Evaluation of sensitivity and setting of the MACRO 5.2. model on direct lysimeter studies of leachate

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Abstract. The water assembly of the MACRO model, making allowance regarding the double porosity of soils, was parameterized according to experimental laboratory data and tested according to the results of studying the water regime of sod-podzolic middle loamy soils of large lysimeters of MSU. Testing of pesticide migration models is necessary to improve forecast accuracy and justify their use. The analysis of the sensitivity, estimated from the data on the lysimetric runoff at the lower point (1.5 m) of the soil, showed that the WRC parameters are the main physical support of the models, which sets the forecast accuracy. These are the parameters that must be used to customize the model. The MACRO model has showed itself better at describing lysimetric runoff during the growing season by taking into account the fast flows along macropores and fissures that occur during periods of intense precipitation in the model than the models previously used.

1. Introduction
Before a new pesticide enters the market, it should undergo a mandatory state registration procedure. A deterministic approach is often used to characterize the environmental risk, which compares the concentration of the pesticide in the environment (using mathematical modeling) and the toxicity [1-2]. Mathematical models make it possible to obtain predicted pesticide concentrations in various climatic conditions, thus allowing to adjust the schemes and doses of pesticide application for example in the formation of a low-carbon strategy for the development of the country’s economy [3]. In Europe, work on modeling of the migration of substances has been carried out since the end of the last century, for which MACRO, PEARL, PELMO, PRZM models have been adapted [4]. However, in Russia the “Information on pesticide” form was approved only in 2007 (Order of July 10, 2007 N 357), according to which mathematical models began to be used for assessing the environmental risks of registered pesticides [5]. In the Russian Federation, standard soil-climatic scenarios have been created [6]; however, the PEARL (chromatographic models) is used for registration purposes, since the MACRO (predominant flow model [7]) has a rather complex mathematical apparatus. But exclusively chromatographic models have a low prediction accuracy for structurally fractured soils, which has been shown in numerous studies [7-9]; This led to the emergence of a new version of the PEARL model, which allows predicting behavior in such conditions due to a mechanism different from the MACRO model, however, the user does not have the ability to calibrate the parameters describing the geometry of the pore space. While the typical MACRO predominant flow model divides the pore space into two domains: macropores and micropores, each of those is characterized by
its own flow rate and concentration of substances [10-11]. Therefore, the use of the MACRO model can significantly increase the accuracy of predicting the migration of substances in regions prone to groundwater pollution [5].

The purpose of this work is to assess the sensitivity of the MACRO 5.2 model to the input parameters of the soil block based on leachate from the lower soil boundary and to tune the model using experimental data of leachate from the lysimeter.

2. Materials and methods

The MACRO model is a one-dimensional physically based model that takes into account the phenomenon of predominant transport of water and dissolved substances [12]. Macropores penetrate the soil profile throughout the entire depth, the process of non-equilibrium sorption is taken into account for the micropore domain and a “two-site” model is used [13-14]. The model used pedotransfer functions [15-16].

Assessing the sensitivity of the model is described in the articles [17]. Sensitivity can be estimated for different output state variables.

Lysimeter studies. In order to study the migration of pesticides and their possible penetration into groundwater, the experiments are being carried out in the last few years on a simulative soddy-podzolic medium loamy soil of large soil lysimeters of the Moscow State University named after M.V. Lomonosov (coordinates are 55.709047, 37.523406) [18]. The size of each lysimeter is 2.8m x 2.8 m x 1.75 m, the soil was brought from the Podolsk district of the Moscow region (60 years ago), quartz sand and gravel were laid under the soil profile [10].

3. Results

Assessing the sensitivity of the model. In this work, the influence of such input parameters as the physical properties of soils (soil density, particle size distribution, filtration coefficient), the parameters of the BHC approximation and the parameters of the pore space that determine the boundary between micropores and macropores in MACRO onto the cumulative leachate from the lower boundary of the soil profile were investigated. Pore space parameters of MACRO used in the sensitivity assessment: XMPOR – the bulk moisture at the boundary between macropores and micropores, that is, the water content in micropores at saturation, together with the water content in macropores, which is TPORV moisture content of full saturation; KSM – filtration coefficient in micropores; ASCALE – effective diffusion path length, which controls the exchange of water and solution between micro and macropore domains; CTEN – the potential of soil moisture at the boundary between micropores and macropores.

The lower boundary condition is free drainage, the upper boundary condition is daily weather data from the MSU meteorological station (precipitation, solar radiation, maximum and minimum temperatures, wind speed and relative humidity) from January 1, 2014 to May 5, 2017.

In order to assess the sensitivity, a simulative uniform soil profile with a thickness of 100 cm was used (table 1), irrigation, tillage and cultivation were absent. The parameters in relation to which the sensitivity of the model was assessed varied within the limits of their variation according to the literature [14; 18-19].

![Table 1. Basic properties of the simulative soil profile.](image-url)

| Property* |
|---|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 |
| Value | 35/30/35 | 7 | 1.3 | 4 | 51 | 0.05 | 2.7 | 0.05 | 46 | 30 | 63.1 | 1 | 77.5 |

* 1-Particle-size composition (%: sand - silt - clay); 2-pH (-); 3-GAMMA soil density (g/cm3); 4-Organic carbon content (%); 5-TPORV full saturation moisture (%); 6-RESID residual moisture (%); 7-n (-); 8-α (cm-1); 9-XMPOR micropore saturation moisture (%); 10-CTEN tension of soil moisture at the border between micropores and macropores (cm); 11-KSATMIN Filtration coefficient, (mm/hour); 12-KSM filtration coefficient in micropores (mm/hour); 13-ASCALE effective diffusion path length (mm).
With a change in the moisture content of full saturation, the saturation moisture of micropores was also changed so that the number of macropores in assessing the sensitivity to TPORV would remain unchanged and equal to 5%. When assessing the sensitivity to XMPOR, there is no clear criteria for the number of macropores in the soil, therefore, changes were made from the value equal to TPORV, that is, there are no macropores, to the amount of 10% macropores in the soil.

As a result of the work carried out, the cumulative values of the leachate volume from the lower boundary of the profile were obtained for the period from January 2, 2014 to May 4, 2017. Sensitivity analysis showed that the model results for the water block were significantly influenced by a small number of input parameters (\(\alpha, n, CTEN, TPORV\)). In previous works [17], it was also noted that the volume of leachate from the lower boundary of the profile is affected by a small number of input parameters and to a relatively small extent, and the main contribution to the forecast of the water balance is supposedly made by meteorological conditions.

Adjustment of the model according to the experimental data of the lysimeter experiment. The migration of substances in the soil is associated with the movement of water, therefore it is important to assess how accurately the MACRO 5.2 model predicts the amount of leachate from the lysimeter. In order to do this, the calculated and experimental data on the volume of leachate from the lower boundary of the lysimeter profile for the period from 06/13/2016 to 05/30/2017 was compared.

The upper and lower boundary conditions are the same as those used for the sensitivity assessment. The main properties of the soil horizons and the parameters of approximation of laboratory determinations by capillarimeter methods and equilibrium over saturated solutions of salts of the basic hydrophysical characteristic (BHC) by means of the van Genuchten function using the RETC model are presented in table 2.

The MACRO 5.2 model can take into account the movement of moisture along the predominant migration routes due to its complex mathematical apparatus, but it requires the introduction of additional input parameters responsible for the description of the pore space. These physical parameters are difficult to determine, therefore, the model implements pedotransfer functions for their calculation. It is possible to calculate KSATMIN, KSM, ASCALE for each horizon separately as well as TPORV, XMPOR, ALPHA, N, CTEN together. Since the BHC parameters are determined for this soil, XMPOR and CTEN and the associated KSM were not calculated by means of pedotransfer functions (PTF), but the values were used according to the Parameter Estimation Guide for the MACRO 4.2 preferred flow model [14]. The CTEN value is set based on the clay content in the profile, there are also grades of the parameter based on texture for KSM, but there are no values for silt or silt loam, a non-international classification by granulometry is used. The texture of the horizons is determined in the model automatically when entering the particle size distribution, according to the correspondence of the names in the international classification to the names in the Russian classification [20-21], silt is medium clay (silty), and silt loam is medium clay (silty). Based on the abovementioned, as well as according to the description of the soil profile [10], it was decided to use the KSM values for the clay loam for the first 40 cm, and those for the clay for the lower horizons [21]. As for XMPOR, the data of a tomographic study of agrosod-podzolic soil was used [22], according to which the average number of macropores in the humus horizon is 7.3%, and in the underlying layers of macropores it is 3.3%. The ASCALE parameter was also set according to grades based on soil structure [14]. The ZN parameter equal to 2 is typical for clays and some coarse sands, and it is equal to 4 for light loams [14]; therefore, ZN is set equal to 3 for the upper 40 cm, and it is set equal to 2 for lower depth along the profile. ZM is set to 0.5 based on the Mualem approach [12]. ZP is equal to 0, which indicates the absence of shrinkage. ZA is set to 1 by default with no effect of shrinkage [12; 14].

4. Discussion
Assessing the sensitivity of the model. While analyzing the graph of the relative leachate volumes in relation to the cumulative leachate at initially average values (50%) for the input parameters, it can be established that the parameters of the BHC approximation by means of the van Genuchten equation
have the greatest influence on leachate volumes, which was also noted by other researchers [20]. ALPHA parameter, the reciprocal value of the air inlet pressure, significantly reduces the leachate at a value below 50%, but practically does not affect the volumes when the values are increased from 0.05 to 0.1. A directly proportional relationship is observed between the value of N, which reflects the pore size distribution, and the amount of leachate, however, just as for the ALPHA parameter, a change from low values to medium values of the N parameter has a greater response, the leachate volume decreases to 23%. The dependence of the leachate on TPORV, as well as on parameters (CTEN, XMPOR, KSM), which determine the boundary between micropores and macropores in MACRO, is noted as well. An increase in the moisture content of full saturation leads to a decrease in the leachate to 868.65 mm (compared to 1162 mm). The influence of the filtration coefficient in micropores is ambiguous, when the parameter changes from 0.227 to 2 mm/h, the leachate volume slightly increases from 97 to 103%, however, a decrease in KSM to 0.03 mm/h leads to an increase in leachate to 109%, which can probably be explained by critically low filtration value in micropores, at which it is possible that the mathematical apparatus of the MACRO model takes into account only the flow through macropores, which leads to an increase in leachate. The potential of soil moisture at the boundary between micropores and macropores with increasing values leads to a decrease in leachate. An increase in the number of macropores naturally leads to an increase in leachate volumes, which has already been noted by other scientists [17]. The filtration coefficient (total) has practically no effect, except for the minimum values, reducing the leachate by 5%; Shein et al. [20] noted that in the MACRO model, the dependence of the leachate on the coefficient is much weaker than on the BHC parameters. With the constancy of other parameters, the granulometric composition and soil density do not affect the cumulative leachate, this is explained by the fact that these parameters are used by the model to calculate the physical parameters responsible for the movement of water in the soil based on pedotransfer functions (PTF). In the current work, PTFs were not used, the values of the physical support of the model were entered independently according to the ranges of variation, which led to the results described above. The ASCALE parameter, which controls the exchange of water and solution between the domains of micro and macropores, does not affect the volume of leachate from the lower boundary of the soil profile; it is expected that this parameter will affect the pesticide block of the model, as with the dispersivity length in the PEARL model, on the release time and peak concentrations [20].

### Table 2. Some chemical and physical properties of soddy-podzolic soil of lysimeters.

| Parameter                        | A          | A’         | EL         | B1         | B2         | B3         |
|----------------------------------|------------|------------|------------|------------|------------|------------|
| Depth, cm                       | 0-10       | 10-20      | 20-40      | 40-60      | 60-80      | 80-100     |
| Organic carbon, %                | 2.5        | 1.7        | 0.7        | 0.6        | 0.6        | 0.8        |
| Bulk density, g/cm³              | 11.2       | 11.2       | 7.0        | 7.3        | 7.2        | 6.8        |
| Clay (<2 μm)                     | 84.8       | 85.3       | 89.8       | 87.8       | 87.0       | 76.5       |
| Silt (2–50 μm)                   | 0.7        | 0.7        | 0.54       | 0.36       | 0.18       | 0.08       |
| Saturated hydraulic conductivity, m/day | 0.4850  | 0.4850     | 0.4360     | 0.4253     | 0.4355     | 0.4271     |
| * Data on the properties of soddy-podzolic soil for horizons below 20 cm, as well as the filtration coefficient for layers of 0-20 cm, were taken from literature sources [10]. Parameters of BHC approximation for horizons of simulative soddy-podzolic soil below 20 cm were taken from literature sources [20].

Thus, the MACRO 5.2 model with respect to the leachate from the lower boundary of the soil profile is most sensitive to the BHC parameters, the potential of soil moisture at the boundary between
micropores and macropores, and the number of macropores in the soil. These are the parameters that should be used to perform setting of the water block of the model.

Adjustment of the model according to the experimental data of the lysimeter experiment. While comparing the calculated and experimental data (figure 1), it can be argued that the model describes well the shape of the curve and the inflection points of the graph, in contrast to the PEARL 4 model, which smoothes the step structure of the graph in the winter-spring period [20].

![Figure 1](image)

**Figure 1.** 1: Comparison of experimental and predicted cumulative leachate from the lysimeter; 2: Comparison of experimental and predicted cumulative leachate from lysimeter with model setting for the humus horizon: 2a – N increased to 150%, 2b – N increased to 150%, the number of macropores to 200%, 2c – N increased to 150%, the number of macropores to 200%, ALPHA up to 200%, 2d – N increased to 200%, the number of macropores to 200%, ALPHA up to 200%, 2e - N increased to 200%, ALPHA up to 200% and the start date of the forecast of 06/12/2016.

However, the MACRO 5.2 model greatly underestimates the leachate volume, especially in the first month, the model practically does not take into account the leachate. Therefore, it was decided to adjust the water block of the model based on the sensitivity assessment described in the previous section. The initial values of the parameters are taken as 100%, if the parameter is doubled, then its value becomes relative to the initial 200%. It was decided to increase the parameter N of the van Genuchten equation for the humus layer by 50%, which led to an increase in leachate volumes, but still the experimental leachate volumes were not achieved (figure 1.2a). Further adjustment of the parameters was also carried out for the upper 20 cm of the soil layer (figures 1.2b-1.2d). Despite the manipulations with the input parameters, the model underestimated the predicted values of leachate from the lower boundary, the discrepancy increased in winter period.

It is also seen that at the initial stage the model underestimates the leachate values. Therefore, it was decided to change the calculation start date to 06/12/16. The influence of the initial soil moisture content (THETAINI) was previously known, therefore a preliminary run over several months or years should be carried out to allow the model to be balanced against the water content in the soil profile [17]. However, ambiguous results were obtained, where, without adjusting the model, the leachate in the first months, on the contrary, exceeded the experimental values, and after the winter period the total leachate according to the forecast was also less than the real one. An increase in N and ALPHA increases the cumulative offset in the same way as it was shown with the setting of the start date of 01/01/2014. An increase in N and ALPHA by a factor of 2 from the initial input data reduces the difference in leachate volumes in the winter-spring period, but the leachate from the lower boundary of the profile increases even more in the first month (figure 1.2e).
5. Conclusion

Approbation of the MACRO 5.2 model for forecasting the water regime of sod-podzolic soil was carried out. The estimation of the model sensitivity showed that the parameters of the Van Genuchten equation for approximating the WRC have the greatest influence on the output state variable (flow volume). These parameters must be determined by experimental methods and used to model setting when compiling standard scenarios for the migration of pesticides to ground and surface waters for the territory of the Russian Federation, which is a very relevant direction in assessing the risk of pesticides during their state registration.

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