Long-term assessment, modeling and forecast of salinity conditions of reclaimed mine dumps of Western Donbass

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Abstract. The neutralization of toxic mine rocks with additional of soil and loess like loam mass leads to a significant decreasing of salts migration at the contact zone. The mathematical model was working out follow general principle where mine rock is pollution source, but soil and loess like loam take place as volumetric filter for water-soluble salts. MathCAD file with commands for solving the problem forecasting the process of vertical salinization of reclaimed minelands was developed. The prospect for the numerical model using up to the most accepted range of values with experimental data shown. The irrigation of reclaimed minelands in the Western Donbass possible in the case of the dilution of the mine waters of aquifers with the Samara river water.

1 Introduction

Rainfall, evaporation, rock weathering, saltwater intrusion, or chemical contamination can cause the salt source for soil salinization in abandoned and reclaimed minelands [1]. Modelling is a suitable alternative technique that saves time and cost for the environment monitoring [2]. Meantime the performance of the models should base on long-term monitoring data. The fate of chemical substances in the soil is complex and dynamic, depending on such factors as clay level, soil pH, hydraulic conductivity, structure, and many others [3]. From the general convection-dispersion function describing solute transport in porous media, several numerical and analytical models have evolved [4, 5]. These include the finite difference approaches. HYDRUS, SALTMOD, PESTFADE, UNSATCHEM, SODIC and SWAP have been widely used as seasonal models to consider the interaction between soil-water and water-soluble salts [6-8]. HYDRUS-2D demonstrates the relevance of numerical modelling in evaluating the water and salt dynamics under drip irrigated horticultural trees [9]. DRAINMOD-S was useful either for the design of a new drainage system and long-term impacts assessment on the groundwater table and soil salinity [10]. All hydrogeological processes: filtration, mass transfer and moisture transfer are those that have a limit and steady state. Pessimistic options have prospects. They calculate theoretically and prevent in advance [11]. Field experiments established 30-40 years ago in reclamation stations in areas affected by mine works require additional research to justify the choice of a mitigation technology or rock deposits replacement in a way that would guarantee the least negative consequences for the environment. It is necessary to introduce a procedure of environmental impact assessment (EIA) for the recommended technologies of reclamation of disturbed lands [12]. The EIA methodology involves the identification of impacts, the choice of mitigation technology, following modeling and forecasting its positive effect.The main objective of our research was to substantiate decisions to create favorable ecological and reclamation conditions on reclaimed mine dumps in the Western Donbass.

2 Materials and methods

The data on salinization of two land reclamation profiles in 1987, 1995, 2003, 2008 and 2018 obtained in the conditions of the Pavlograd experimental station of the DSAEU. The station founded in 1976 in the floodplain of the Samara River in order to examine the best restoration measures. Typical abandoned site shown in the figure 1.

Other example connected with intention to create dachas for mining workers in Pavlogradsky district just in reclaimed minelands (Fig.2). The scheme for reclamation of disturbed land based on the study of the effectiveness of capping the mine dumps with different layers of black-soil mass (chernozem) both with and without a shielding layer of loess - like loam. The following models of artificial land reclamation profiles were used to look into the peculiarity of upward migration of toxic salts from the mine dumps: 1 Mine rock (MR) + 50 cm of the top black soil (50BS); 2. MR + 50 cm of the loess-like loam (50LLL) + 50BS. Soil and rock samples taken along both

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profiles, mixed thoroughly, air-dried and sieved through a 2-mm diameter stainless steel screen.

Fig. 1. Abandoned mining site in Western Donbass.

Fig. 2. Small dacha in reclaimed minelands in Western Donbass.

Soil pH and EC measured using a soil-to-water ratio of 1:1. pH and EC distribution in two land reclamation profiles are shown in fig 3.

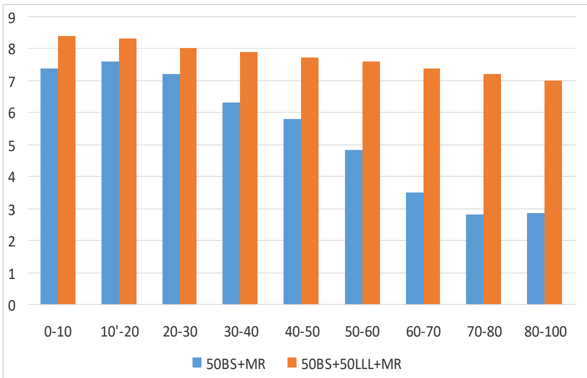


Fig. 3. pH distribution in two artificial profiles.

The differences in pH and EC profile distribution between two profiles demonstrate the negative impact of underlying toxic mining rocks caused with weathering in space and time. The applied model of the moisture-salt transfer process based on the theory of physicochemical hydrodynamics of porous soils. Mass transfer processes are described by differential equations of motion and conservation of matter mass of the second order in partial derivatives of elliptic and parabolic types according to this theory. One - dimensional versions of these equations used for solving practical problems. This process describe by the equation of movement and of mass of matter mass keeping:

$$D\frac{\partial^2 c}{\partial x^2} - V\frac{\partial c}{\partial x} = m_0\frac{\partial c}{\partial t}, \qquad (1)$$

where C – soil salinity, %; D – hydrodispersion coefficient; x – spatial coordinate; t – time; V – infiltration rate, m/day; m_0 – topsoil moisture, %. This is due to the fact of the salt transfer in the aeration zone takes place mainly in the vertical direction.

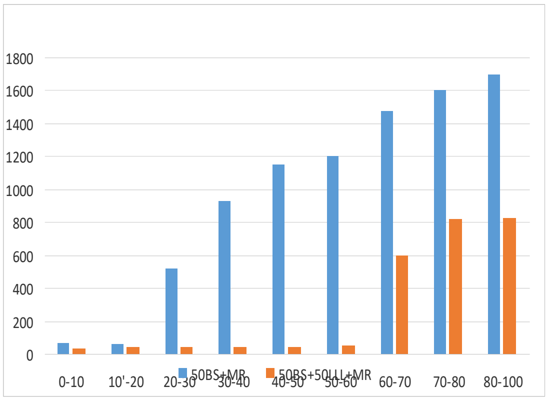
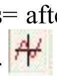


Fig. 4. EC distribution in two artificial profiles, units.

A special MathCAD file created to predict the process of vertical salinization of the topsoil. Commands to solve the simulation problem to this file written. It is enough to substitute the original data into this file. The program itself will calculate the result. Constants and procedures are on the first two sheets of the MathCAD document. They changed under the conditions of introduction of new initial parameters. It is necessary to indicate the depth of the artificial soil profile, modeling time, step in space and time correctly. The operator: = to set the value of the variable used. The name of the variable to the left of it written. Variable value: *upper_border:*=0 and *lower_border*:= 1 is written on the right. Sign (dot) used to separate integer and fractional part in number. Variables *upper_border* and *lower_border* used to establish border boundaries. Value *upper_border* always set to zero. The dimensions along plot are in meters. Variable *dx* used to change the size of the soil layer. The size of the soil layer is set as 10 cm in the section of global constants. This value changed as follows: *dx: =0.1* when the size of the reclamation layer differs. The variable *t* to change the simulation time used. Simulation time in days is measured. The number of year's t: = translated into the number of days. The number of simulation steps (periods into which the simulation time is divided) must also be set. The number of steps from 10 to 16 recommended. It is possible to use other values as well. The variable steps: = 32 used to set the number of steps. The variable *n* used to find the number of steps in space. It calculated automatically by the command:

$$n := \frac{(lower\_border - upper\_border)}{dx}.$$

 https://doi.org/10.1051/e3sconf/202128006007

This command can not be deleted. The most important step in future modeling is to enter the initial salinity values. The character C denotes salinity. It inserted in a slightly different way than all other data since salinity is not one value. Character *C* selected in toolbar in the menu after entering C: = Item "Insert - Matrix". It is necessary to select the number of horizontal and vertical values in the window that appears. The number of values horizontally is always set to 1. A step plus one vertically should indicate the height of the soil profile. A blank for entering salinity data of the soil profile will appear on the screen. The results are displayed on the screen using the command res= after that. Name *res* used in the previous command (or  - on the toolbar) used to construct the surface of the results Command "Insert - Graph – Surface Plot". 3D a surface with three coordinates (y (*C*) is the salinity of the soil, z (t) is time, x is the spatial coordinate, dm) appears on the screen.

3 Results

The choice of measure to neutralize potentially toxic rocks related to the ratio of precipitation and evaporation at each site. Evaporation is a negative component of the water balance. Evaporation involves a complex water vapor between the ground surface and the atmosphere. Its value depends on the depth of groundwater, lithological composition of the rocks, vegetation cover and complex climatic factors. The maximum evaporation for the Dnipropetrovsk province is 800 – 820mm [13]. The ratio between precipitation and evaporation is 0.5. The rate of vertical moisture - salt transfer preliminarily estimated by the balance method according to the formula (2):

$$\boldsymbol{V} = \frac{\boldsymbol{P-(E-W)}}{\boldsymbol{1000T}}, \quad (2)$$

where P - precipitation, mm, E – evaporation rate, mm, W – water accumulation (moisture removal with plant biomass), T – grass vegetation period, days. The coefficient of water consumption (W) varied depending on the type of plant – from 450 to 550 m^3/t. In subsequent calculations, the formula used to calculate the hydrodispersion coefficient (3):

$$D = V \cdot \frac{x}{2 \cdot ln\left(\frac{C_2}{C_1}\right)}, \quad (3)$$

where V – velocity of vertical moisture transfer, m/day; C_2 – salinity at a point with the coordinate of the mine dump (x, m), C_1 – mineralization depending on the surface of the dump. The mathematical model was refined in the second stage by solving multivariate forecast problems to the best coincidence of the calculated values with the experimental data. The use of such an approach in the mathematical model of vertical salt transfer along profile of the dump of mine rocks allowed taking into account the surface runoff. Equation (1) proved for this to the form of boundary differences:

$$D\left(\frac{C_{i+1}^{\tau+1} - 2C_i^{\tau+1} + C_{i-1}^{\tau+1}}{(\Delta x)^2}\right) - V\frac{C_{i+1}^{\tau+1} - C_i^{\tau}}{\Delta x} = m\frac{C_i^{\tau+1} - C_i^{\tau}}{\Delta t} \quad (4)$$

where τ – time grid point number; i – spatial grid point number. The boundary condition of the 3rd kind Dankwerts - Brenner [14] was given at the upper bound:

$$[C(0,t) - C_n] \cdot V = D\frac{\partial C(0,t)}{\partial x} \quad (5)$$

Boundary condition of the 1st kind (C_0 = const) was set at the lower limit. Consider more carefully the boundary condition at the upper bound. Write the formula (5) in another form:

$$(V_2 - V_1)(C_n - C_0) = D\frac{\partial C}{\partial x} \quad (6)$$

After giving the equation in the form of finite differences and opening the brackets in the left part of the formula we get the following formula:

$$V_2C_n - V_2C_0 - V_1C_n - V_1C_0 = D\frac{C_0 - C_1}{\Delta x}. \quad (7)$$

We proceeded from the position that the third component in the left part was equal to zero, because the evaporation of salts from the soil surface under natural conditions does not occur. The boundary condition in this case takes the following form:

$$DC_0 + \Delta x V_2 C_0 + \Delta x \cdot V_1 \cdot C_0 = D \cdot C_1 + \Delta x \cdot V_2 \cdot C_n, (8)$$

where V_1 – ascending flow rate of the substance, m / day;
V_2 –downward flow rate of the substance, m / day;
C_p –mineralization of precipitation, %
C_0 –salinity on the top soil, %;
Δx –step along the spatial coordinate, m

The vertical transfer rate was calculated as the speed difference V_2-V_1 taking in account that this boundary pre-condition is used. The salinity forecast scenarios was made for the two- and three layers reclamation profiles during a period of three decades (Fig. 5 and 6).

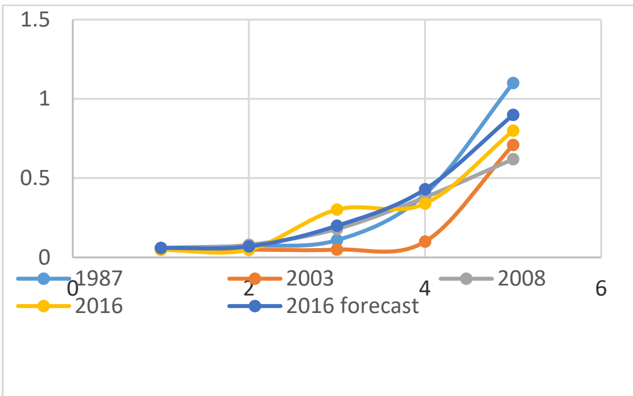


Fig. 5. Estimation and forecast of salinization of the two-layers profiles, %.

The results of the forecasts for one of the two recommended reclamation profiles are in good agreement with the data of experimental observations for 1987, 2003, 2008 and 2016. The analysis of changes in the content of water-soluble salts at the contact of the lower layer of the soil with the mine rock in the trial MR + 50cm Black Soil indicates a slow decrease in the soil mineralization. The tendency of slow increase in salinization of the upper soil layers of the artificial reclaimed profile is recorded. At the same time, the comparison of soil salinization data in the options MR + 50cm Black soil and MR+ 50 cm Loess Like Loam + 50 cm Black Soil testifies in favor of the three - layer reclamation profile. The same conclusion made after trend analyse analysis of water-soluble salts vertical migration in technogenic edaphotops of reclaimed mine dumps [15].

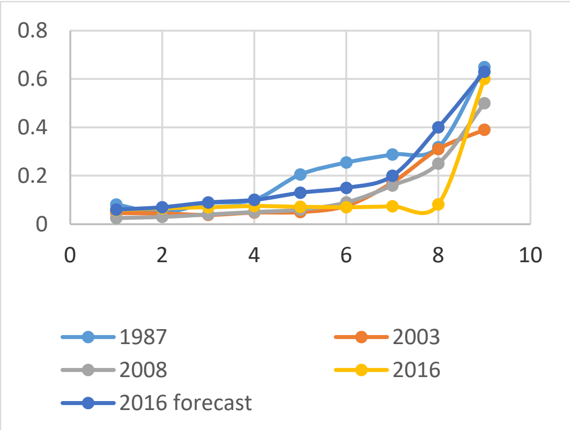


Fig. 6. Estimation and forecast of salinization of the three layers profiles, %.

It is obviously also that there is a certain pattern of growth of the content of soluble salts in the layers in the chernozem, which was dumped on the mine rock, approaching the mine rock. The topsoil looks like a volumetric filter of soluble salts migrating from the lower layer of mine rock. Thus, the salt concentration on the surface will be lower the larger the soil layer. This observation led to the theoretical assumption that the mine rock is a source of salinization, and black soil as volumetric filter for salts migration and absorption by the soil. Therefore, the obtained experimental data allowed building a mathematical model of the generalized dependence of the content of soluble salts in the layer of black soil of different heights, poured on top of the mine rock. The database grouped by the distance of a certain layer, starting from the mine rock, and the corresponding values are plotted on a scatter plot (Fig.7).

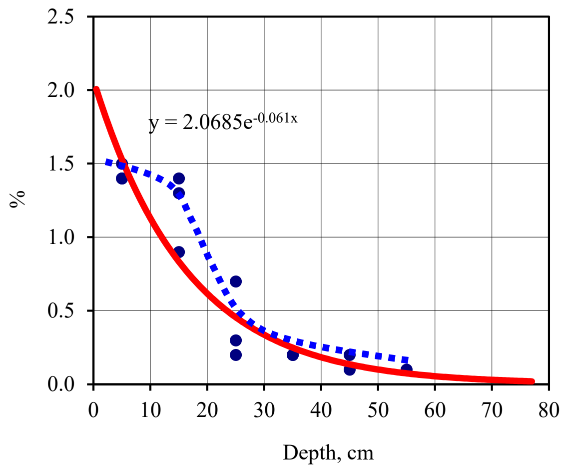


Fig. 7. Dependence of the content of soluble salts on the thickness of the soil layer.

The trend in the form of an exponent represent by a solid line. The possible real dependence presented by a dotted line. The smoothing of the discrete series of values performed by the exponent described above-mentioned assumption. Quantitatively, the molecular diffusion of substances described by first and second laws of the Fick. Under the above conditions, the differential equation of mass transfer of pollutants looks like the equation of diffusion of matter everywhere per unit area (Fick's first law):

$$j = -D\frac{dC}{dx}, \text{ mg/cm}^2, \quad (9)$$

where C is the mass concentration of the flow of the transferred substance through the selected plane, mg / m^3; x is the current coordinate in the direction of flow, m; D is the diffusion coefficient, m^2 / s.

Therefore, according to the law of diffusion, the salts drift into the region with a lower concentration. This process written in the form of an equation for a steady state in the soil in which there is no time factor, namely:

$$\frac{dC}{dl} = -k \cdot C, \quad (10)$$

where C is the concentration of the migrating substance, mg / m^3 or%; l is the thickness of the layer of loose soil), m (cm); k is the filtration coefficient of dissolved salts in the soil, m^{-1}. Analytical solution of equation (10) with initial conditions, for (salt concentration at the boundary of the soil with the mine rock) has a general form

$$C = C_0\, exp(-k \cdot l). \quad (11)$$

Since the nature of salt migration influenced by various factors, the real dependence of the salt content describe by a second-order differential filtration equation. For practical conditions, in our opinion, it is sufficient to apply a simplified version of the exponential dependence, which represent in an approximate normalized form (12):

$$C = C_0\, exp(-0{,}05 \cdot l), \quad (12)$$

where l - the salt content in the topsoil adjacent to the surface of the mine dump or at a depth selected for the initial level of reference in the soil, %. According to the properties of the exponent, a decrease in the salinity of chernozem in *e* times, ie 2.7 times, will be observed at a layer thickness of 20 cm. Almost zero concentration will decrease at a layer thickness of black soil at (3-4) 1 / k , i.e. 3-4 times larger, namely - 60-80 cm.

Verification of this model and its subsequent identification for chernozem was performed three times on the basis of experimental data obtained in the Pavlograd reclamation hospital every eight years. The results of the distribution of salt content in soil samples taken in the reclaimed profiles of the two-layer variant are presented in Figure 8.

As we can see, the content of soluble salts in chernozem depends not only on the soil layer, but also on the period from the beginning of reclamation. In this case, over time, there is an increase in the maximum concentration of salts (curve 2 in Fig. 8), coming from the lower layers of the rock to the chernozem, and then, over the years - a gradual decrease (curve 3).

The calculations showed that in real conditions, when the mode and duration of salinization are unknown, it is possible to use a model that takes into account all available experimental data.

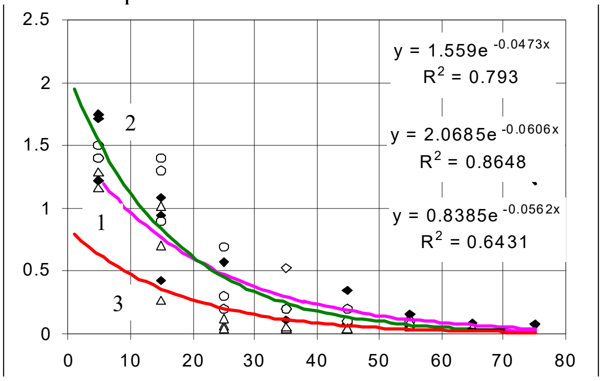


Fig. 8. Profile distribution of salt content (y,%) depending on the thickness of the layer (x, cm) of black soil.

This dependence represented in the form (11), where the coefficient k is approximately in the range of 0.05-0.06 m – 1, and the value will depend on the level of the initial salt concentration in the rock. The introduction of a 50 cm layer of loess-like loam in the option 50BS + 50LLL + MR led to a significant decreasing of the chemical weathering process of underlying mining rocks (Fig. 9).

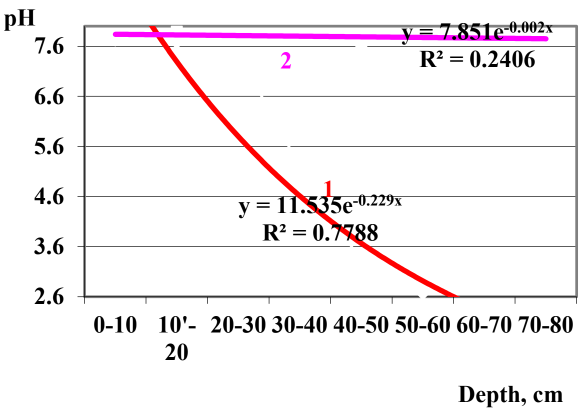


Fig. 9. Modeling of pH distribution along two land reclamation profiles: 1-50BS+MR; 2-50BS+50LLL+MR.

Therefore, pH stabilization in the trial 50BS + 50LLL + MR is possible in the range of 7.6-7.7. Estimation of quality of waste mine waters of the Western Donbass has shown that a certain part of weakly mineralized waters can be suitable for irrigation under conditions of dilution of mine water of artificial ponds by water of the Samara river (Fig. 10).

The results of the calculation of salt migration for the trial with dilution shown in Fig. 11.

The forecast of the salt regime of the reclaimed mine dump with systematic irrigation in the option with water dilution of the irrigation source up to 1.6 g / dm^3 was performed for a period of 5, 10, 20 years in the steady state for the initial salinity of 0.6 and 0.8%. The process characterized by a constant content of salts of the topsoil with slow salinization of the upper part of the mine rock heap. The calculation of the required amount of gypsum as an ameliorant performed by the formula:

$$R = E \cdot \left[Ca^{++} - C^{++}{}_f\right] \cdot N, \ldots \qquad (13)$$

where R – ameliorant dose, t / ha; E – the equivalent of ameliorant, which is equal to 1 mg - eq Ca^{++}; Ca^{++}– the amount of Ca, which is equal to 43.4mg-eqv/dm^3; N – irrigation rate, thousand m^3 / ha. The dose of gypsum for case study of the Samara river as a source for topsoil irrigation is following:

$$R = E \cdot \left[Ca^{++} - C^{++}{}_f\right] \cdot N =$$
$$8.6 \cdot [16.6 - 11.1)] \cdot 1000 = 0.5\,ton / ha$$

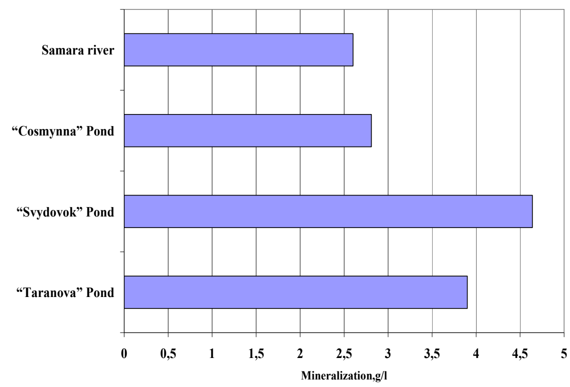


Fig. 10. Water mineralization in river and mine ponds.

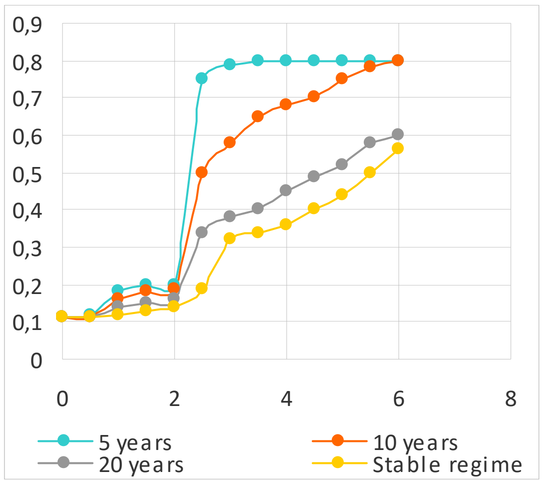


Fig. 11. Dynamics of salt transfer on a reclaimed mine dump with irrigation, %.

The implementation of the environmental protection measures recommended for production took place as follows. On the one hand, some reclaimed territories transferred to the balance of private farms in Pavlograd district. At the same time, a certain share of reclaimed areas given to several horticultural societies with a total area of more than 100 hectares. All of them are located in the floodplain of the Samara River.

The calculations proved that in any case of reclaimed mine dump salinization of the top soil is inevitable. It is necessary to create a flushing mode to prevent it. Irrigation carried out with the minimum norms.

4 Discussion

The main problem in identifying the optimal scheme of land reclamation in the coal mining regions is the prevention man-made pollution of artificial landscapes [16, 17]. Given the trend of transition from land use as arable land to the state of natural meadows, the latter type of nature management of reclaimed land in the Western Donbass seems less risky for the development of soils vertical salinization.

The solution of the migration problem for reclaimed mine dumps in the steady state with the maximum values of the initial salinity of dump rocks (0.8-1.0%) should be considered as an extreme negative option, leading to intensive accumulation of salts in the soil.

Analysis of vertical migration of salts with the depth of the reclaimed profile showed that none of the options with a top layer of chernozem 30, 50 and 70 cm did not provide complete stabilization of the distribution of pH and water-soluble salts. Predictive calculations based on the theory of migration proved the possibility of salinization of the topsoil without irrigation due to the pulling of salts by the upward flow of moisture.

Therefore, stable and favorable ecological and reclamation conditions created with the use of systematic irrigation. Three types of irrigation regimes used in different natural and climatic zones of Ukraine: compensatory, evaporating and washing [11]. Conditions for the application of compensation and evaporation regimes are more typical for the Central Donbass, where mine rocks are not saline.

The flushing regime of irrigation of reclaimed dumps is more suitable, as they are everywhere to varying degrees saline. Irrigation by brackish water is a possible solution to alleviate freshwater shortages [18]. The simulated results were helpful to provide a basis for assessing the environmental effect under long-term brackish water irrigation.

During long term, salts leaching under the effects of rainfall can contaminate groundwater [19-20]. On the other hand, the salinization phenomenon in the topsoil can be cyclic, and the effect of salinity on crops attenuated with proper management that involves appropriate irrigation for salt leaching [21-23]. This risk reduces in the case of special irrigation strategy. This requires lower irrigation doses and the use of a drip irrigation system associated with proper management practices such as increasing irrigation frequency.

5 Conclusion

Slow salinization of the topsoil described for the three-layer reclamation profile. The introduction of a carbonate-containing layer of loess like loam is a reliable geochemical barrier to counteract the process of vertical migration of water-soluble salts from the surface of the mine dump. Creating a leaching regime with a downward flow of moisture is a guarantee to prevent the development of the process of soil salinization. In this case, irrigation carried out with minimum standards. Irrigation with ponds-accumulators water diluted by water of the Samara River can be tolerable to the grass and induces a low topsoil salinization risk in the artificial land reclamation profile. Given the trend of transition from land use as agricultural land to the state of natural meadows and plantations for second generation energy crops cultivation, the latter type of nature use of reclaimed land in the Western Donbass is less risky.

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