International Journal of Plant & Soil Science
5(2): 117-126, 2015; Article no.IJPSS.2015.066
ISSN: 2320-7035

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LINN Simulation Model for Health/Environmental Impacts Associated with the Presence of Dangerous Minerals in Agricultural Soils

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Authors' contributions

This work was carried out in collaboration between all authors. Author WML designed the study, wrote the protocol, and wrote the first draft of the manuscript. Authors NJI, NKN and APN proofread and managed preparation of the final manuscript. All authors read and approved the final manuscript.

Article Information

DOI: 10.9734/IJPSS/2015/13970
Editor(s):
(1) Francisco Cruz-Sosa, Biotechnology Department, Metropolitan Autonomous University Iztapalapa Campus Av. San Rafael Atlixco 186 México City 09340 México.
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(4) Anonymous, Institute for Medical Research, Croatia.
Complete Peer review History: http://www.sciencedomain.org/review-history.php?iid=780&id=24&aid=7402

Short Communication

Received 12th September 2014
Accepted 22nd November 2014
Published 17th December 2014

ABSTRACT

In this study, a brief history related to mathematical modeling of minerals uptake by plants from soil is presented. Thereafter, a simulation model called LINN is developed that will have the main task of providing a link between the results predicted by the existing mathematical models and/or measured values (from real experiments) and health impacts as stipulated elsewhere in the literatures. LINN model is built on MS-OFFICE (Access). Six metallic trace elements (MTE) that are known to be dangerous to the ecosystem (As, Cd, Cr, Hg, Ni and Pb) can be evaluated by LINN. This program provides general descriptions on impacts that may happen to plants and/or human beings when these elements are present in the soils at levels exceeding the standard limits set by the regulatory organs i.e. World Health Organization (WHO). However, LINN does not differentiate

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impacts related to MTEs present at levels just above the standard limits from levels extremely higher than the standard limits.

Keywords: Metallic trace elements; mathematical/simulation modeling; modeling; LINN; plants; human beings.

1. INTRODUCTION

Two major groups of dangerous minerals that are taken up by plants through the process of plant mineral uptake from agricultural soils have been identified; heavy metals i.e. Chromium, Arsenic and Lead [1-4] and radionuclides i.e. Uranium, Thorium and Radon [5-10]. Both groups possess health risks to plants, animals (especially human beings) and the general environment [1-2,9,11-13]. In lieu of that, many researchers have developed mathematical models to predict concentrations of minerals taken up by plants from agricultural soils [14-17]. These models have a long history of developments (Table 1).

Table 1. Development of mathematical models related to radionuclides since 1970

Sn	Model	Year
1	Hermes	1971
2	Food	1976
3	Airdos-epa	1979
4	Ecosys	1982
5	Terfoc-N	1990
6	Ecosys-87	1993
7	Resrad/Erica tool	Recent ones

Source; [14-17]

Most existing mathematical models (Barber-Cushman, HERMES, FOOD, ECOSYS, TERFOC-N, AIRDOS-EPA and ECOSYS-87) were developed to predict concentrations of various nutrients taken up by plants from soil through soil-plants interactions [14]. Other recently developed models include RESRAD and ERICA Tool that can be used to assess radiological risks to terrestrial, freshwater and marine biota [15-16]. Although these models are widely used in evaluating the effects of the transfer of such dangerous minerals to humans and the ecosystem in general, these models lack a necessary component relating to a more direct and simpler interpretation of the outcomes of their predictions, of which are always in terms of numbers (i.e. Bq/Kg or mg/Kg). Furthermore the existing mathematical models lack a comparative component in them, in that, their outcomes do not inform us whether the measured/predicted values exceed the standard limitations provided by the regulatory organs.

2. THE HISTORY OF MATHEMATICAL MODELING OF RADIONUCLIDES AND METALLIC TRACE ELEMENTS (MTEs) IN SOIL

2.1 Mathematical Modeling of Radionuclides in Soil

Radioactive elements that are found in many soils of the world are dangerous to both plants and animals [18]. However, research [5-10] has shown that the amount of these radionuclides taken up by plants do not pose significant health impacts to plants grown in the agricultural soils of the world. The danger to plants is considered minimal. Likewise, human beings are less prone to radiations from agricultural soils due to the fact that, plants' edible parts contains little contamination from the soil and also the exposure time is very short (people do not stay in their farms for 365 days a year) [5,7]. This is the main reason to why many mathematical models for radioactivity levels were developed to investigate radiological effects caused by fallouts from nuclear devices as well as accidents from nuclear power plants i.e. Chernobyl [14,19-21].

Mathematical models that can be used for evaluating and preventing radiological health risks were developed since 1960 [22], although the first widely accepted mathematical model came in 1971 [23]. These models are exchangeably referred to as environmental transfer models. Most of these models were developed to prevent radiological effects caused by fallouts from nuclear devices [19-21,23-25]. These models are divided into two categories namely equilibrium models and dynamic model [14]. According to Yasuda (1995), equilibrium models are used in normal situations where contamination was caused by normal operations while dynamic models are meant for emergence situations where rapid prediction is needed due to accidental pollution. Table 1 represents a trend in the development of mathematical models related to the prediction of levels of radioactive minerals present in soil.

One of the oldest mathematical models in this category is HERMES (Table 1). This model has widely been used to study potential radiation doses to people from nuclear facilities. In HERMES, radionuclides are assumed to reach food edible parts of a plant through direct deposition from air, irrigation and from mineral uptake from contaminated soil [23]. The equation to calculate radionuclide concentration in a crop was as follows:

$$C_{crop} = \frac{f.f_{ret}}{Y_c}\sum_{m=a}^{h}\left[\left(Q_{c-dep} + r_{irr}C_{irr}\right)e^{\lambda_{crop}t}\right] + \frac{T_f}{W_{soil}}\left(Q_{s-air} + Q_{s-irr}\right)$$

Where;

C_{crop}: Concentration in crop edible parts (Bq.Kg^{-1})
C_{irr} :Concentration in irrigation water during month (Bq.L^{-1})
F :Translocation factor to crop edible parts
f_{ret} :Deposition retention factor (fraction of deposited activity retained on crops)
λ_{crop} : Effective removal rate constant from crops (T^{-1})
t :Time (T)
m :Constant giving best fits
a :Month of appearance
h :Month of harvest
T_f :Soil-to-plant transfer factor (concentration ratio between crop edible parts and soil at time of harvest) (Bq.Kg^{-1}-crop per Bq.Kg^{-1}-soil)
Y_c :Yield of edible parts of crops (kg.m^{-2})
Q_{c-dep}:Deposition amount on crop per unit soil surface area (Bq.m^{-2})
R_{irr} :Irrigation rate during month (L. m^{-2})
Q_{s-air} :Concentration in plowlayer of radionuclide deposited from air (Bq. m^{-2})
Q_{s-irr} :Concentration in plowlayer of radionuclide deposited from water (irrigation) (Bq. m^{-2})
W_{soil} :Amount of surface soil (plowlayer) per unit area (kg.m^{-2})

2.2 Mathematical Modeling of MTEs in Soil

Heavy metals and metalloids in soils, above the allowable limits [13,26-27] are harmful to both plants and animals [2,11,28-31]. Many mathematical models [1,32-41] have therefore been developed to evaluate and prevent health effects associated with the presence of such dangerous elements in agricultural soils. These models seem to integrate values for root size and its increase with time, nutrient inflow into the roots as related to nutrient concentration in the root zone soil solution and nutrient transport in the soil by convection or diffusion [18]. The earliest model in this category, which has been the basis for development of all other models related to the uptake of heavy metals to plants from agricultural soils, is Barber-Cushman model [17]. This model was developed in 1980 by Barber and Cushman. Many studies [1,32,35,38-39] from 1980 to 2003 have used Barber-Cushman platform and Michaelis-Menten kinetics of nutrient uptake from soil solution by plant roots to simulate uptake of minerals by plants from agricultural soils of the world.

Barber-Cushman model is governed by the following formulae;

i. The concentration in the liquid is linearly related to the solid concentration

$$C_i^t = b * c_{liquidi}^t$$

Where;

C_i^t = Nutrients concentration in solid phase at time, t
$C_{liquidi}^t$ = Nutrients concentration in liquid phase at time, t
B =buffer power of nutrients on the solid phase for nutrients in solution, dimensionless.

ii. The flux of a nutrient from one node to another is described by the combined effect of diffusion (Ficks law) and mass flow (works on liquid concentration and needs therefore be multiplied with b)

$$F_{lt} = D_e * \frac{\partial C^t}{\partial r} + \frac{V_l^t}{b} * C_{l,l+1}^t$$

Where;

B =buffer power of nutrients on the solid phase for nutrients in solution, dimensionless.
F_{it} =Nutrients flux from one node to another
V_i^t = Volume of the solution at time, t (sec)
C^t = Nutrients concentration
$C_{i,i+1}^t$ =Nutrients concentration in solid phase
D_e = Effective diffusion coefficient for the nutrients in the soil, (cm^2/s).

iii. The flux from the most inner node into the root is described by Michealis-Menten kinetics.

$$F_{0t} = \frac{J_{max} * C_1^t}{K_m * C_1^t} - Efflux$$

Where;

Efflux is independent of the concentration outside the root. Sometimes it is represented by a minimum uptake concentration C_{min} for which C is corrected.

F_{ot} = Nutrients flux from the most inner node to the root
K_m = Nutrient concentration in the solution (μmol/L)
J_{max} = Maximum diffusive flux (μmol)
C_i^t = Nutrients concentration in solid phase

iv. The flux over the outside boundary is zero.

$$F_{kt} = 0$$

Where;

F_{kt} = Flux over the outside boundary, which is zero

As it has been shown above, outputs from the two models (HERMES and Barber-Cushman) are concentrations of minerals present in the medium. These concentrations are presented in the form of $BqKg^{-1}$ or $mgKg^{-1}$, in which it is very difficult for one to conclude whether the values are harmful in terms of health/environmental risk. A comparison of the predicted values to the standard limits set by regulatory authorities needs to be undertaken before a conclusion is made on the fate of the predicted values. Also, further description on the type of health risks that might be associated with the predicted values to both plants and animals needs to be addressed.

In that regard, LINN simulation model is developed to fill the above addressed gaps related to mathematical modeling in health/environmental impact assessment.

3. DEVELOPMENT OF LINN SIMULATION MODEL

3.1 Background

Radionuclides and heavy metals in soil can be dangerous to both plants and animals esp. human beings [5-12,26-27]. Unlike radionuclides which many studies [5-10] have revealed little danger through soil-plant-man pathway, MTEs possess a significant danger to both plants and human beings. Plants and animals can both be contaminated directly from agricultural soils through plants mineral uptake (for plants) and soil-eating, inhalation, skin contact and drinking water (for humans) [42]. Moreover, human beings can be contaminated through indirect pathways such as the food chain (eating plants or other animals that are already contaminated from agricultural soils). This kind of contamination may lead to health impacts both to plants and animals. From a scientific research point of view, most research scholars take soil samples to laboratories for different analyses related to measurements of contents of dangerous elements including MTEs. These researchers, on the other hand may decide to use the existing mathematical models, created by others, to predict such contents in agricultural soils. The main aim for both methods is to find out whether the contents in the study sites are safe as stipulated by regulatory boards i.e. World Health Organization (WHO).

From the laboratory analysis and predictions from the available mathematical models, one is able to come up with a value/number i.e. 10 in mg/Kg that tells the amount of MTEs present in the study site. However, if this value is presented as it is, it is very difficult for one to interpret its meaning in terms of health/environmental perspective, in that, the value does not give us any information on how safe is the study site. It only gives us a mere value, that one needs to compare with some standard value to judge whether the site is safe or not. Even after comparison with standard values, it is still difficult for a person to clearly understand what are the possible consequences of the presence of such elevated levels of MTEs. This is where the idea of developing LINN Simulation Model started. This model acts as a link between the three levels/stages (1. measurements/predictions 2. comparison with standards and 3. description of the health impacts) explained above. LINN Simulation Model is therefore meant to link the three stages so that a common man can easily understand the true meaning of the measured/predicted values.

3.2 LINN Simulation Model

LINN is a short form of Lema-Ijumba-Ndakidemi-Njau. These are four names of four colleagues who are co-founders of the LINN Simulation Model. This model is very simple and anyone can use it. LINN is built on MS-OFFICE (Access) and is based on the predictions/measurements performed earlier in agricultural soils. This program has a strong database (Table 2-3) containing a description of health/environmental impacts that may be cause by the existence of elevated levels of MTEs in agricultural soils to both animals and plants. This database is also fed with data on standard limits of MTEs in soil that are believed to cause negative impacts to plants and animals (Tables 2-3). The values obtained through laboratory measurements or through mathematical modeling (i.e. Ni=56.50mg/Kg) Lema et al. [18] are fed into LINN through the interface shown on Fig. 2, one at a time. The following is a simple procedure to be followed while using LINN Simulation Model;

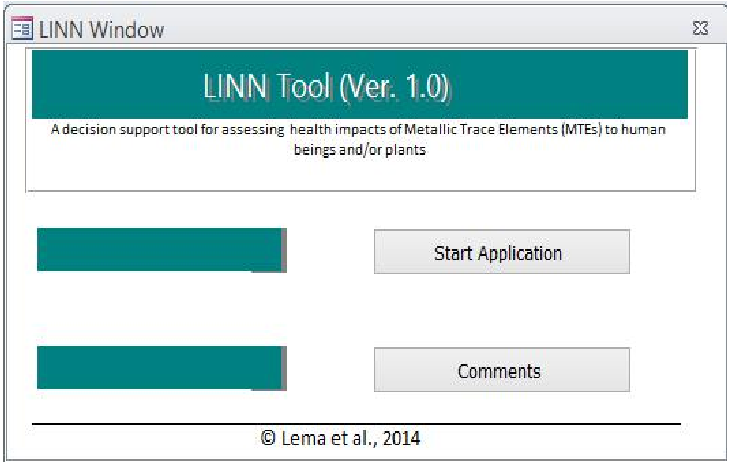
From LINN Tool Interface (Fig. 1), select “Start Application” and then a new window (Fig. 2) will appear, that will require you to follow the following steps to accomplish your task;

i. Choose MTE that you want to evaluate from the available list of MTEs i.e. As, Cr, Ni, Cu, Zn and Pb.
ii. Enter the value obtained from laboratory measurements or from mathematical modelling predictions i.e. 20 mg/Kg
iii. Choose one category (either animals {human beings} or plants) to get a description of health impacts for one of the two categories.

From the three steps above, LINN is capable of giving a brief description on health impacts related to the MTE of concern by pressing the button “Evaluate Impacts”. However, this program has limitations, in that, the evaluation of impacts does not consider differences in the values fed to it by users, i.e. if the standard limit for As is 10mg/Kg, and the measured value is 12mg/Kg or 60mg/Kg, LINN will give the same description on impacts related to the two values without considering that 12mg/Kg might have lesser impacts than 60mg/Kg. The following is an example of an output from LINN Model (also see Fig. 3).

“Arsenic is associated with the following impacts on plants;”

- *causes growth inhibition in roots and shoots*
- *affects P and Mn status in plants,*
- *reduces chlorophyll “a” concentration*
- *increases MDA and thiol levels”*



A decision support tool for assessing health impacts of Metallic Trace Elements (MTEs) to human beings and/or plants

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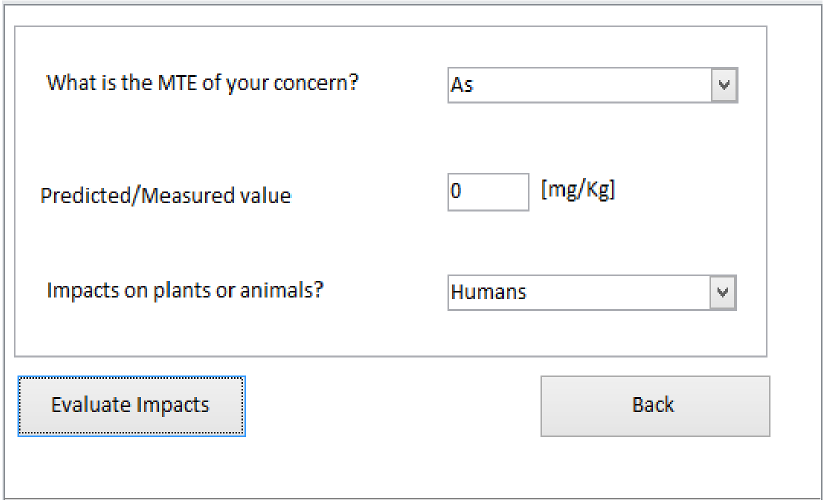
Figure 1. LINN Simulation Program Interface

Table 2. Impacts on plants

MTE	Standard Limits (mg/Kg)*	Possible Impacts**
Cr	1	Chromium can cause alterations in the germination process, stunted growth, reduced yield and mutagenesis.
Ni	30	Nickel can cause decrease in leaf area, chlorosis, necrosis and stunting.
As	10	Arsenic causes growth inhibition in roots and shoots, affects P and Mn status in plants, reduces chlorophyll “a” concentration and increases MDA and thiol levels.
Cd	3	Cadmium can cause chlorosis, necrosis, purple coloration.
Hg	0.3	Mercury is known to affect photosynthesis and oxidative metabolism by interfering with electron transport in chloroplasts and mitochondria. It also inhibits the activity of aquaporins and reduces plant water uptake.
Pb	50	Lead is associated with dark-green leaves.

**Source: [30,43] **Source: [31,44-45]*



What is the MTE of your concern? As

Predicted/Measured value 0 [mg/Kg]

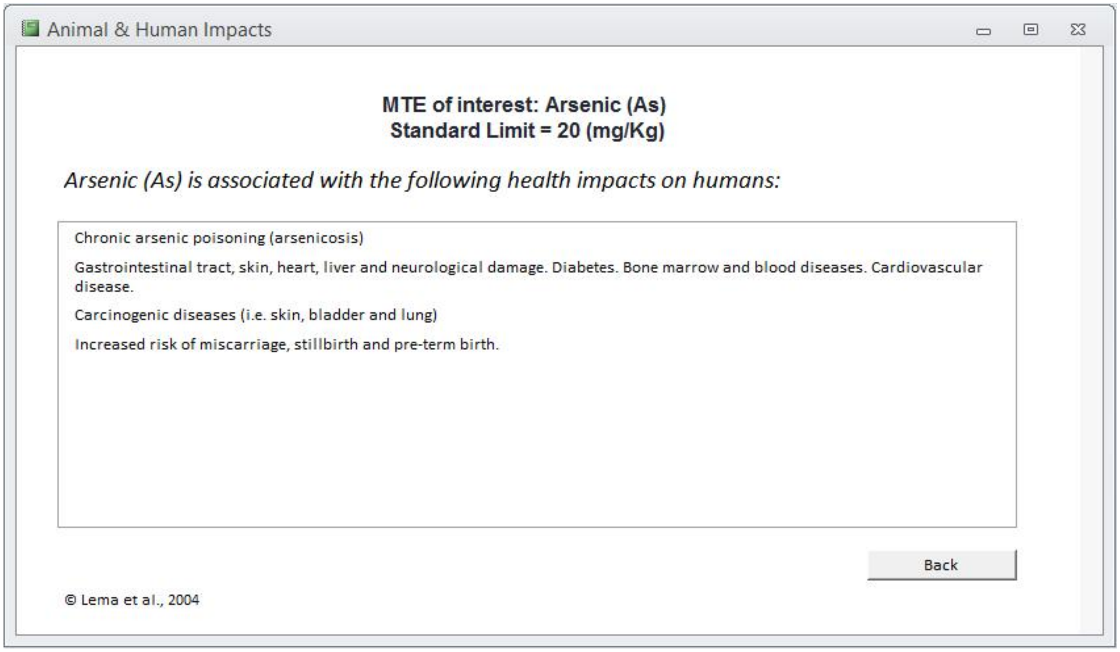
Impacts on plants or animals? Humans

Figure 2. Inputs on LINN Simulation Program

Table 3. Impacts on Animals esp. human beings

MTE	Standard Limits (mg/Kg)+	Possible Impacts++
Cr	30	Chromium, especially Cr (VI) is associated with; Both carcinogenic (causing cancer) and noncarcinogenic diseases. Allergic skin reactions (dermatitis) and malfunctioning of lung and blood system problems, gastrointestinal burns, hemorrhage, diarrhea, ulcers, abdominal pain, indigestion, vomiting, liver damage, and kidney damage that may lead to death. Asthma, nasal septum ulcers and even nasal septum perforations
Ni	600	Nickel is associated with; Induced respiratory tract irritation, chemical pneumonia, lung damage, emphysema and varying degrees of hyperplasia of pulmonary cells, and fibrosis (pneumoconiosis). Allergic skin reactions (dermatitis), renal effect and crossing the placental barrier, thus being able to influence prenatal development by direct action on the embryo.
As	20	Arsenic is associated with; Chronic arsenic poisoning (arsenicosis), gastrointestinal tract, skin, heart, liver and neurological damage. Diabetes. Bone marrow and blood diseases. Cardiovascular disease, carcinogenic disease (i.e. skin, bladder and lung). Increased risk of miscarriage, stillbirth and pre-term birth.
Cd		Cadmium is associated with; Liver and kidney damage, low bone density and is carcinogenic disease (i.e. lung) and renal tubular damage.
Hg	23	Mercury is associated with; Central nervous system (CNS) and gastric system damage, affects brain development in children, resulting in a lower IQ, affects co-ordination, eyesight and sense of touch Liver, heart and kidney damage, reduced reproductive success, impaired growth and development, behavioral abnormalities, hearing loss, reduced immune response and decreased survival.
Pb	300	Lead is associated with; Neurological damage, lowers IQ and attention, hand-eye co-ordination impaired,, encephalopathy, bone deterioration, hypertension, kidney disease, the incomplete development of the blood-brain barrier in fetuses, stunt growth rates, learning disabilities, impairing hearing acuity, and behavioral problems, convulsions, coma or death.

$^{+}$*Source: [30,43]* $^{++}$*Source: [13,28,46-51]*



MTE of interest: Arsenic (As)
Standard Limit = 20 (mg/Kg)

Arsenic (As) is associated with the following health impacts on humans:

Chronic arsenic poisoning (arsenicosis)

Gastrointestinal tract, skin, heart, liver and neurological damage. Diabetes. Bone marrow and blood diseases. Cardiovascular disease.

Carcinogenic diseases (i.e. skin, bladder and lung)

Increased risk of miscarriage, stillbirth and pre-term birth.

© Lema et al., 2004

Figure 3. LINN simulation program output

4. CONCLUSION

Existing mathematical models i.e. HERMES and Barber-Cushman have been used for years, since 1970 to predict impacts related to presence of radionuclides and MTEs in agricultural soils of the world. The outcomes from these models have so far been values/numbers of which researchers used to further interpret and come up with the predicted impacts after several steps including comparison of the obtained results with the available standard limits as well as relating the obtained values with the impacts stated in the existing literature. LINN Simulation Model is meant to utilize the predicted/measured values to give a more direct, clearer, simpler and understandable description of the meaning of the obtained values for the health/environmental decision makers and planners through linking all the required step/stages (1. measurements/predictions 2. comparison with standards and 3. description of the health impacts). However, LINN model will not be able to give a clear difference between health impacts associated with the presence MTEs at levels just above the standard limits and those related to levels that are extremely higher than the standard limits.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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