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SOIL REMEDIATION FROM HEAVY METALS USING MATHEMATICAL MODELLING

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Abstract. The essence of the contemporary mathematical modelling methodology is the replacement of a real object in question (a process, phenomenon or system) with its "image" – a mathematical model. The mathematical modelling programme REC (Risk Reduction, Environmental Merit and Cost) is based on the comparison of alternative cleaning technologies (to clean contaminated areas). The programme REC is aimed at adapting efficient soil decontamination technologies. The aim of this paper is to analyse the ability of a grassy vegetation mixture to absorb heavy metals from soil in this way decontaminating it. Initial concentrations of heavy metals (copper, lead, manganese, zinc, nickel and chromium) – the concentrations, used during the experiment when performing the investigation into the efficiency of soil remediation using the mixture of grassy vegetation, were input into the programme. During the entire chosen period of 10 years, soil would be decontaminated from copper and lead. The zero concentration of manganese in soil is achieved after 8 years, and that of zinc – after 9 years when soil is cleaned with the mixture of grassy vegetation and no additional contamination is present. Soil is most rapidly decontaminated from nickel – in 6 years. At the initial chromium concentration of 79.5 mg/kg in soil, the zero concentration of this metal would be achieved in 7 years.

Keywords: heavy metals, soil remediation, *Lolium perenne L., Poa pratensis L., Festuca pratensis Huds,* mathematical modelling.

1. Introduction

Soil contamination is a problem of a global scope, and yet no universal solution has been discovered to deal with it. There are lots of soils contaminated with heavy metals all across the world (Peters 1999; Hooda 2003; Barazni *et al.* 2004; Morel 2002). Despite the fact that some contaminants naturally access the soil, all human activities, including mining, metal melting, industries, agriculture, transport, waste water sludge treatment, fertilizer manufacturing and others, are accompanied by contamination . All these activities produce contaminants, which in one or other way access the environment: as gas, solid particles or solutions. Heavy metals are the consequences of modern industry (Sun *et al.* 2001; Khan 2005; Boularbah *et al.* 2006; Wu *el al.* 2006; Pereira *et al.* 2006). Such soils become barren and heavily contaminated, and contaminants may penetrate into the layer of underground waters. Consequently, contamination by heavy metals is one of the most critical environmental problems. Heavy metals are discovered in various chains of food, what finally results in serious health problems of micro-organisms, plants, animals and humans. The removal of metals using usual physical and chemical methods is expensive and in the majority of cases unsuitable (Yun-Guo *et al.* 2006; Calace *et al.* 2005; Weber and Karcazewska 2004; Malik 2004; Liphadzi and Kirkham 2006; Jankaitė and Vasarevičius 2005). The removal of toxic contaminants is complicated due to abundance and variety of contaminants (Glick 2003).

Transport of trace metals from the soil to a plant involves chemical, physical and biological processes (such as diffusion, adsorption, absorption, growth of a plant, transpiration rate, etc.) in the soil, the soil rhizosphere and in the plant itself (Baltrėnaitė and Butkus 2007). Mathematical modelling is a part of applied mathematics intended for doing tasks in different areas using the methods of a virtual experiment. It is based on the formation and primary analysis of mathematical models, composition and analysis of digital algorithms, processing of natural observations and experimental findings as well as reception and analysis of new information about the processes, systems and phenomena being modelled. The essence of the contemporary mathematical modelling methodology is the replacement of a real object in question (a process, phenomenon or system) with its "image" – a mathematical model and later – a virtual object (computer-aided realization of the mathematical model). In this way, a major part of the real object's features is obtained when making experiments with the virtual object. This third method of knowledge (forecasting, designing) contains a number of qualities of the first two research methods, i.e. the methods of theory and experiment. Working with the model but not with the real object itself allows us to perform investigation on its features and behaviour in different possible situations inexpensively and sufficiently rapidly (advantages of the theory). In the meantime digital (computer, simulation, imitation) experiments with the models of objects, allow us, on the basis of contemporary digital methods and information technologies, to perform a detailed, deep and sufficiently full investigation into objects, which cannot always be achieved with the help of purely theoretical methods (advantages of the experiment) (Mathematical modelling … 2007; Baltrėnas *et al.* 2006). The mathematical modelling programme REC (Risk Reduction, Environmental Merit and Cost) is based on the comparison of alternative cleaning technologies (to clean contaminated areas). The programme REC is aimed at adapting efficient soil decontamination technologies.

The mixture of grassy vegetation used for modelling consists of perennial ryegrass (*Lolium perenne L.*), meadow-grass (*Poa pratensis L.)* and fescue grass *(Festuca pratensis Huds.)* mixed at a ratio of 8:1:1. These species were selected due to the fact that such plants do not require much care and boast good conditions for growing. Separate species of these plants are most frequently found on Lithuanian roadside soils.

Lolium perenne L. is a species of grass belonging to the *Poaceae* family. It grows up to 15–90 cm high and is an important feeding plant and a perennial.

Poa pratensis L. is a species of grass belonging to the *Poaceae* family. Usually it is a perennial plant, rarely annual. This plant is native to temperate and cool climate zones, and mountains in the tropical zones. The *Poa pratensis L.* grows to 30–90 cm high, its leaves are flat and narrow, and the panicle is up to 20 cm long.

Festuca pratensis Huds. is a perennial plant belonging to the *Poaceae* family. The stem is 50–100 cm high, leaves are flat and 3–5 mm in width with a roughish upside. The plant is resistant to cold weather, mostly found in humid and fertile areas. These species were selected due to the fact that such plants do not require much care and boast good conditions for growing. Separate species of these plants are most frequently found on Lithuanian roadside soils (Jankaitė and Vasarevičius 2007).

The aim of this paper is to analyse the ability of a grassy vegetation mixture to absorb heavy metals from soil and in this way decontaminate it.

2. Formation of the mathematical model to calculate the permeability of metals in plants and soil

REC modelling programme is divided into sections: the input section and the output section. Initial data have to be entered in the input section, and the output section shows data about soil contamination and changing concentrations of contaminants depending upon time.

When forming the calculation model, the following initial data have to be input:

1. Characteristics of a contaminated soil layer (content of organic substances, %; pH; clay content, %; humidity content, %; contaminated soil volume, m^3; depth of aqueous layer, mm; porosity, %).
2. Characteristics of contaminants (the highest concentration of heavy metals, mg/kg; class of hazardousness; soil permeability coefficients, depending on the type of heavy metals (obtained within the programme according to metal).
3. Period selected for modelling change of heavy metals, in years.
4. Characteristics of soil layers of the plants in question (species of sown plants; average depth of roots, mm; average period of plant vegetation, days/years).
5. Meteorological conditions (average winter temperature, °C; average summer temperature, $^{\circ C}$; precipitation per year, mm).

Current soil contamination is evaluated by calculating the load of contaminants:

$$L_j = \rho V_j \left(c_j - s_j\right), \tag{1}$$

here: $L_j - j$ loads of the components of contaminants mixture, mg; V – volume of contaminated soil, m^3; ρ – density of dry soil, kg/m^3.

The total load of contaminants is standardised and summed up when determining a soil quality index:

$$QI = \sum_j \frac{L_j}{\rho \cdot t_j}, \tag{2}$$

here: QI – soil quality index, m^3.

$$t_j = \frac{B_j + Q_{MTR,j}}{2}, \tag{3}$$

here: B – background value, mg/kg; $Q_{MTR,j}$ – MTR (Maximal Tolerable Risk) level, mg/kg.

The soil quality index can be understood as the equivalent of one cubic meter of contaminated soil at the level t.

The access of contaminants from soil to plants is calculated using the method of mass equilibrium.

Total quantity per year (n+1) – total quantity per year (n) = clean-up + plant sorption.
Or:

$$A \cdot d \cdot \rho \cdot \left(Q_{n+1} - Q_n\right) = prec.surpl. \cdot C \cdot A + Q_{plant} \cdot yield_{plant} \cdot A, \tag{4}$$

here: A – area of contaminated surface, m^2; d – depth of contaminated layer, m; ρ – density of dry soil, kg/m^3; Q_n – quantity of contaminants per year n, mg/kg; *prec. surpl.* – precipitation amount, mm; C – contaminant concentration in pores water, mg/l; Q_{plant} – quantity of contaminants in a plant, mg/kg; $yield_{plant}$ – plant yield in the site in question, kg.

Soil density and porosity are calculated according to the functions of transfer showing relationship between the structure and properties of soil. The following formulas are used to calculate soil density and porosity:

$$\rho_{soil} = \frac{2670}{1 + 0{,}0128205 \cdot OM}, \tag{5}$$

$$\theta_{soil} = 0{,}28 + 0.111 \cdot OM^{0{,}35} + 0{,}000395 \cdot clay^2, \tag{6}$$

here: OM – organic substance quantity, mg/kg; $clay$ – clay quantity, mg/kg.

The concentration of contaminants in pore water is calculated using the functions of soil-pores transfer, which represent relationship between contaminant content, soil properties and contaminant concentrations. The following general form of equation is used in the REC model:

$$\log Q_{soil} = n \log C_{porewater} + \alpha + \beta \log OM + \gamma \log clay + \delta \cdot pH. \tag{7}$$

The coefficients *n,* α, β, γ, δ for heavy metals (such as cadmium, copper, lead, nickel and zinc) are recorded in the programme itself. Such coefficients for other metals should be determined experimentally or found in literature.

In the case of organic contaminants, concentration in pore water depends only on the contents of organic substances. In such cases the coefficients have the following values: n, $\beta = 1$; $\gamma, \delta = 0$; $\alpha = \log(Kom/1000)$.

The quantity of contaminants in plants is calculated according to contaminant concentration in pore water instead of contaminant concentration in a solid phase of soil. This is an advantage because changes in soil composition should not be mixed up with the functions, describing the sorption of contaminants to plants. The capacities of plant sorption depend only on plant species but not on soil composition. The applied relationship between concentrations in pores water and plant contents is described by a simple formula:

$$\log Q_{plant} = a + b \cdot \log C\,. \tag{8}$$

The coefficients *a* and *b* were determined experimentally. During these experiments plants were grown in soils with different levels of contamination. After some time the quantities of contaminants in soils with different levels of contamination and in plants were determined. The obtained results (coefficients) were entered into the programme.

Contaminants from the contaminated layer finally access the groundwater. The concentrations of contaminants that reach the groundwater are smaller than concentrations determined in the contaminated soil layer. Leaching to the groundwater is calculated according to the formula:

$$C_{groundwater} = \frac{C_{toplayer}}{R} \cdot \frac{d_1}{d_2}, \tag{9}$$

here: R – retention coefficient; d_1 – depth of contaminated layer, m; d_2 – distance from the contaminated layer to groundwater, m.

The retention factor is determined as follows:

$$R = \frac{Q_{soil} \cdot \rho_{soil} \cdot \left(1 - \Theta_{soil}\right)}{C_{porewater} \cdot \Theta_{soil}}. \tag{10}$$

The concentrations of contaminants obtained experimentally are entered into the model and, therefore, the calculations, using theoretical, i.e. already entered calculation versions of heavy metals transfer to plants and self-cleaning in soil for particular selected metals, are made first of all. Depending on the initial concentration of the applied contaminant and entered results, obtained experimentally, the programme produces the correlation coefficient (Bonten *et al.* 2004). The programme shows that the experimental data being used correlate with the data used, i.e. calculated by the modelling programme. The most exact congruity of the data was noticed when calculating the results of the transfer of copper and lead to plants, while the biggest deviations were obtained when modelling how chromium accesses plants.

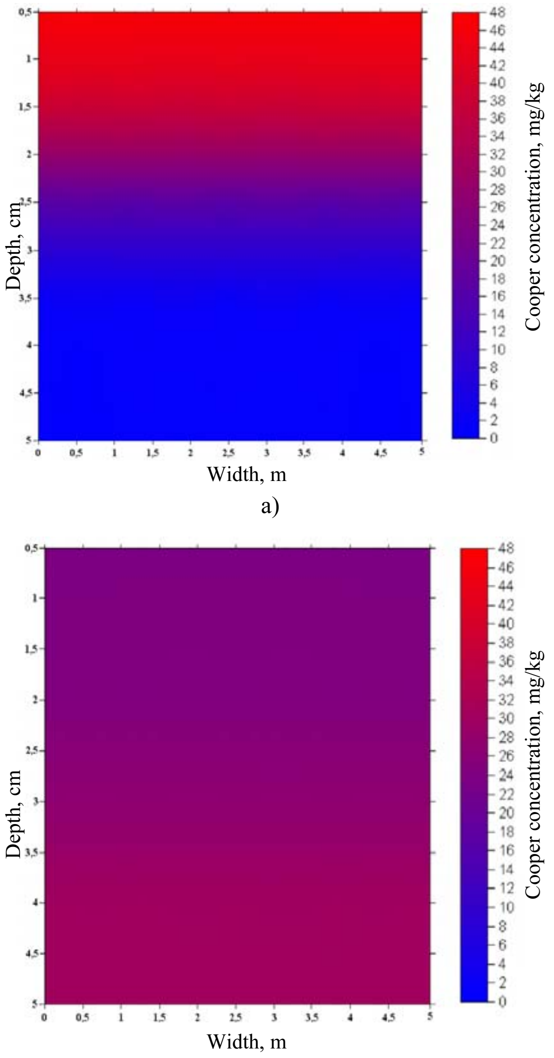
3. Modelling results of how heavy metals access grassy vegetation from the soil

Depending on the modelled contaminant, soil properties and plants applied for soil decontamination, the distribution of heavy metals at depth is being modelled. When calculating the transition of contaminants to plants, the programme does not single out plant roots as a separate layer but upon setting the study layer of 5 cm in the task being modelled, plants (including their roots) are modelled at 1–2 cm, further separating a soil layer being cleaned, also containing roots, i.e. at 3–4 cm, and further the soil, that was not reached by plant roots and where contaminants migrate depending on their nature and soil properties, is being modelled.

During modelling, the initial copper concentration in soil reached 46.5 mg/kg. As Fig. 1a shows, at the time of introducing contaminants, the contamination of soil surface layer is 46.5 mg/kg, but in deeper layers this concentration decreases. Copper concentration starts decreasing at a depth of 2–3 cm, and at a depth of 5 cm from the surface copper concentration is equal to 14 mg/kg. After 6 months from initial soil contamination, copper concentration in the surface layer falls to 28 mg/kg.

This is preconditioned by grassy vegetation applied for soil cleaning and natural processes of migration when contaminants migrate to deeper layers of the soil. Upon setting the task for this programme to show the quantity of copper remaining in soil after one year, it shows that cooper concentration in the surface layer decreases up to 24 mg/kg after a year. The concentration of copper at a depth of 5 cm is 30 mg/kg (Fig. 1b). These results allow us to make an assumption that a part of heavy metals is removed from the soil with the help of grassy vegetation applied, and another part of contaminants naturally migrate to deeper layers.

After setting the task for this programme to show soil clean-up possibilities after 10 years, it shows that, without additional contamination, soil is cleaned from copper to the zero concentration after the mentioned period. As Fig. 2 shows, the soil cleaning process is occurring continuously. After the first year of cleaning the concentration of copper in soil is 17.3 mg/kg, and in grassy vegetation – 26.42 mg/kg. After five years from the beginning of contamination the content of copper after decontamination in soil would reach 9.2 mg/kg, and after further soil decontamination with grassy vegetation the concentration of copper in soil would fall to 5.9 mg/kg. After 10 years the surface layer of soil would be completely cleaned from copper. The obtained results show that when soil is cleaned with grassy vegetation the copper concentration in it decreases and, therefore, we can draw a conclusion that the selected mixture of grassy vegetation may be applied for the removal of copper from soil (Fig. 2).



a)

b)

Fig 1. Copper distribution in soil: a) immediately after the introduction of copper into soil; b) after a year from the beginning of contamination

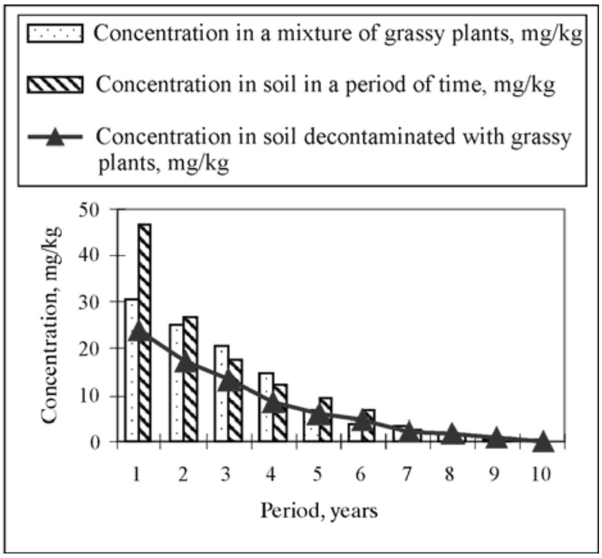
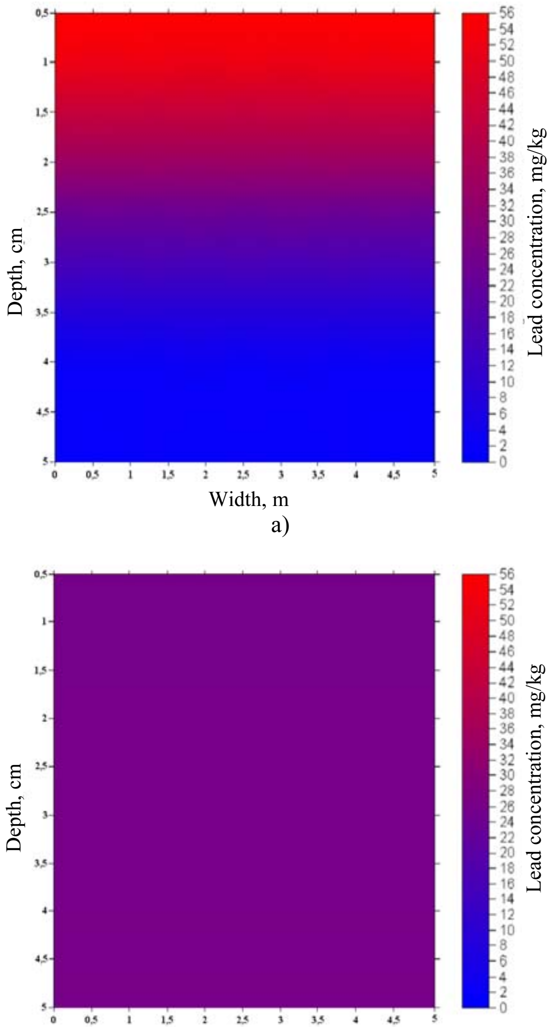


Fig. 2. Soil decontamination from copper in the course of time

The concentration of lead input into the modelling programme was 56 mg/kg. As Fig. 3a shows, immediately after introduction of contaminants into soil, their major part thereof remains in the surface layer. In the layer of 3 cm, the lead concentration is around 26 mg/kg. After 6 months, the lead concentration in the surface layer decreases to 31 mg/kg when grassy vegetation is applied for soil decontamination. After a year, the lead concentration reaches 25 mg/kg on the soil surface (Fig. 3).



a)

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Fig. 3. Lead distribution in soil: a) immediately after the introduction of copper into soil; b) after a year from the beginning of contamination

As Fig. 4 shows, during 10 years the soil is cleaned from lead to its zero concentration if additional contamination is not present. Soil cleaning is a continuous process – if the initial lead concentration in soil is 56 mg/kg, after a year this concentration falls to 25.85 mg/kg. At that time the lead concentration in grassy vegetation would reach 22.05 mg/kg. After 5 years from the beginning of decontamination the lead content in soil would be 5.15 mg/kg. After 10 years, the surface layer of the soil would be completely cleaned from lead. As the results obtained show, when soil is cleaned from lead with the help of grassy vegetation, the lead concentration in it decreases, especially during the first 5 years (Fig. 4).

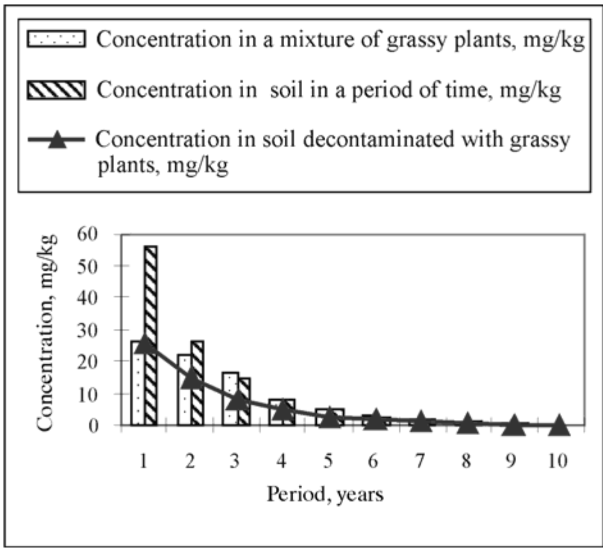
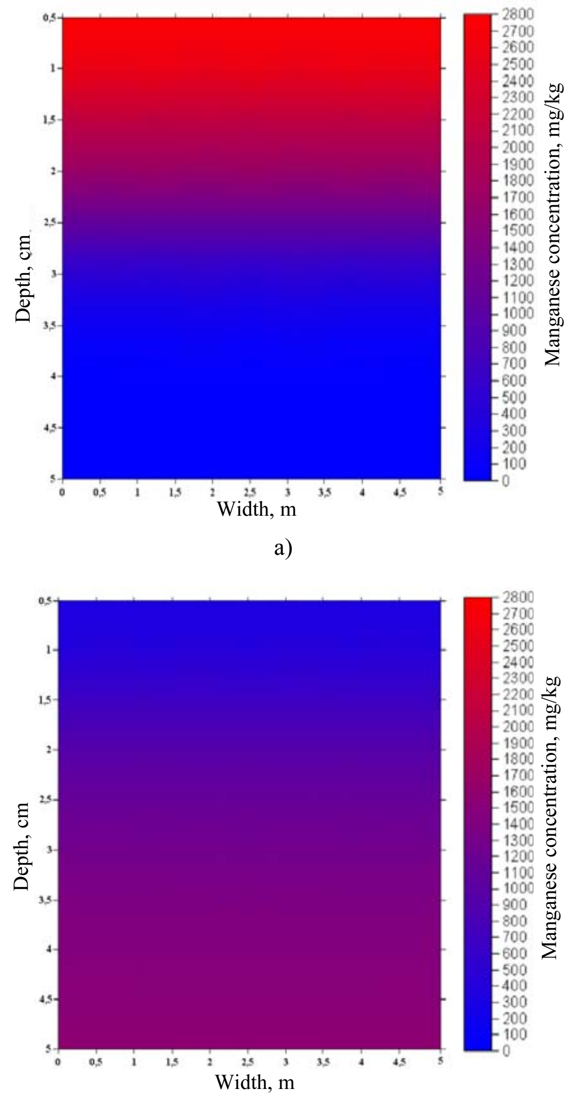


Fig. 4. Soil decontamination from lead in the course of time

The initial concentration of manganese in soil was 2751.5 mg/kg. As Fig. 5a shows, upon introducing the contaminant into soil, the soil contamination with manganese in its surface layer reaches the initial concentration of contamination which decreases in deeper layers. At a depth of 2.5 cm the manganese concentration starts decreasing (around 1800 mg/kg), and at a depth of 5 cm from the surface, the manganese concentration is equal to 150 mg/kg. After 6 months from the initial soil contamination, the manganese concentration in the surface layer falls to 1300 mg/kg. Upon setting the task for the programme to show the quantity of manganese remaining in soil after one year, it shows that that the manganese concentration in the surface layer of soil decreased to 310 mg/kg. At a depth of 5 cm the manganese concentration reaches 1400 mg/kg (Fig. 5).

As Fig. 6 shows, soil, without additional contamination, would be cleaned from manganese to its zero concentration in 10 years. The soil-cleaning process is the most rapid during the first three years – during this period the manganese concentration falls to 11.32 mg/kg when using grassy vegetation for soil decontamination. After three years the concentration in grassy vegetation would be 37 mg/kg. After 4 years from the beginning of contamination the content of manganese in soil is 2.15 mg/kg, and upon cleaning the soil with grassy vegetation for another year, the manganese concentration in soil would not reach even 1 mg/kg. After 8 years, the surface layer of soil would be completely cleaned from manganese. The obtained results show that the concentration of manganese is rapidly decreasing when soil is cleaned with grassy vegetation, and the lower concentration of manganese is in soil, the lower concentrations are in the mixture of grassy vegetation (Fig. 6).



a)

b)

Fig. 5. Manganese distribution in soil: a) immediately after the introduction of copper into soil; b) after a year from the beginning of contamination

The initial concentration of zinc in soil was 176 mg/kg. As Fig. 7 shows, soil contamination with zinc in its surface layer upon introduction of this contaminant reaches the initial concentration of contamination, and going deeper this concentration decreases. At a depth of 2 cm the zinc concentration starts falling, 120 mg/kg, and at a depth of 5 cm from the surface the concentration of zinc is equal to 10 mg/kg. After 6 months from the initial soil contamination, the concentration of zinc in the surface layer falls to 106 mg/kg. Upon setting the task for the programme to show the content of zinc remaining in soil after one year, it shows that after a year the zinc concentration in the surface layer of soil decreases to 95 mg/kg. At a depth of 5 cm the concentration of zinc is equal to 100 mg/kg (Fig. 7).

As Fig. 8 shows, if no additional contamination is present, soil would be cleaned from zinc to its zero concentration in 10 years. The soil-cleaning process is the most rapid during the first four years – the concentration

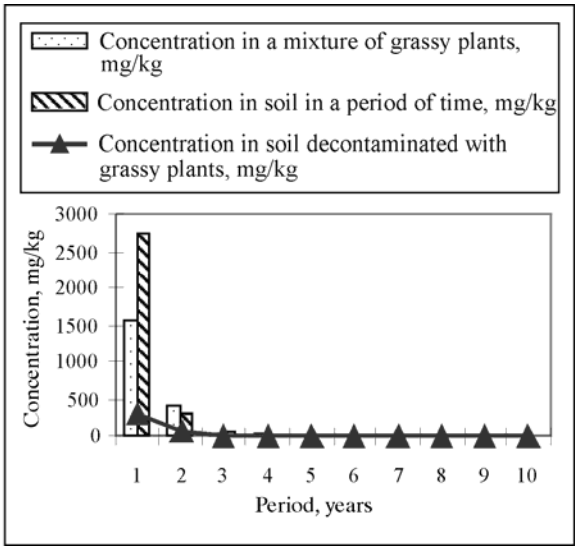
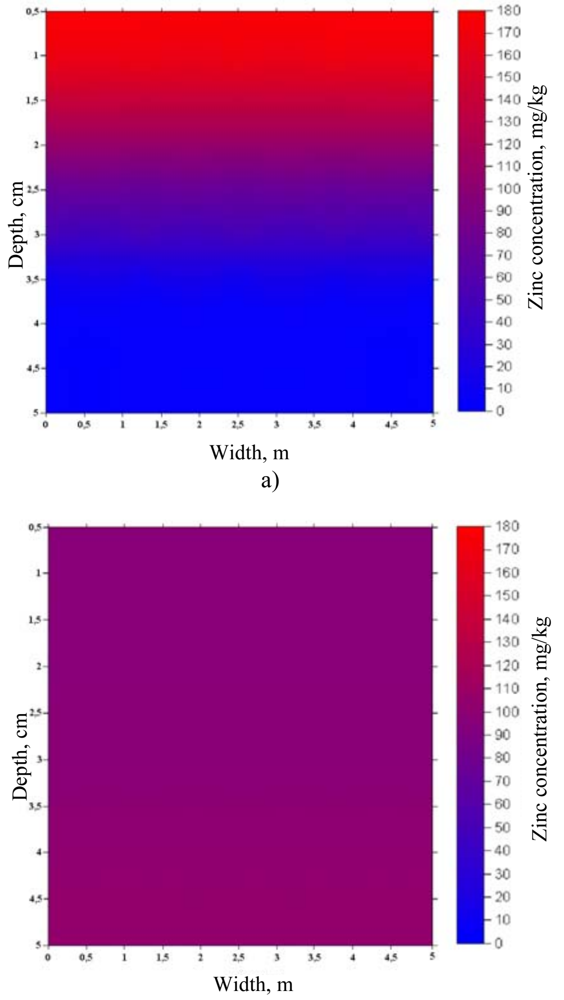


Fig. 6. Soil decontamination from manganese in the course of time



a)

b)

Fig. 7. Zinc distribution in soil: a) immediately after the introduction of copper into soil; b) after a year from the beginning of contamination

of zinc in this period decreases to 11.95 mg/kg when grassy vegetation is used for decontamination. After four years the concentration in grassy vegetation would reach 12.03 mg/kg. After 8 years from the beginning of contamination, the content of zinc in soil would be 2 mg/kg, and upon further cleaning of soil with grassy vegetation for another year, the concentration of zinc in soil is nearly equal to zero. After 10 years, the surface layer of soil would be completely cleaned from zinc. When cleaning soil with grassy vegetation, the concentration of zinc decreases in both the soil and the mixture of grassy vegetation (Fig. 8).

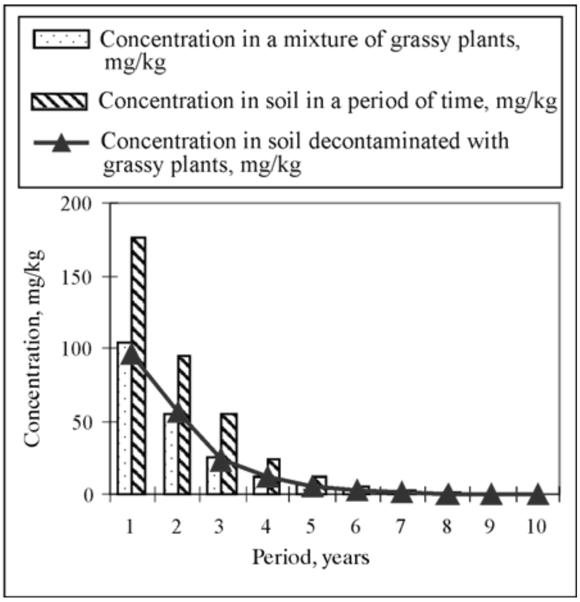


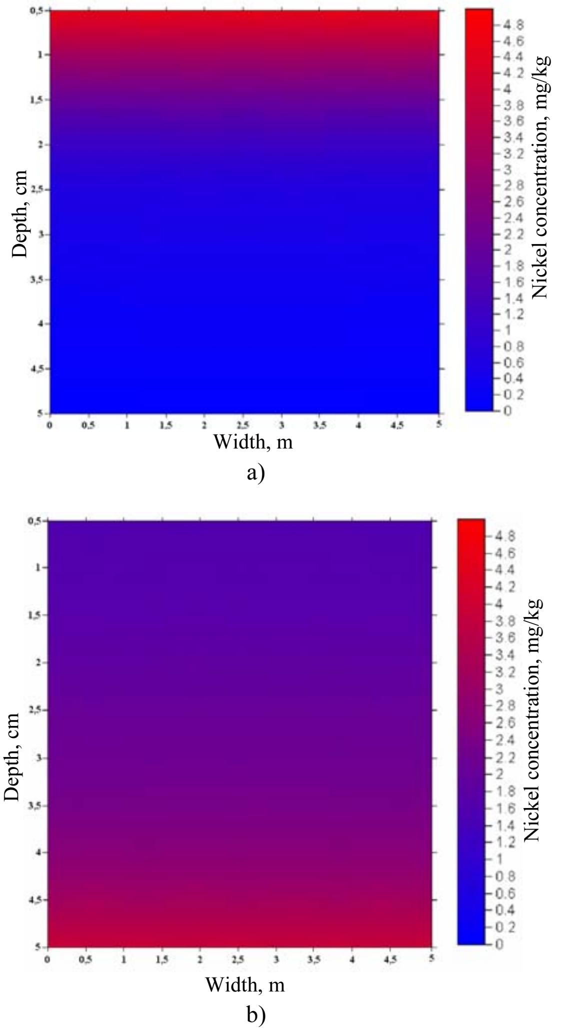
Fig. 8. Soil decontamination from zinc in the course of time

The initially input concentration of nickel in soil was 4.65 mg/kg. As Fig. 9 shows, soil contamination by nickel in its surface layer, at the time of the contaminant introduction, reaches the initial concentration of contamination and going deeper this concentration decreases. At a depth of 3 cm, the concentration of nickel falls to 1.8 mg/kg. At a depth of 5 cm from the surface the nickel concentration is equal to 0.4 mg/kg. After 6 months from the initial soil contamination, the concentration of nickel in the surface layer falls to 2.6 mg/kg. Upon setting the task for the programme to show the content of nickel remaining in soil after one year, it shows that after a year the nickel concentration in soil decreases to 1.6 mg/kg in the surface layer. At a depth of 5 cm the concentration of nickel reaches 3.3 mg/kg (Fig. 9).

As Fig. 10 shows, if no additional contamination is present, in 10 years soil would be cleaned from nickel to its zero concentration. Soil cleaning is a continuous process – if the initial nickel concentration in soil is 4.65 mg/kg, after a year this concentration falls to 1.6 mg/kg, and the concentration of nickel in soil cleaned with the help of grassy vegetation is 1.8 mg/kg. Presently, the nickel concentration in grassy vegetation would reach

3.56 mg/kg. After 5 years from the beginning of contamination, the content of nickel in soil would reach 0.48 mg/kg, and the nickel concentration in grassy vegetation in soil would be 1.12 mg/kg. After 8 years, the surface layer of soil would be completely cleaned from nickel. As the obtained results show, when soil is cleaned with the help of grassy vegetation, the concentration of nickel in soil decreases, in particular during the first 5 years (Fig. 10).

The initial concentration of chromium in soil was 79.5 mg/kg. As Fig. 11 shows, immediately after introduction of the contaminant, soil contamination in its surface layer was the same, i.e. 79.5 mg/kg, and was decreasing in deeper layers. At a depth of 2.5 cm, the chromium concentration starts significantly falling (35 mg/kg), and the depth of 5 cm from the surface, the concentration of chromium is equal to 5 mg/kg. After 6 months from the initial contamination of soil, the chromium concentration in the surface layer decreases to 25 mg/kg. This is preconditioned by the use of grassy vegetation for soil decontamination and natural processes of migration when contaminants migrate to deeper layers of soil. Upon setting the task for the



a)

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Fig. 9. Nickel distribution in soil: a) immediately after the introduction of copper into soil; b) after a year from the beginning of contamination

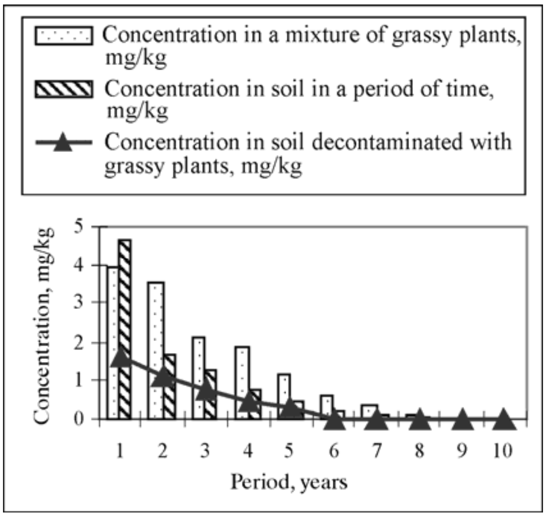
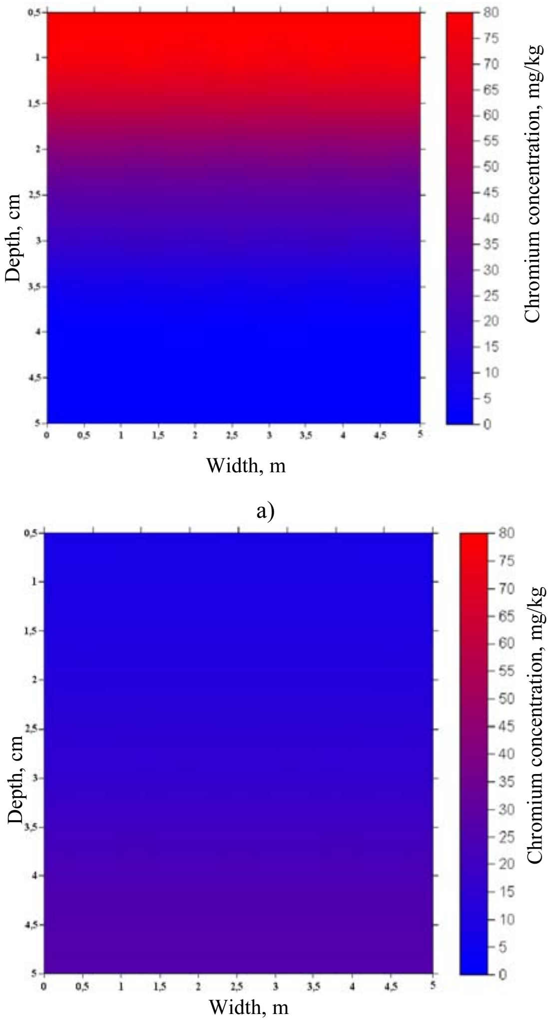


Fig. 10. Soil decontamination from nickel in the course of time



a)

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Fig. 11. Chromium distribution in soil: a) immediately after the introduction of copper into soil; b) after a year from the beginning of contamination

programme to show the content of chromium remaining in soil after one year, it shows that the concentration of this metal in soil after one year falls to 10 mg/kg in the surface layer. At a depth of 5 cm, the concentration of chromium was 26 mg/kg. These results allow us to make an assumption that a part of heavy metals is removed from soil by grassy vegetation, and another part naturally migrate to deeper layers (Fig. 11).

As Fig. 12 shows, at the absence of additional contamination, the soil would be cleaned from chromium to its zero concentration in 10 years. Soil cleaning is a continuous process – if the initial chromium concentration in soil is 79.5 mg/kg, after a year this concentration falls to 10 mg/kg. Presently, the chromium concentration in grassy vegetation would be 6.52 mg/kg. After 5 years from the initial contamination, the chromium concentration in soil would reach 0.06 mg/kg. After 6 years, the surface layer of soil would be completely cleaned from chromium. The obtained results show that when soil is decontaminated by grassy vegetation the chromium concentration in it decreases, in particular during the first 3 years (Fig. 12).

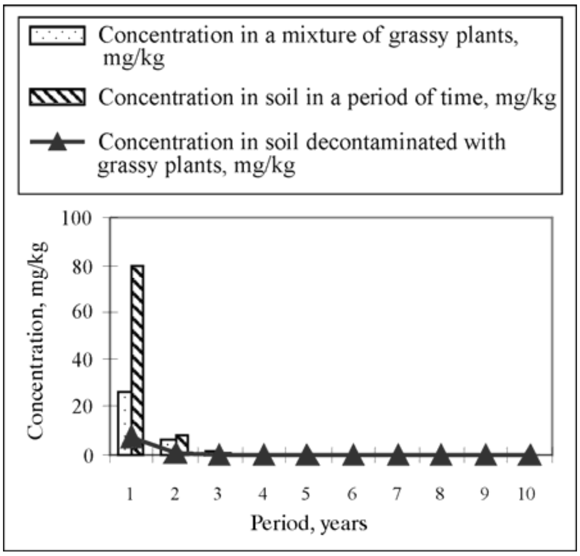

Fig. 12. Soil decontamination from chromium in the course of time

On the basis of the obtained results of modelling, it can be stated that soil remediation by using the mixture of grassy vegetation is a sufficiently efficient solution. When using this mixture of grassy vegetation and at the absence of additional contamination, the soil would be cleaned from copper and lead to their zero concentrations in 10 years, from manganese – in 8 years, from zinc – in 9 years, nickel – 6 years, and chromium – 7 years.

4. Conclusions

1. The mixture of grassy vegetation used for modelling consists of perennial ryegrass (*Lolium perenne L.*), meadow-grass (*Poa pratensis L.)* and fescue grass *(Festuca pratensis Huds.)* mixed at a ratio of 8:1:1.

2. According to the obtained results of the performed mathematical modelling of soil remediation with regard to heavy metals, it can be stated that the remediation of soil using the mixture of grassy vegetation to decontaminate the soil from heavy metals is a productive and efficient solution.

3. The results obtained with the program of mathematical modelling REC show that when the method of phytoremediation is applied, 10 years, i.e. the entire period analysed, would be necessary to clean soil from copper and lead to the lowest concentrations.

4. Manganese is totally removed from soil after 8 years, while zinc is removed after 9 years when soil is cleaned with the mixture of grassy plants and is not additionally contaminated.

5. Nickel is a metal which is removed from soil in the shortest period, i.e. in 6 years. The concentration of chromium in soil reaches zero after 7 years.

Acknowledgements

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SUNKIŲJŲ METALŲ VALYMAS IŠ DIRVOŽEMIO REMIANTIS MATEMATINIAIS MODELIAIS

A. Jankaitė

Santrauka

Matematinio modeliavimo metodologijos esmė yra tiriamo realaus objekto (proceso, reiškinio, sistemos) pakeitimas jo „atvaizdu“ – matematiniu modeliu. Matematinio modeliavimo programa *REC* (angl. *Risk reduction, Environmental merit and Cost*) pagrįsta alternatyvių valymo technologijų (užterštam plotui valyti) lyginimu. Programos *REC* tikslas – pritaikyti efektyvias ir veiksmingas dirvožemio valymo technologijas. Šio darbo tikslas – išanalizuoti žolinės augalijos mišinio gebą sorbuoti sunkiuosius metalus iš dirvožemio ir tokiu būdu valyti iš jo teršalus. Programoje nusistatomos pradinės sunkiųjų metalų (vario, švino, mangano, cinko, nikelio ir chromo) koncentracijos, eksperimentų metu naudotos tiriant dirvožemio kokybės atkūrimo žolinės augalijos mišiniu efektyvumą. Iš esmės per visą pasirinktą laikotarpį – 10 metų iš dirvožemio būtų valomas varis ir švinas. Mangano nulinė koncentracija dirvožemyje, valant jį žolinės augalijos mišiniu ir nesant papildomo teršimo, pasiekiama po 8 metų, cinko – po 9 metų. Greičiausiai iš dirvožemio išvalomas nikelis – per 6 metus. Chromas, esant 79,5 mg/kg pradinei jo koncentracijai dirvožemyje, iki nulinės koncentracijos būtų išvalytas per 7 metus.

Reikšminiai žodžiai: sunkieji metalai, dirvožemio atkūrimas, *Lolium perenne L., Poa pratensis L., Festuca pratensis Huds*, matematinis modeliavimas.

ОЧИЩЕНИЕ ПОЧВЫ ОТ ТЯЖЕЛЫХ МЕТАЛЛОВ С ПРИМЕНЕНИЕМ МАТЕМАТИЧЕСКОГО МОДЕЛИРОВАНИЯ

А. Янкайте

Резюме

Суть методологии математического моделирования заключается в замене исследуемого реального объекта (процесса, явления, системы) его отображением – математической моделью. Программа математического моделирования *REC* (англ. *Risk reduction, Environmental merit and Cost*) основана на сравнении альтернативных технологий по очищению загрязненных территорий. Целью программы *REC* является приспособление эффективных и действенных технологий для очищения почв, а целью настоящей работы – анализ способности смеси из травянистых растений сорбировать тяжелые металлы из почвы и таким образом способствовать ее очищению от загрязнителей. По программе задаются начальные концентрации тяжелых металлов (меди, свинца, марганца, цинка, никеля и хрома), применявшиеся во время экспериментальных исследований эффективности восстановления качества почв благодаря применению смеси из травянистых растений. Практически за весь установленный промежуток времени – 10 лет – почвы будут очищены от меди и свинца. При очищении почв с помощью смеси травянистых растений и при отсутствии дополнительного загрязнения нулевая концентрация марганца достигается спустя 8 лет, цинка – 9 лет. От никеля почва очищается спустя 6 лет, а от хрома при начальной его концентрации в почве, равной 79,5 мг/кг, спустя 7 лет.

Ключевые слова: тяжелые металлы, восстановление почвы, *Lolium perenne L., Poa pratensis L., Festuca pratensis Huds*, математическое моделирование.

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