humana. O programa Etrace Express segue a mesma metodologia do documento preparado para o The Fertilizer Institute (TFI, United States) para o cenário norte-americano, intitulado “Health Risk Evaluation of Selected Metals in Inorganic Fertilizers Post Application”. Concentrações baseadas em risco calculadas pelo Etrace Express usando dados provindos dos documentos do TFI e do cenário brasileiro foram idênticos aos originalmente publicados. Adicionalmente, o programa permite personalizar parâmetros para cenários específicos com muita rapidez.

Termos de indexação: metais pesados, contaminação do solo, segurança alimentar, plataforma Delphi.

Etrace Express: software for risk analysis of trace elements in inorganic fertilizers – user's manual and reference guide

Abstract

Trace Elements are generally present in inorganic fertilizers as 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 (nutrients or not) might pose a health risk to humans. This risk may be estimated by assessment models. Thus, this work presents a tool, the software Etrace Express, for easy calculation of Risk Based Concentrations of trace elements in inorganic fertilizers, which suggest safe limits for agricultural use. The main purpose of this software 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 follows the same approach shown in the document prepared by The Fertilizer Institute (TFI, United States) for the US scenario, entitled "Health Risk Evaluation of Selected Metals in Inorganic Fertilizers Post Application". RBCs calculated by Etrace Express using data from the TFI and from a Brazilian scenario reports were identical to the original. Additionally, the software allows customization of parameters for specific scenarios, very rapidly.

Index terms: heavy metals, soil contamination, food safety.

Embrapa

Cerrados

Ministry of Agriculture,
Livestock and Food Supply



CGPE 9174