1. Description of the ROMUL model

1.1. General description

ROMUL is represented as a system of differential equations based on known descriptions of main processes and a set of assumptions about connections between leading variables. ROMUL approach is based on a generalized description of soil organic matter (SOM) pools dynamics in different soil horizons without division into detailed compounds but taking into account successive SOM transformations by soil pedobionts whose activity depend on dynamics of soil nutrition elements and environmental factors. It allows for a calculation of coefficients being sometimes nonlinear and which includes direct account of microorganisms activity and soil animals contribution to the SOM and nutrition elements' dynamics (Chertov et al., 2001).

The theoretical background of the ROMUL model is (i) a concept of fast mineralization of fresh plant debris at an early phase of decomposition, and its transformation into partially humified material that decomposes slowly; (ii) the consideration of the role of soil fauna in the process of SOM transformation, and (iii) the simulation of SOM dynamics simultaneously in organic layer and in mineral topsoil. The approach corresponds to the concepts of humus forms (types) and their different functional properties (raw humus, moder and mull) (Figure 1).

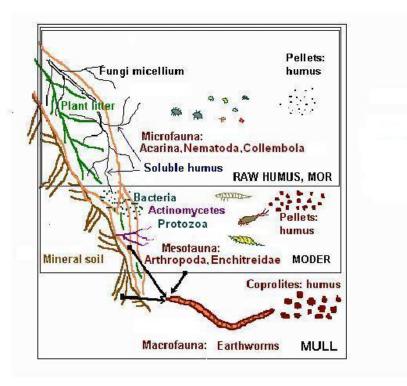


Figure 1. Conceptual scheme of soil biota functioning and SOM formation at three main humus forms. The dominating functional groups of organisms-destructors are only reflected on the scheme.

This approach allows for a successful use of standard soil descriptions and physico-chemical parameters of organic and mineral horizons for model initialization. We assume that main processes of

SOM transformations are reflected by soil profile and soil horizons, and humus forms mark different patterns of soil processes.

The different fresh aboveground litter fractions (leaves, needles, etc.) reflected in the model as undecomposed litter **L** (kg/sq.m). It is a pool of organic matter, corresponding to **L** horizon of forest floor (Figure 2). It contains undecomposed and partially decomposed litter with big plant fragments. Microorganisms and fungi compose a main complex of organisms-destructors with a rate of mineralization k_1L and transformation into a next pool with a rate k_3L (both depending on nitrogen and ash concentration and on forest floor moisture and temperature). The domination of this process at plant debris decomposition leads to the formation of raw humus.

 L_u (kg/sq.m) is a pool of SOM, which contains undecomposed and partly decomposed fine and coarse root litter. Rate of mineralization is k_1L_u and transformation into the next pool is k_3L_u (depends on ash concentration and mineral soil temperature and moisture). Part of this pool is metabolized by the decomposing organisms and the corresponding carbon is released as gaseous CO₂. This process controls formation of labile humus in mineral topsoil.

The majority of the organic matter ends up in a more slowly decomposing complex of partly decomposed organic matter with new-formed humic substances (CHS) (kg/sq.m), which is a pool of organic matter that contains partly decomposed litter with small decomposed plant fragments and corresponds to \mathbf{F} horizon of the forest floor. The transformation of this pool goes by two groups of organism-destructors:

1. The community of Bacteria, Fungi and Arthropoda with rate \mathbf{k}_4 transforms part of SOM into **H** pool of forest floor and a rest part in a stable humus in mineral horizons **Sh** (Stable humus) and produces SOM with a C/N ratio 15. Moder humus develops at a domination of this way at decomposition.

2. Transformation (humification) of SOM by the community of earthworms and macroarthropods forms mull humus **Sh** in mineral horizons with a C/N ratio 8, rate of this transformation is k_{5} .

A specific parameter **d** is a ratio to divide SOM flow between these ways. This parameter depends on C/N ratio in F: the larger is C/N the greater part of humified matter stays in H of organic layer.

Labile humus **Lh** (kg/sq.m) is a belowground analogue of organic layer. Transformation of this pool also goes by two groups of organism-destructors. \mathbf{k}_4 is rate of transformation by Bacteria and Arthropoda, \mathbf{k}_5 is rate of transformation by earthworms.

The transformation of organic matter into the stable humus ("recalcitrant soil C") **Sh**, i.e. mass flows $\mathbf{k_4}$ and $\mathbf{k_5}$, is based on the assumption that all the organic matter in the compartment "**Sh**" is mostly produced by the metabolism of the decomposing organisms (Fungi, Bacteria, Protists, Arthropods and Lumbricidae).

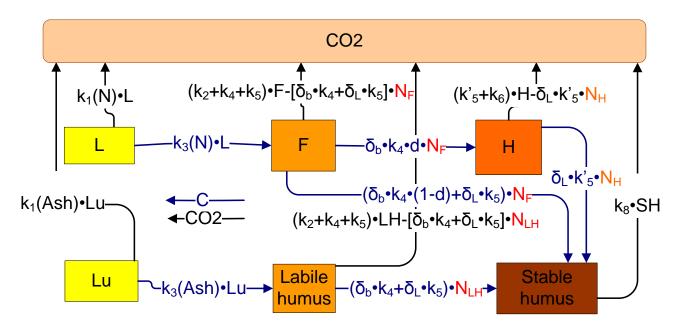


Figure 2. Flow-chart of the ROMUL model. Explanations of symbols are in the text

Nitrogen has a special role in this phase: the rate of nitrogen moving from compartments N_F into the compartment N_{SH} is calculated using some modifiers (δ_j and γ) in the main scheme of SOM decomposition (Figure 3). We postulated that 20% of nitrogen consumed by soil fauna is transformed into their biomass and 80% - into stable humus ($\gamma = 0.8$) with a C/N ratio 15 for Bacteria and 8 for Arthropods. Thereafter an amount of nitrogen in the humified material was used to calculate the SOM flow from the compartments **F** to the compartment **Sh** using parameters δ_j that is equal to 24.0 for Bacteria and Arthropoda community and 12.8 for Lumbricidae dominated one.

The "stable" humus **Sh** is also decomposing, at a rather slow rate, modified by the soil temperature and moisture. The decomposition flux has a range from a minimum 1-2% annually up to 15% annually, depending on the soil texture, actually clay content. Maximal rate of **Sh** decomposition was observed in arable soils. However, as roughly a half of the soil organic matter in the Boreal zone is in the compartment **Sh**, the value of the rate factor \mathbf{k}_5 has a significant effect on the total storage of organic matter and nitrogen in the soil.

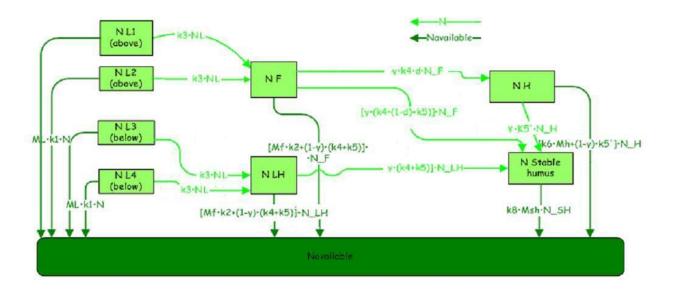


Figure 3. Flow-chart of nitrogen in the ROMUL model. Explanations of symbols are in the text

1.2. The general system of equations

The system of equations at its present state is as follows:

$$\begin{aligned} \frac{dL_{i}}{dt} &= Litterfall_{i} - (k_{1} + k_{3}) \cdot L_{i} \\ \frac{dLu_{j}}{dt} &= Litterfall_{u_{j}} - (k_{1} + k_{3}) \cdot L_{-}u_{j} \\ \dots \\ \frac{dN_{Li}}{dt} &= Litterfall_{i} \cdot N_{-}con_{i}/100 - (M_{L} \cdot k_{1} + k_{3}) \cdot N_{Li} \\ \frac{dN_{Lu_{j}}}{dt} &= Litterfall_{u_{j}} \cdot N_{-}con_{u_{j}}/100 - (M_{L} \cdot k_{1} + k_{3}) \cdot N_{Lu_{j}} \\ \dots \end{aligned}$$

$$\frac{dF}{dt} = \sum_{i} k_3 \cdot L_i - (k_2 + k_4 + k_5) \cdot F$$
$$\frac{dN_F}{dt} = \sum_{i} k_3 \cdot N_{Li} - M_F \cdot k_2 \cdot N_F - (k_4 + k_5) \cdot N_F$$
$$\frac{dLH}{dt} = \sum_{i} k_3 \cdot Lu_j - (k_2 + k_4 + k_5) \cdot LH$$

$$\begin{aligned} \frac{dN_{LH}}{dt} &= \sum_{j} k_{3} \cdot N_{Lu\,j} - M_{LH} \cdot k_{2} \cdot N_{LH} - (k_{4} + k_{5}) \cdot N_{LH} \\ \frac{dH}{dt} &= \delta_{a} \cdot k_{4} \cdot d \cdot N_{F} - (k_{6} + k_{5}^{'}) \cdot H \\ \frac{dN_{H}}{dt} &= \gamma \cdot k_{4} \cdot d \cdot N_{F} - (k_{6} + k_{5}^{'}) \cdot N_{H} \\ \frac{dSH}{dt} &= [\delta_{a} \cdot k_{4} \cdot (1 - d) + \delta_{L} \cdot k_{5}] \cdot N_{F} + (\delta_{a} \cdot k_{4} + \delta_{L} \cdot k_{5}) \cdot N_{LH} + \delta_{L} \cdot k_{5}^{'} \cdot N_{H} - k_{8} \cdot SH \\ \frac{dN_{SH}}{dt} &= \gamma \cdot [k_{4} \cdot (1 - d) + k_{5}] \cdot N_{F} + \gamma \cdot (k_{4} + k_{5})] \cdot N_{LH} + \gamma \cdot k_{5}^{'} \cdot N_{H} - M_{SH} \cdot k_{8} \cdot N_{SH} \end{aligned}$$

where subscript *i* denotes the *i*-th cohort of above-ground litter, u_j denotes the cohort of below-ground litter, L_i are running undecomposed masses of different litter fractions, *Litterfall_i* are the inputs of corresponding above-ground litter fractions, N_{Li} are their nitrogen amounts ; similar variables with subscript u_i are the similar amounts of below-ground litter and its nitrogen.

F and N_F are transformed complex of humic substances (CHS) originating from above-ground litter cohorts and its corresponding nitrogen contents, *LH* and N_{LH} are similar masses and their nitrogen of below-ground partially decomposed litter cohorts (labile humus, particulate organic matter). It should be noted that at this stage all cohorts are merged and total mass of organic matter and their nitrogen masses in *F* and separately in *LH* cohorts are summed up.

Relations between *H* and *SH* together with multiplier *d* dividing different flows between these carbon and corresponding nitrogen pools N_H and N_{SH} are described earlier. Note that rates of mineralization of these pools k_6 and k_8 are similar in their role in organic matter transformations but they depend on different temperatures and moistures: *H* and N_H depend on forest floor conditions, and *SH* and N_{SH} on mineral soil conditions.

It should be noted that there are different and independent ways of decomposition for above- and below-ground litter cohorts for the first two stages of litter transformation and one united pool of humus bonded with the mineral matrix of topsoil. Coefficients δ_B , δ_L and γ reflect the relations between the spending of nitrogen to the soil faunas' biomass and humus formation (Chertov et al., 2001). The dimensions of *L*, *Lu*, *F*, *LH*, *H*, *SH*, *N_L*, *N_{Lu}*, *N_F*, *N_{LH}*, *N_H* and *N_{SH}* are (kg m⁻²), *k_i*, (day⁻¹). The coefficients k_i are different for above- and below-ground litter fractions (not marked in the system of equations above). *k*₁ is the rate of fresh litter mineralization by a complex of soil destructors consisting of *Fungi*; *k*₂ is the rate of mineralization of CHS ; *k*₃ is the rate of litter transformation to *F* as a process of organic debris humification; *k*₄ is the rate of *F* (different for above and below-ground fractions) consumption by a community of *Bacteria*+*Arthropoda*; *k*₅ is a rate of F consumption by earthworms; *k*₆ is a rate of H

mineralization; k_8 is a rate of SH mineralization; M_L , M_F , M_{LH} , M_{SH} are relative rates of nitrogen mineralization in L, L_u , F, F_u and H pools. It should be noted that the coefficients k_{iL} and k_{iS} are calculated using different temperature and moisture data as an input parameters. The coefficients with index L use litter temperature, with an index S they use soil temperature. All coefficients k_{iL} are dependent on litter moisture, k_{iS} use soil moisture.

1.3. Rates of the SOM transformation which are specified on the basis of organic debris (litter or transformed litter) chemical properties

Dependencies of kinetic parameters on ash and nitrogen contents are listed in Table 1. Necessary nitrogen and ash contents for several plant species are listed in a Table in Appendix 1.

k _i	Above-ground litter	Below-ground litter	Correction for Nitrogen/lignin ratio	Correction for pH
	$\psi(Nitr)$	$\theta(Nitr, Ash)$	µ(Nitr / Lignin)	$\eta(ph)$
<i>k</i> ₁	0.0005+0.0054*nitr	0.0136+0.0006*Ash, Ash≥0 0, Ash<0	$0.092 \cdot (lignin / nitr)^{-0.7396}$, lignin $\neq 0$, nitr $\neq 0$ 1, else	$0.701 \cdot ph - 1.618$ -0.038 $\cdot ph^2$, $3 \le ph \le 5.2$ 1, else
<i>k</i> ₃	0.0089+0.0078*nitr	0.0394-0.0021*Ash, 0≤Ash≤18.762 0, Ash>18.762	$0.0622 \cdot (lignin / nitr)^{-0.397}$, lignin $\neq 0$, nit $\neq 0$ 1, else	-
<i>k</i> ₂	0.000496	0.00126	$0.0027 \cdot (lignin / nitr)^{-0.3917},$ $lignin \neq 0, nitr \neq 0$ 1, else	$0.701 \cdot ph - 1.618$ -0.038 \cdot ph^2, $3 \le ph \le 5.2$ 1, else
<i>k</i> 4	$0.0005 * nitr, nitr \le 2$ $0.001, else$	$0.0005*nitr, nitr \le 2$ $0.001, else$	-	
k ₅₌ k'5	$0.007 * \frac{2.0 * nitr - 1}{3.0},$ $0.5 < nitr \le 2$ 0.007, nitr > 2 0, else	$0.007 * \frac{2.0 * nitr - 1}{3.0},$ $0.5 < nitr \le 2$ 0.007, nitr > 2 0, else	-	-

Table 1. Dependencies of kinetic parameters on ash and nitrogen contents, N to lignin ratio and pH

1.4. Other coefficients which are specified from external sources (literature or regional traits

 k_6 and k_8 values vary from 0.0006 [d⁻¹] in sandy soils to 0.00006 [d⁻¹] in heavy loams and clays (the only parameter is to be calibrated in some cases).

Coefficients $\delta_a \ \delta_l \ and \ \gamma$ reflect nitrogen expenditures for calculation humus formation by soil fauna (Chertov et al., 2001).

$$\delta_a = 24.0$$

 $\delta_l = 12.8$
 $\gamma = 0.8$

٢

 M_L , M_F , M_H = M_{LH} , - corrections for nitrogen mineralization rates in relation to SOM mineralization rates in L, F, H и LH. M_L=0.1

$$M_{F} = \begin{cases} 0.1, & N_{F} / F \cdot 100 - 1.16 \cdot N _ con _ ab \le 0.44 \\ 0.5, & 0.44 < N_{F} / F \cdot 100 - 1.16 \cdot N _ con _ ab \le 1.50 \\ 1.0, & 1.5 < N_{F} / F \cdot 100 - 1.16 \cdot N _ con _ ab \end{cases}$$

$$M_{LH} = \begin{cases} 0.1, & N_{LH} / LH \cdot 100 - 1.16 \cdot N _ con _ be \le 0.44 \\ 0.5, & 0.44 < N_{LH} / LH \cdot 100 - 1.16 \cdot N _ con _ be \le 1.50 \\ 1.0, & 1.5 < N_{LH} / LH \cdot 100 - 1.16 \cdot N _ con _ be \end{cases}$$
$$M_{SH} = \begin{cases} 1.0, SH \cdot 0.5 / N_{SH} \le 8 \\ 0.5, else \end{cases}$$

N_con_ab is average weighted nitrogen content of above-ground litter fractions (in %):

$$N_con_ab = \frac{\sum_{i=1,2...} N_Litter_i}{\sum_{i=1,2...} Litter_i} \cdot 100$$

N_con_be is average weighted nitrogen content of below-ground litter fractions (in %):

d is a coefficient which reflects relation between reallocation of organic matter flow between H horizon in forest floor and SH pool in mineral soil. In north taiga soils where SOM content in mineral horizons is small **d** is equal to 1, and flow defined by coefficient k_4 goes completely to forest floor H horizon. Inversely in temperate zone where forest floor is almost (or temporarily) absent this coefficient is equal to zero (or to small value). At the moment, assigned value is an expert evaluation but it could be further a special procedure developed where \mathbf{d} will be calculated in dependence of hydrothermal conditions and soil biota activities.

1.5. Moisture functions *F*(*W*)

For more general approach, and more simplicity of further modification, the function G(W), that describe dependences of ROMUL coefficients k_i on soil moisture should be written as: $F_i(W, W_{WP}, W_{FS}, W_{Sat})$, where W – actual moisture value, W_{WP} – moisture at permanent wilting point, W_{FC} – moisture at field capacity, W_{Sat} – total capacity (moisture value at full saturation).

At the current stage, we used "normalized" values of moisture $W_N = W/W_{FC}$. The functions been used before (Chertov et al., 2007) were transformed into the new form, with some general assumptions about W_{FC} for soils and plant litters used in the old experiments (W_{FC} ~300% mass for plant litters used for estimates of $k_1 - k_4$ and ~30% for loamy soils – for k_5). For k_6 and k_8 (coefficients of mineralization of organic matter in H and in SH correspondingly) we now use the same dependence, that was elaborated for coefficients $k_1 - k_3$, but in the new "normalized" form. We suppose, that it allows to apply more correctly the dependences, obtained for substrates with different physical properties, than the usage of dependences, based on mass water content.

Advantage of such normalized moisture values is that there are no differences between moisture units (mass %, volume % or mm H₂0 per layer) we use initially; the result should be the same. We only have to use the same units both for *W* as well as W_{FC} (or other soil hydrological constants if they are used). So, while we use soil moisture values expressed as mass % in our climate scenarios, we should use input values of hydrological constants for ROMUL expressed in the same units.

Dependencies of the kinetic parameters on soil (litter) temperature and soil (litter) moisture are listed in Table 2.

	f(t)	$\varphi(w)$
k ₁	$\begin{array}{l} 0.1595 + 0.0319 * t, -5 < t \leq 1 \\ 0.1754 * e^{0.087 \text{i}t}, 1 < t \leq 35 \\ 8.791 - 0.1465 * t, 35 < t \leq 60 \\ 0, else \end{array}$	$\begin{array}{ccc} 0, & W_N < 0.023 \\ 9.297 * (W_N)^{2.5492} & 0.023 \leq W_N < 0.417, \\ 1 & 0.417 \leq W_N < 1.333, \\ & 29.53 * 0.07889^{W_n} & 1.333 \leq W_N, \end{array}$
k ₃		$\begin{array}{ccc} 0, & W_N < 0.023 \\ 9.297 * (W_N)^{2.5492} & 0.023 \leq W_N < 0.417, \\ 1 & 0.417 \leq W_N < 1.333, \\ & 29.53 * 0.07889^{Wn} & 1.333 \leq W_N, \end{array}$

Table 2. Dependencies of the kinetic parameters on soil (litter) temperature and soil (litter) moisture

k ₂	$\frac{1.3}{(1+1.97 \cdot t^2)}, -3 < t \le 0$ $1.3, 0 < t \le 7$ $\frac{78.0 - 1.3 \cdot t}{53.0}, 7 < t \le 60$ $0, else$ $0.1595 + 0.0319 * t, -5 < t \le 1$	$0, W_N < 0.023$
2	$0.1754 * e^{0.087 ^{\text{b}}t}, 1 < t \le 25$ $1.534,25 < t \le 35$ $3.69 - 0.0615 * t,35 < t \le 60$ 0, else	$9.297 * (W_N)^{2.5492} \qquad 0.023 \le W_N < 0.417,$ $1 \qquad 0.417 \le W_N < 1.333,$ $29.53 * 0.07889^{W_N} \qquad 1.333 \le W_N,$
k ₄	$0.1595 + 0.0319 * t, -5 < t \le 1$ $0.1754 * e^{0.087 * t}, 1 < t \le 20$ $1,20 < t \le 40$ $2.0 - 0.025 * t, 40 < t \le 80$ 0, else	$7.5* W_N$, $W_N < 0.133$,1 $0.133 \le W_N < 1.333$, $2.333 - W_N$ $1.333 \le W_N < 2.333$ 0 $2.333 \le W_N$,
k ₅	$0.078 + 0.0156 * t, -5 < t \le 1$ $0.0675 * e^{0.2088t}, 1 < t \le 13$ $1,13 < t \le 25$ $2.0 - 0.04 * t, 25 < t \le 50$ 0, else	$\begin{array}{cccc} 0 & & W_N < 0.067, \\ 2.307^* W_N - 0.1538 & 0.067 \leq W_N < 0.500, \\ 1 & & 0.500 \leq W_N < 2.333, \\ 2.40 - 0.6^* W_N & & 2.333 \leq W_N \end{array}$
k ₆ , k ₈	$0.1595 + 0.0319 * t, -5 < t \le 1$ $0.1754 * e^{0.087 ^{\text{P}t}}, 1 < t \le 27.5$ $1.95,27.5 < t \le 35$ $4.68 - 0.078 * t, 35 < t \le 60$ 0, else	$\begin{array}{llllllllllllllllllllllllllllllllllll$

1.6. Additional procedures as an interface with ecosystem models

The amounts of mineralized humus and nitrogen available for plants are important outputs from ROMUL. At every time step, the mineralized amount of humus is calculated for each litter fraction (aboveor belowground) as

$$\begin{split} H_{\min er} &= \sum_{i} k_{1} \cdot L_{i} + \sum_{j} k_{1} \cdot Lu_{j} + \left(k_{2} + k_{4} + k_{5}\right) \cdot F - \left(\delta_{B} \cdot k_{4} + \delta_{L} \cdot k_{5}\right) \cdot N_{F} + \\ &+ \left(k_{2} + k_{4} + k_{5}\right) \cdot LH - \left(\delta_{B} \cdot k_{4} + \delta_{L} \cdot k_{5}\right) \cdot N_{LH} + \left(k_{6} + k_{5}^{'}\right) \cdot H - \delta_{L} \cdot k_{5}^{'} \cdot N_{H} + k_{8} \cdot SH \end{split}$$

Correspondingly the nitrogen available for plants is defined as:

$$\begin{split} N_{avail} &= \sum_{i} M_{L} \cdot k_{1} \cdot N_{Li} + \sum_{j} M_{L} \cdot k_{1} \cdot N_{Luj} + \left[M_{F} \cdot k_{2} + (1 - \gamma) \cdot (k_{4} + k_{5}) \right] \cdot N_{F} + \\ &+ \left[M_{F} \cdot k_{2} + (1 - \gamma) \cdot (k_{4} + k_{5}) \right] \cdot N_{LH} + \left[k_{6} + (1 - \gamma) \cdot k'_{5} \right] \cdot N_{H} + M_{F} \cdot k_{8} \cdot N_{SH} \end{split}$$

2. Guide to ROMUL program

ROMUL is a program working in the operational environment of Microsoft Windows. It is intended for modeling processes of mineralization and humification (recalcitrance formation) of soil organic matter. An interaction with the program is based on algorithms that are typical for Windows applications, and most operations in the program would be clear for users of OS Windows family.

2.I. Preparation of input files for the ROMUL model

2.1.1. Preliminary information

For the program start-up it is necessary to have the special file named "scheme" and describing configuration of the program configuration and three input files:

- 1. file with cohorts of litter fall (dead organic debris input),
- 2. file with climatic data,
- 3. initial soil parameters and conditions.

If you have a number of experimental measurements of variables or even one measurement then you can place them on the graphic for visual comparison of the measured data with modeling results. For this purpose an additional special file with measured data can be added.

What is the scheme of the current configuration of the program ("modSoil_v7_0_2_users.dlessch" file)? This version of the ROMUL program is included in DLES platform (Bezrukova et al. 2012) intended for a development of the program complex that is joining a large number of simulation or analytical models of various processes in terrestrial ecosystems. The scheme indicates what models participate in computer experiment according to the user's scenario and how data from one program are transferred to another. In this version a prototype of the prepared project is described. It consists of input files, united by some scenario, which is realized by the ROMUL model and a shell with incorporated graphic interface.

The DLES platform has a number of advantages:

• It allows for uniting easily various models and has a number of built-in tools for simplification of the accounting of spatial interactions when modeling natural processes and the phenomena in various ecosystems.

• All parameters of system have standard description made with the use of the XML standard.

• DLES allows carrying out data exchange between the models written in different programming languages and working with the different spatial and temporary resolution, and for this purpose, the general area of memory of the system's kernel is used. Also the kernel provides an automatic transformation of the data expressed in various dimension units.

• The platform allows running simultaneously several simulation experiments with different input data and/or models and provides facilities for comparison of results of modeling.

The ROMUL program works with a monthly time step. It should be noted that values of model's coefficients are calculated for a daily step. For example, k8 is equal to 0.0001 day⁻¹ (used later as an input value), indicates the rate of mineralization of stable pool of soil organic matter in one day of the vegetative period under certain conditions.

Warning

The file with the working scheme of modeling $(modSoil_v7_0_2 users.dlessch)$ is stored in the $DLES_user \rightarrow data \rightarrow ROMULS$ folder (this folder may contain different ROMUL projects and it is prescribed in the project scheme with this name.. Please do not rename and do not change location of this file in order to avoid failures in the work of the program.

Files with test data are prepared in the same folder: LitterFall.csv, InitValues_users.txt, climate.csv. You can do the following using these files: 1) to carry out the test run to compare results with given in this manual; 2) to prepare your own data files used test files as templates. Please don't change anything in initial test files of the project at preparation of input files with your data, let these files be always fixed in the folder: data \rightarrow ROMULS. Save your data with other names but keep specific extensions.

Please firstly rename test files "LitterFall.csv, InitValues_users.txt, climate.csv and exp_data.csv" for creation of files with your own data and only after that you would incorporate your data.

Parameter	Type of input file					
Type of data, File name	File with litter cohorts (LitterFall_x.csv)	File with initial soil data (InitValues_users_x.txt)	File with climatic data (climate_x.csv)	File with experimental points (xxx_x.csv)		
File type:	Comma- Separated Values	Text	Comma- Separated Values	Comma- Separated Values		
File extension	.CSV	.txt	.CSV	.CSV		
Separator between data	comma	blanc	comma	comma		
Separator between integer and fractional part in number:		Decimal point				
Names of parameters:	names of parameters should be written down by Latin letters and - if consist of several words - then use underlining instead of blanc					
In the 2nd line of the file (1 modelling step)	all numbers have to be written down as real numbers for example: zero as 0.0, unit as 1.0, etc.					

Table 3. Main files properties

2.1.2. File with scenario of litter input (LitterFall.csv).

It consists of the consecutive description of cohorts (fractions) of plant litter (kg/m²/month⁻¹). Cohorts consist of monthly values of litter biomass (not carbon!) of different fractions of vegetation: leaves, branches, roots, etc. Fractions have to differ accordingly to nitrogen, ash and lignin contents. So the seasonal dynamics of litter flow has reflected in the scenario. For example, birch leaves fall in autumn, and dry branches fall evenly all year.

The file with litter flow is arranged as follows: every line contains data on miscellaneous litter cohorts (leaves, branches, etc.) for one step of modeling (with comma as a separator). The number of cohorts can be no more than 14 (it is stated in the program scheme). Number of monthly time modeling steps must be minimally 1, if litter flow is constant, or 12 (if it is unevenly distributed within a year). I If litter flow is distributed unevenly during the year but not changes in sequence of years then it ids convenient to use the follow program's property: if the program doesn't find on any step the next line, it takes last row again and continues input further. If litter flow changes during the modeling time then number of file rows must correspond to number of modeling steps to avoid repeating of the last row. At the preparation of the input file, an important point is that the sequence of litter cohorts can not be broken. If any litter cohort is absent then its value shall be written as zero (0.0). Thus, each column data corresponds to litter cohort of a certain type. Names of columns and their order cannot be changed.

Simplest way to prepare this file is as follows:

1) open the file *LitterFall.csv* in Excel program, and rename it, for example, into *LitterFall_1.csv*;

2) insert your data into Excel then convert them in the table form. For this purpose mark the data by cursor and rewrite them using menu *Data* \rightarrow *Text on columns* (with comma as a separator) to a tabular form;

3) replace demonstration litter flow data with your own data;

4) save file (in our example: LitterFall_1.csv) with .csv expansion in the same ROMULS folder.

Warning

After saving of LitterFall_x.csv file with litter cohorts, it is necessary to open it in Notepad or similar editor and to check whether commas are really separators and decimal points are separators in numbers (it could depend on regional settings of Excel). Change them if necessary. If not all 14 cohorts (it is a maximal number for our ambient scheme) are used then you need to check that on the first step (the 2nd line of the file) all figures (the last cohort) must be zero with decimal point 0.0 because Excel keeps simply 0 in the form of an integer! It is obligatory only for second line!

5) open the prepared file (*LitterFall_1.csv*) in the Notepad and check separators again: comma between of cohorts, and decimal point before fractional part of numbers. You may do necessary changes by Replace menu in Edit \rightarrow Make necessary changes (Fig. 4):

📮 LitterFall_1.csv - Notepad			<u> </u>
File Edit Format View Help			
Step;Lit_00;Lit_01;Lit_02;Lit_03;Lit_04;Lit_05;Lit_06; 1;0.0;0.00347;0.0;0.0;0.0;0.0;0.00163;0.00379;0.0003 2;0;0.00347;0;0;0;0;0;0.00163;0.00379;0.00038;0.0006 3;0.00766;0.00347;0.003;0;0;0;0.00163;0.00379;0.00 4;0.00766;0.00347;0.003;0;0;0;0.00163;0.00379;0.00 5;0.02 Constraints 6;0.00 Replace 7;0.00; Find what: 9;0.00; Replace with: 11;0.0 11;0.0 12;0;0 Match case	38;0.00065;0.0 5;0.00043;0;0; 038;0.00065;0 038;0 0 038;0 0 038;0 0 038;0 0 038;0 0 038;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	10043;0.0;0.0;0.0 0 .00043;0;0;0	

Figure 4. Checking correctness of litter flow files (LitterFall.csv) in the Notepad: the given format is

incorrect: there are semicolons instead of commas, correct it.

Now the file looks so (Fig. 5):

LitterFall_1.csv - Notepad	
File Edit Format View Help	
Step,Lit_00,Lit_01,Lit_02,Lit_03,Lit_04,Lit_05,Lit_06,Lit_07,Lit_08,Lit_09,Lit_10,Lit_11,Lit_12,Lit_1	13 🔺
1,0.0,0.00347,0.0,0.0,0.0,0.0,0.0,0.00163,0.00379,0.00038,0.00065,0.00043,0.0,0.0,0.0,0.0	
2,0,0.00347,0,0,0,0,0.00163,0.00379,0.00038,0.00065,0.00043,0,0,0	
3,0.00766,0.00347,0.003,0,0,0,0.00163,0.00379,0.00038,0.00065,0.00043,0,0,0	
4,0.00766,0.00347,0.003,0,0,0,0.00163,0.00379,0.00038,0.00065,0.00043,0,0,0	
5,0.02298,0.00347,0.010,0,0,0,0.00163,0.00379,0.00038,0.00065,0.00043,0,0,0	
6,0.00766,0.00347,0.003,0,0,0,0.00163,0.00379,0.00038,0.00065,0.00043,0,0,0	
7,0.00766,0.00347,0.003,0,0,0,0.00163,0.00379,0.00038,0.00065,0.00043,0,0,0	
8,0.00766,0.00347,0.003,0,0,0,0.00163,0.00379,0.00038,0.00065,0.00043,0,0,0	
9,0.00766,0.00347,0.003,0,0,0,0.00163,0.00379,0.00038,0.00065,0.00043,0,0,0	
10,0.01532,0.00347,0.010,0.04,0.02,0,0.00163,0.00379,0.00038,0.00065,0.00043,0,0,0.04	
11,0.00766,0.00347,0.003,0,0,0,0.00163,0.00379,0.00038,0.00065,0.00043,0,0,0	
12,0,0.00347,0,0,0,0,0.00163,0.00379,0.00038,0.00065,0.00043,0,0,0	
<u> </u>	►
Ln 1, Col 1	11.

Figure 5. File of litter flow (LitterFall.csv) in the Notepad after corrections

6) check that all zeros in the second line were written down as real numbers "0.0";

7) save file (in our example as *LitterFall_1.csv*).

2.1.3. The file of initial soil characteristics (InitValues_users.txt).

Representation of the soil horizons in ROMUL and calculation of pools of carbon and nitrogen for soil horizons

The ROMUL model calculates transformation of generalized pools of soil organic matter and nitrogen according to the following scheme. The soil profile is separated into organic and mineral horizons. The organic horizons are understood as three horizons of forest floor (L, F, H), (Figure 6) and also grass sward and peat. The detailed description of these horizons is provided in (Chertov et al. 2001; Modelling of

Organic Matter ..., 2007). All soil organic matter of mineral horizons up to the depth of 1 meter is united in one pool, designated AB. For poor soils with shallow profile, the calculation within a root-inhabited layer is acceptable. However it is necessary to point out that values of all variables, including hydrological constants, must be given for the whole modeled soil layer.

. [Russian	taxonomy	International	taxonomy
	Previous	Recent*	Previous	Recent**
Undecomposed plant litter	01	Excluded	L	OL
Partially decomposed organic material, fermentation layer	02	20	F	OF
Decomposed organic layer, humified forest floor	03 /	for all organic layer***	н	он
Humus horizon of mineral topso	il A1	A (AO,AH,AJ,AY e	tc.) Ah	A, AE
Elluvial horizon, often as podzol horizon	A2	E	E	E
Illuvial horizon	в	B (BMF, BFM etc.)) В	В

Notes:

* There is a great number indices for transitional and specific horizons as a combination of basic indices

** These basic indices have a great number of subscript indices showing various specific features of basic ones

*** There are some other indices for organic layers of different kind without their sub division

Some horisons can absent in describing soil profile



Pools of organic matter or nitrogen in soil horizons can be calculated with the following formula if we know bulk density of the soil horizon D_v (dm3 kg) (see below list of necessary parameters), thickness of soil horizon Z and percent of the content of organic matter (or nitrogen) in the horizon (name it as P) pool of SOM organic matter (or nitrogen)

$SOM = D_v * Z * P * S,$

where S is area unit (for example, m^2 , ha etc.).

Sometimes there are no data for F or H horizons or they are absent in the profile. Therefore it is convenient to consider a whole organic layer being F or H as input parameter in the model. If there are no both horizons then obviously corresponding pool is equal to 0.0.

Pool of organic matter AB of mineral layer in ROMUL consists of labile and stable parts. Division into these fractions can be made at initialization in two ways.

1. If there were experiments on decomposition of soil organic matter from AB horizon then loss of weight V can be presented as the sum of two negative exponents:

$V = A1^{*}exp(-R1) + A2^{*}exp(-R2).$

Maximal A_i coefficient in this equation describes fast decaying component and corresponding term of the equation can be taken for an estimation of labile organic matter. The second term respectively is the estimation of a stable component.

2. The amount of a labile organic matter in this horizon depends on vegetation dominants and originates presumably from root litter fall. It can be calculated by expert way (for example, for a spruce tree root litter in the mineral soil is assumed to be 10-15% from all organic matter in this horizon, for a pine respectively it represents 30% from measured full amount of organic matter in the mineral topsoil (horizon of AB). In general, this portion varies between 50 and 30% in natural soils in all climatic zones (in wet rich soils this portion can be higher, for example, in dark-colored meadow gley soils). The degraded arable and pasture soils can have a portion of labile fraction even less 0.1 (10%). This pool appears to be a calibrating parameter at initialization of soil characteristics. Sometimes AB horizon does not contain organic matter, consequently this value in the input file will be set to 0.0.

It is necessary to know the size of soil bulk density and horizon thickness of the mineral soil horizons for recalculation of analytical concentration of organic matter and the corresponding nitrogen to their pools. In this case, it is possible to use the previous equation, and then to summarize pools in all mineral horizons to 100 cm of depth. If data represent soil carbon, value of organic matter can be calculated with conversion coefficient 1.774 or 2.0 (for taiga soils).

The nitrogen pool of a labile fraction is calculated assuming at the first approximation that C/N ratio in the labile fraction is the same as in the H horizon of forest floor. Then nitrogen pool can be easily estimated from labile organic matter pool by formula

$N_{labile} = C_{AB}/C/N_H,$

where C_{AB} is a pool of carbon in labile organic matter, C/N_H is C/N ratio in H horizon of forest floor. Respectively, value of nitrogen pool of stable organic matter is equal to

$N_{stable} = N_{AB} - N_{labile,}$

where $N_{AB}\xspace$ is the total pool of nitrogen in the mineral horizons.

This file contains initial values of model variables, soil characteristics, characteristics of litter cohorts, some coefficients and soil and hydrological constants. These data are collected altogether in this file with the ".txt" expansion (Fig. 7), the detailed description of variables is given below.

InitValues_users.txt - Notepad	_ 🗆
ijle Edit Format Yiew Help	
/AR VALUE	
#number of litter cohorts:	
LITTER_COUNT 9	
#names of litter cohorts:	
names Leaves_Oak twigs flowers acorns Ash_leaf Ash_keys insect hazel fine_root n n n n n	
#is cohort above (0) or below (1):	
key00000001100000`	
#nitrogen content in each cohort:	
nitr 1 23 0.97 2 33 0 84 1 3 1 7 3 18 1 26 2 8 0 0 0 0 0 0 0 0 0 0	
#ash content in each cohort:	
ash 2.8 1.65 0.9 0.29 2.45 2.4 2.7 2.8 3.2 0.0 0.0 0.0 0.0 0.0	
#lignin content in each cohort, %:	
ignin 0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.	
#organic matter content in sub-horizon L:	
[kg/m2] 0.00 0.00.00.00.00.00.00.00.00.00.00.00	
angening of one that the state the state of one of the state of the st	
N_L[kg/m2] 0.0 0.0 0.0 0.00 0.00 0.0 0.0 0.0 0.0	
≰organic matter content in sub-horizon F:	
F(kg/m2) 0.91	
#nitrogen content in sub-horizon F:	
N_F[kg/m2] 0.011 #organic matter content in sub-horizon H:	
-	
H(kg/m2) 0.0	
#hitrogen content in sub-horizon H:	
N_H(kg/m2) 0.0	
#organic matter stock of labile humus:	
Labile_humus[kg/m2] 0.028	
#nitrogen stock of labile humus:	
N_Labile_humus[kg/m2] 0.001	
#organic matter stock of stable humus:	
Stable_humus[kg/m2] 16.956	
#nitrogen stock of stable humus:	
N_Stable_humus[kg/m2] 0.606	
#density of organic layer, kg/dm3:	
D_ORG 0.1	
#density of mineral soil, kg/dm3:	
D_MIN 0.99	
#acidity:	
oh 4.04	
#parameter for transformation by earthworms from F subhorizon and labile to stable humus - 1 - activity of earthworms, 0 - earthwor	ms are absent:
k5_soil 1.0	
#parameter for transformation by earthworms from H subhorizon to stable humus - 0.001 - activity of earthworms, 0 - earthworms ar	re absent:
<5_soil_H 0.001	
#coefficient of mineralization for H:	
(8_soil 0.00006	
#coefficient of mineralization for stable humus:	
<8_soil 0.00006	
#redistribution of SOM flow between H and stable humus; if d=0.0 and k5=0.0 - the absence of H sub-horizon:	
10.0	
#soil hydrological constants:	
N_WP_ff5.2	
N_FC_ff 25.0	
N_Sat_ff95.0	
N_WP_ms 23.7	
N_FC_ms 38.9	
N_Sat_ms 62.2	
 d	
1 	
Ln 1, Col 1	

Figure 7. File of initial soil characteristics (InitValues_users.txt)

Specification for preparation of InitValues_users.txt file

The short comments are in the lines beginning with symbol # and being after a line with numerical values in the text of input file.

Please pay attention that lines "names" are names of cohorts, "key" are indicators of above- (0) or belowground (1) cohort, "nitr" contains values of cohorts' nitrogen, "ash" includes data on cohorts' ash concentration, "lignin" has records on lignin contents. Cohort numbers have to be identical and

correspond to the number of cohorts in the file with litter flow (no more than 14) in all these lines. It should be filled by figure 0.0 in a case of absence of data.

Simplest way to prepare the file of initial soil characteristics is as follows:

1) please open the InitValues_users.txt file (*data →ROMULS* folder) in the Notepad and save it under other name, for example: InitValues_users_1.txt;

2) replace soil data in this file by your own data;

3) save the file (in our example: InitValues_users_1.txt) with the.txt expansion (with blanks as separators) in the same ROMULS folder;

Warning

Please check whether there are no excess gaps especially in the ends of lines, and whether there are no excess empty lines at the end of the file; count number of cohorts in above specified lines.

Below is an example with values of parameters from one project.

LITTER_COUNT 10

it is integer value indicating number of all litter cohorts in considered data (14 cohorts are the greatest value, 10 are in this example)

names need1 twigs need2 leaf grass t_root_b t_root_a g_root_b sh_root_a sh_root_b n n n n

names of litter cohorts written with blank as a separator. If the name consists of several words then underlining should be used as a separator between words belonging to the same name! The number of names should correspond to number of declared litter cohorts in the first line (in this example – 10). Absent cohorts can be designated by any letter (in this example - n)

key 0 0 0 0 0 1 0 1 0 1 0 0 0 0

indicator of above- (0) or belowground (1) cohort; litter cohorts in the model are separated on above-(foliage/needles, branches, cones and so forth) and belowground (coarse and fine roots). It should be done because above- and belowground cohorts are in different temperature and moisture conditions. The number of values has to correspond 14; if data is not present on any cohort, then the value must be equal to 0.0 (a real number).

nitr 0.82 0.69 1.1 1.26 1.38 0.6 0.6 1.8 1.1 1.1 0.0 0.0 0.0 0.0

nitrogen content in litter cohort (%) - this line contains nitrogen content for each litter cohort. The number of values has to correspond 14; if data is not present for any cohort then the value must be equal to 0.0 (a real number).

ash 3.83 1.16 1.71 3.74 3.44 1.7 1.7 2.8 1.79 1.79 0.0 0.0 0.0 0.0

ash content in litter cohort (%) - this line contains ash content for each litter cohort. The number of values has to correspond 14; if data is not present for any cohort then the value must be equal to 0.0 (a real number).

lignin content in litter cohort (%) - this line contains lignin content for each litter cohort. The number of values has to correspond 14; if data is not present for any cohort then the value must be equal to 0.0 (a real number). If there are no data at all then set 0.0 for all cohorts.

$L[kg/m^2] \ 0.0$

sometimes it is possible to estimate pools of organic matter in L horizon proportionally to litter cohorts – from the modeling point of view, the first stage of fresh litter decomposition is different for different litter cohorts and still depends on their nitrogen, ash and lignin contents separately. Sometimes it is possible to distinguish their origin: the remains of leaves, needles, branches, etc. Fractions of belowground litter, with rare exception, are absent and then it is more correct to consider these fractions as equal to zero. In some cases this horizon can be absent as, for example, in the deciduous forests, litter is transformed quickly and this horizon, as a rule, is not observed in the spring yet. Taking these compartments into account is needed because rate of decomposition of organic matter in the L horizon depends on the rates of decomposition of components that didn't yet lose their properties, and it differs for different fractions. Distribution of organic matter in the L horizon between fractions can be done proportionally to the masses of litter cohorts. The number of values has to correspond 14; if data is not present for any cohort then value must be equal to 0.0 (a real number).

pools of nitrogen of the L horizon with corresponding redistribution of nitrogen of the L horizon on litter fractions similarly to described above redistribution of organic matter. The number of values has to correspond 14; if data is not present for any cohort then value must be equal to 0.0 (a real number).

$F[kg/m^2] 0.0$

pool of organic matter of the F soil horizon (the organic matter is not split into fractions in F horizon because owing to the impact of biological, physical and chemical processes it represents relatively homogenous mass and is characterized by variables described below.

```
N_F[kg/m<sup>2</sup>] 0.0
# pool of total nitrogen in F horizon;
H[kg/m2] 0.0
# pool of organic matter of the H horizon of forest floor;
N_H[kg/m<sup>2</sup>] 0.0
# pool of total nitrogen of the H horizon of forest floor;
Labile_humus[kg/m<sup>2</sup>] 0.0
# pool of labile organic matter in mineral soil (as described above);
N_Labile_humus[kg/m<sup>2</sup>] 0.0
# pool of total nitrogen in labile organic matter;
Stable_humus[kg/m2] 0.0
# nool of stable organic matter which is calculated as a difference between the measured nool of the stable organic matter which is calculated as a difference between the measured nool of the stable organic matter which is calculated as a difference between the measured nool of the stable organic matter which is calculated as a difference between the measured nool of the stable organic matter which is calculated as a difference between the measured nool of the stable organic matter which is calculated as a difference between the measured nool of total not of the stable organic matter which is calculated as a difference between the measured nool of the stable organic matter which is calculated as a difference between the measured nool of total not of the stable organic matter which is calculated as a difference between the measured nool of total not of the stable organic matter which is calculated as a difference between the measured nool of total not of the stable organic matter which is calculated as a difference between the measured nool of total not of total not
```

pool of stable organic matter which is calculated as a difference between the measured pool of organic matter in whole AB horizon and labile organic matter;

N_Stable_humus[kg/m²] 0.0

pool of total nitrogen in stable organic matter;

D_ORG 0.15

bulk density of the soil organic layer, kg/dm³. Density of soil organic and mineral horizons are necessary for calculation of dependences of rates of decomposition on moisture.

D_MIN 1.5

bulk density of mineral soil, kg/dm^3

 $pH_{\rm H2O} \ 5.00$

soil pH because some rates of organic matter decomposition depend on pH;

k5_soil 1.0

- parameter of organic matter transformation by earthworms from F horizon and labile organic matter into stable organic matter: if it is equal to 1 then activity of worms is considered, if it is 0.0 then worms don't influence the rate of organic matter transformation. In soils of temperate zone, Lumbricidae actively mixing soil and transforming soil organic matter but in boreal zone they are mostly absent. Therefore this indicator of their activity is inserted. Can take intermediate values in dependence on soil fauna activities.

k5_soil_H 0.001

parameter, reflecting organic matter transformation by worms from H horizon to stable humus: if it is equal to 0.001 then the activity of worms is considered, if 0.0 then worms do not influence the rate of organic matter transformation. Thus, it is possible to consider or exclude activity of worms at this flow of organic matter similarly to the previous comment.

k6_soil 0.00006 coefficient of organic matter mineralization in H horizon of a forest floor. This coefficient is a calibration one and changes from 0.00016 till 0.00001 in dependence on soil texture of organic floor. The more clays then the rate of decomposition of organic matter in this horizon is smaller. It depends on temperature and moisture of organic horizon contrarily to k8_soil. It depends on temperature and moisture of organic horizon contrarily to k8_soil. It depends on temperature and moisture of organic horizon contrarily to k8_soil.

k8_soil 0.00006

coefficient a mineralization of organic matter in the mineral horizon AB. This coefficient is calibration and changes from 0.0006 till 0.00001 it dependences on soil texture of mineral soil, mostly of clay percent. It depends on temperature and moisture of mineral horizon not on temperature and moisture of forest floor contrarily to k6_soil. The more clays then the rate of decomposition of organic matter in this horizon is smaller.

d 1.0

d is a parameter of redistribution of flow of soil organic matter between organic H horizon and stable humus in mineral soil. This parameter is equal to 1.0 in the absence of forest floor or H horizon. It is calculated by empirical function depending on C/N of F horizon and manages redistribution of humified matter between forest floor and mineral horizons. See table below with correspondence between d and k5_soil_H.

d	What means
d = 0.0 k5_soil_H = 0.0	All humic substances remain in H horizon
d = 1.0	All humic substances move to mineral horizons AB due to activity of soil macrofauna (earthworms)and H horizon of forest floor is absent

W_WP_ff 7.1

forest floor moisture content at the permanent wilting point, in volume %;

W_FC_ff 33.0

forest floor moisture content at field capacity, in volume %;

W_Sat_ff 62.8

forest floor moisture content at saturation (the total porosity), in volume %;

W_WP_ms 8.0

mineral soil moisture content at the permanent wilting point, in volume %;
W_FC_ms 32.2
mineral soil moisture content at field capacity, in volume %;
W_Sat_ms 52.4
mineral soil moisture content at saturation (the general porosity), in volume %.

2.1.4. File with climatic data (climate.csv)

File with climatic parameters contains average monthly temperature and moisture of forest floor and mineral soil. This input file (climate.csv) is with .csv expansion, commas as separators (Table 3). These parameters are calculated by the climatic generator SCLISS (see its Manual). t_lit is average monthly forest floor temperatures, C°, t_soil is average monthly mineral soil temperatures, C°, m_lit is average monthly moisture of forest floor in volume %, m_soil is average monthly moisture of mineral soil in volume %. Month is a time step. Reading from file is looped (if the program does not find next line at any step then it takes the first line from the scenario again). The minimum number of steps is 12 for 1 year, or bigger in dependence on number of modelling steps. The order of columns and their headings cannot be changed. Detailed preparation of this file is described in SCLISS Manual. Structure of the file is described in Table 4.

step	t_lit	t_soil	m_lit	m_soil
1	4.9	6.0	27.0	54.1
2	3.0	5.0	28.1	56.2

Table 4. Sequence of columns at preparation of the climatic input file for ROMUL

2.1.5. File with experimental data

There is an example of file in the ROMULS folder. Data have to be written down in the file with the.csv expansion. At the preparation of the file, please check commas between variables and decimal points between integer and fractional parts of the values. In the second line, all zero have to be written down as real numbers "0.0". Structure of the file is as follows. First column contains modeling step, values of the measured variable are written in the second one, third column contains its standard deviation (if it was not measured then in this column it is necessary to put value 0.0), further columns are filled similarly (see Table 4). The number of variables (columns) is unlimited.

step	Exp_value_min_soil	Exp_value_min_soil_SD	
1	16.956	2.434	
49	20.408	3.758	
121	17.542	2.5760	
181	16.426	1.9730	

Table 4.-Sequence of data in file with experimental data

3. Description of the ROMUL model interface

3.1. Work with demonstration data

1. Start shell (prShellGUILes_user.exe) then a main window of the program will be open on the screen (Fig. 8).

A DLES 1.0.1		
File Simulation Tools Display + 1 1 1	Main menu Toolbox	_

Figure 8. Main window

At the main window, the program name (DLES) is displayed as a heading; *main menu* and *toolbar* are located below.

2. The new project start. For this purpose, please press the button + at toolbar or make this operation through *Simulation* \rightarrow +*Add* project menu. After this a *New Project* dialog box will arrive (Fig. 9).

-	ols Display			
New Project			E	
Project Name			Prefix	
sim_a			а	
Project Descr	ption			
22:58:06 01	01.2013		*	
Model Scheme				
Input Data:				
Data type	Input File			
		OK	Cancel	

Figure 9. New Project dialog box

First of all you have to specify the scheme of the project by pressing button — near *Model Scheme* window. Choose modSoil_v7_0_2_users file (Fig. 10) from folder DLES_user/data/ROMULS. Then load test files with input data: InitValues_users.txt, Climat.csv, LitterFall.csv (Fig. 11).

🎎 DLES 1.0.1			
File Simulation Tools Display + 1 1 1			
New Project	🔮 Open Model S	ลา Scheme	X
Project Name sim_b	Папка:	🔋 ROMULS 👻	G 🗊 📂 🎞 •
Project Description	(Ana	Имя	Дата изменения Тип
22:49:29 01.01.2013		\mu Alice-Holt	15.12.2012 18:21 Папка с ф
	Недавние места	modSoil_v7_0_2_users	26.12.2012 13:04 Файл "DL
Model Scheme			
Input Data:	Рабочий стол		
Data type Input File			
	Библиотеки		
	Компьютер	•	4
OK		Имя файла: mod Soil_v7_0_2_users	• Открыть
		Тип файлов: DLES Scheme Files	• Отмена

Figure 10. Addition of the new project, loading of the scheme of the project

ULES 1.0.1				23
File Simulation	Tools Display			
+ []* 1	Image:			
New Project		2		
Project Name		Prefix		
sim_b		b		
Project Descript	tion			
22:49:29 01.0)1.2013			
		-		
Model Scheme				
	\Downloads\DLES_user\DLES_user\data\ROMULS\modSc	il li		
Input Data:				
Data type	Input File			
InitValues	D:\DLES_user\Data\ROMULS\InitValues_users.txt	•••		
Climate	D:\DLES_user\Data\ROMULS\Climate.csv			
LitterFall	D:\DLES_user\Data\ROMULS\LitterFall.csv			
	ОК	Cancel		

Figure 11. Loading of test files with input data

After loading of the scheme of the project in heading of main window, the name of the open project $(modSoil_v_7_0_2 users)$ and the name of the model scheme experiment (dlessch – sim_a) are displayed.

On information line below a data report *Project successfully loaded* (Fig. 12) is also displayed.

LLES - modSoil_v7_0_2_users.dlessch - sim_a	
File Simulation Tools Display	
Project successfully loaded	

Fig. 12. Main window with loaded scheme of the project

3. Initialization the project. It is carried out by the button at toolbar or through *Simulation* \rightarrow *Init all projects* menu. Please initialize the project each time from the beginning when it is necessary to make model experiment.

4. Set up the number of model steps. At the toolbar, there is an entry form of number of model steps

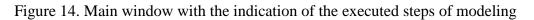
1 _____, by default it is equal to "1". One model step corresponds to one month; respectively 12 steps correspond to 1 year. Enter the necessary number of steps (Fig. 13). The number of the executed steps of modeling and information message of *Project initialized*, *0 calculated step (s)* is displayed in the bottom of a window in Information line.

LLES - modSoil_v7_0_2_users.dlessch - sim_a	
Eile Simulation Tools Display + $[12]$	
Project initialized: 0 calculated step(s)	

Figure 13. Main window indicating duration of modeling - 12 months (1 year)

5. Simulation starts by pressing the button \checkmark at the toolbar, or through *Simulation* \rightarrow *Step all projects* menu. In the bottom of window in *Information line* the number of modeling steps and information report *12 calculated step* (*s*) (Fig. 14) have to appear.

LES - modSoil_v7_0_2_users.dlessch - sim_a	
Eile <u>S</u> imulation <u>T</u> ools <u>D</u> isplay + []≱ 12 ▶ []⊉ [翻]]♥	
12 calculated step(s)	



If to press the *Step* button again, the program will add and execute the same number of steps. It is possible not to specify all period of modeling, and to consider it as short pieces. It can be convenient if the period of simulation run is very long.

If it is necessary to begin the run from the beginning, please press the initialization button and the simulation will start again (from the first step).

6. Choice of data for visualization. The choice of data for vizualization in the form of graphs or tabular data is made in tool palette "Available Data" (the button \rightarrow Selecting data menu). The list of categories of data is provided in the opened menu on the right side (Fig. 15). The double click of mouse on category opens the list (Fig. 16). In revealing lists, you need to mark by ticks the required output data. To clear all marks, it is necessary to click the corresponding category twice. It should be noted that the program remembers marks of the variables made at the previous call to the program. Therefore at the first call of the program, it is necessary to remove by double cliques on all categories the marks made at the previous calls.

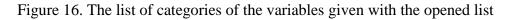
LES - modSoil_v7_0_2_users.dlessch - sim_a	
File Simulation Iools Display + ① 12 ▶ □ ₩ Ⅲ ▶	Available Data
12 calculated step(s)	

Figure 15. List of categories of data

Three categories of data are provided in the program: 1) *Climate* contains data from climate input file, 2) *Litterfall* contains data from the input file with litter fractions, 3) *modSoil_7_0_0* contains the list of the model outputs variables. Choice of all variables belonging to the category may be done if you will mark it by tick. The double click on category opens the complete list of variables of this category. If you mark the variables by ticks then they will be selected for presentation on the graphs (in the given example, an organic matter of a forest floor and size of a pool of organic matter in the mineral soil, "humus" are marked) (Fig. 16).

Please press the *Accept and View* button for a confirmation of the choice (Fig. 16). The chart with graphs will appear (Figure 17).

BLES - modSoil_v7_0_2_users.dlessch - sim_a	
File Simulation Tools Display + $[12]$ \blacktriangleright \blacksquare \blacksquare \blacksquare	
	Available Data
	forest_floor h h l fall ▼ Accept and View
12 calculated step(s)	



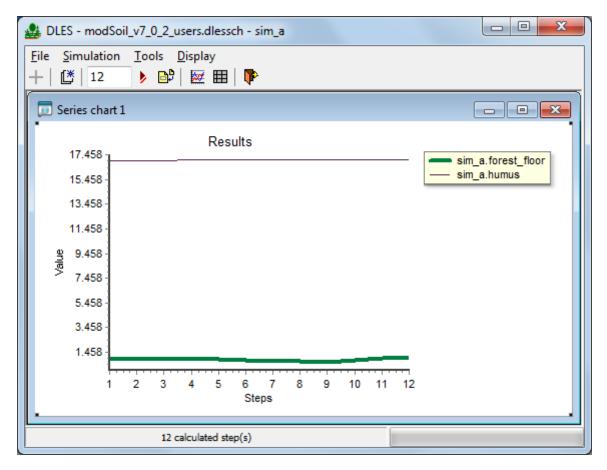


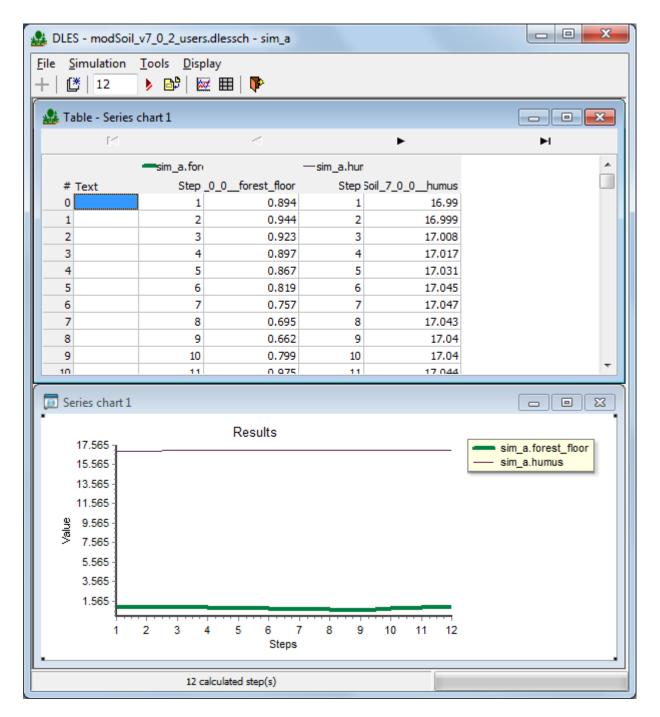
Figure 17. Main window with graphs and a legend with the list of variables

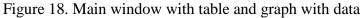
If necessary, it is possible to display the chart with other variables at any time using **Tools** \rightarrow Selecting data menu (button). If you make one click by left mouse button on parameter(s) form, you may add graph(s) by pressing *Accept and View* / After that these parameters will be drawn on the same chart with the graphs drawn earlier. If you make a double click by the left mouse button (as it was already offered earlier) on one selects item then the graphs of this chosen parameter only will be drawn. In the program, all results of the model run irrespectively of choice of data for visualization are remembered.

The chart window also has standard Windows commands \square to minimize, minimizemaximize the screen, and to close. If several windows with graphs are opened on the screen then you can put the cursor in the field of window which you want to close and click by mouse. Also, if you maximized a window in all screen then it is possible to come back to previous view by *Displays* \rightarrow *Windows* \rightarrow *Tile* menu.

If to initialize the simulation once more (pressing button \checkmark at the toolbar), the results of continuation of computed experiment will display on the graphs in addition to previous ones for number of steps specified in the *Entry of number of model steps*. It is possible to enter other number of steps. The total number of steps of modeling is displayed in *Information line* in the bottom of the chart.

Results of simulation experiment can be seen on the table as well (the button \blacksquare or the Displays \rightarrow Table menu) (Fig. 18).





It is possible to open several diagram-charts with different parameters at the same time in the working area of the screen (Fig. 19). For this purpose, choose *Tools* \rightarrow *Selecting data* menu (button) and mark data for other graph.

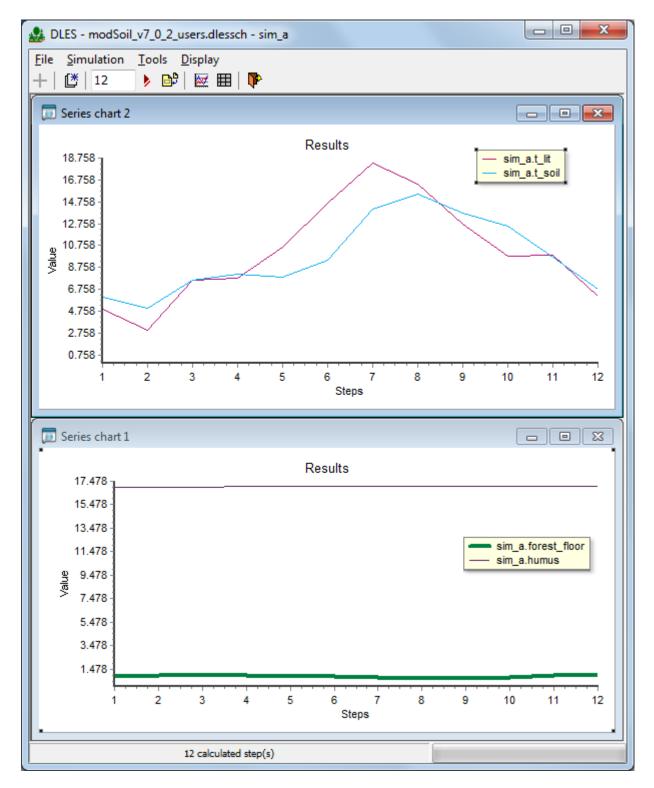


Figure 19. Main window with two charts

the graph windows can occupy the whole screen or be settled down as a cascade, the choice of a mode is carried out in the *Displays* \rightarrow *Windows* menu.

It is possible to close all windows by *Displays* - Close all menu

The chosen list of data for visualization is remembered automatically at program switching off. At following start of the program, it is possible to visualize graphs with the same variables by pressing button

or through *Displays* →*Series Chart* menu.

6. Editing of the chart. You need to call a chart element (an axis, a legend, a series of data, the chart name) with double click and change properties of an element in the appeared palette (Fig. 20). It is possible to change name of charts, names of axes (to add units of measurement of parameters); thickness, color, view of line; look and the size of fonts or to make an element invisible. It is also possible to edit any properties of the chart through the chart editor (*click by the right button of mouse* \rightarrow Editor).

Legend Options 🛛	Axis 33 Title Font Value		
Alignment Top Substance Left Custom Right	Labels 3 🗭 Decimals Font	Series Properties Title sim_c.forest_floor	
Bottom Custom position	Scales 4.975 Max 🗸 Auto	Active	Graph Title Caption
Left 14 Top 31	0.000 Min Auto	Color Pen — X: 4.00; Y: 4.9007 Min: 4.7579; Max: 4.9283	Results Visible Font

Figure 20. Palettes for property changes in the chart (legend, axes, series of data, chart name).

So, for example, if it is necessary to edit the scale of temperatures (Fig. 20-1) then please load the cursor on a scale and after call of pop-up menu click once with right mouse button. Choose object for editing in the editing catalog: *Editor* \rightarrow *Axis (axis)* (Fig. 20-2).

Further please choose menu for left axis editing: $Axis \rightarrow Left Axis$ (fig. 20-2) and change usual way for Windows parameters of axis: *Minimum* (the minimum value on the axis), *Maximum* (the maximum value on the axis), *Increment* (step between the specified values of scale) and choose necessary values by

pressing Change... and bring value in the opened window (fig. 20-3). Confirm choice by OK. If you specify maximum value of scale as an integer in *Maximum* menu, and put "0" in the *Offset* window, then you will see integers on the graph axis (fig. 20-4).

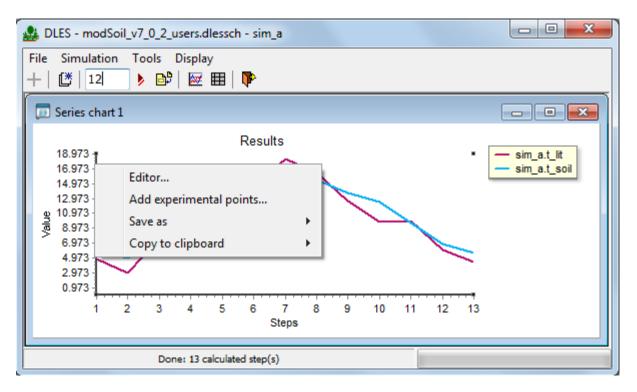


Figure 20-1. Chart editing

BLES - modSoil_v7_0_2_users.dlessch	n - sim_a	
File Simulation Tools Display + 12 12 12 12	•	
Series chart 1		
18.973 □	Visible Visible Behind Axes: Left Axis Right Axis Top Axis Bottom Axis Depth Right +	Scales Title Labels Ticks Gri Options Minimum Maximum Inc Automatic Visible Inverted Logarithmic Log Base: 10
]	Close
Done: 13 calculate	ed step(s)	

Figure 20-2. Chart editing

🔬 DLES - modSoil_	v7_0_2_users.dlessch - sim_a	
File Simulation + []* 12	Tools Display Desired Value Increment	
18.973 - 14.973 -	Increment:	es Title Labels Ticks Gri
ຍ 10.973 6.973	OK Cancel	Change Show all labels sired Increment:
2.973	Panel Paging + -	Close
	Done: 13 calculated step(s)	

Figure 20-3. Chart editing

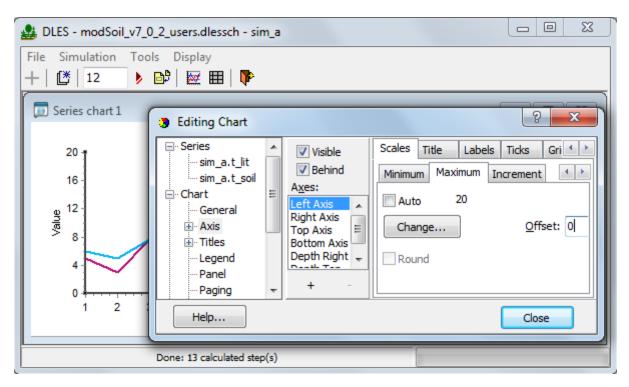


Figure 20-4. Chart editing

By *Tools* ->Close all toolboxes menu it you may close at once all panels opened on the right.

7. If necessary, you may *add points of laboratory or field measurements of parameters on the graph*. The demonstration file contains experimental data of 16 years observation of soil organic matter (humus) dynamics. You may display experimental data using file with experimental data versus simulating soil

dynamics for 20 years (240 steps) at the same graph. Let we display the graph of soil organic matter dynamics (ticking on corresponding variable in invariable list (Fig. 21).

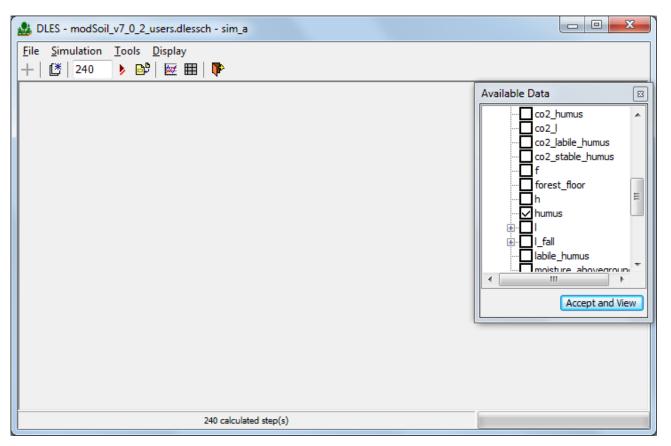


Figure 21. Opening data on humus dynamics in soil (results of computer experiment on 240 steps, i.e. 20 years)

Please open additional menu clicking right mouse button at the window with graph (Fig. 22). From *Add experimental points* \rightarrow menu choose the file with experimental points *exp_data*. The result of experimental points with standard deviations loading on the diagram is presented at Figure 23.

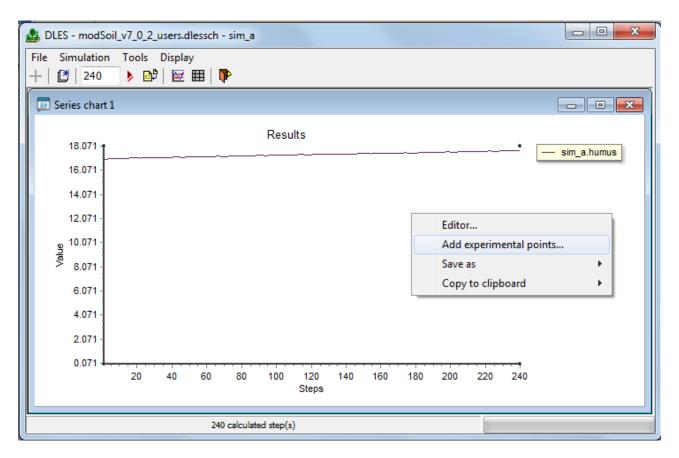


Figure 22. Opening menu for addition of experimental points on the graph

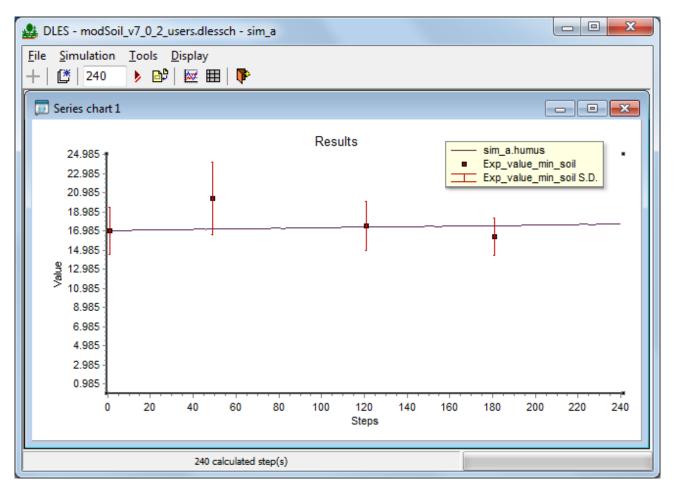


Figure23. Result of loading of experimental points with standard deviations on the graph

The file with experimental points is described in the section "Preparation of Input Files".

8. Results of modeling can be saved in different formats (graphic, text). You should do the following for saving the results: 1) choose the chart (make it active by clicking on it), 2) call additional menu (Fig. 24) (click by the right mouse button) and choose option *"Save as"*, 3) choose format of data export (Bitmap,, Metafile in the form of vector graphics, Comma-separated values in the form of the text with comma separators).

You may choose in additional menu option "Copy to clipboard" for copying and a subsequent insertion to other documents.

The only data that are displayed (Fig. 25) can be saved at any mode of graph saving.

🏭 DLES - modSoi	I_v7_0_2_users.dlessch - sim_a
	Tools Display
+ 12	
👼 Series chart 1	
17.458 1	Results
17.450	sim_a.forest_floor
13.458	
11.458	Editor
<u>위</u> 9.458 · 명 · · · · · · · ·	Add experimental points
⁹⁵ 7.458	Save as Bitmap
5.458	Copy to clipboard Metafile
3.458	Comma-separated values
1.458	
	2 3 4 5 6 7 8 9 10 11 12 Steps
	12 calculated step(s)

Figure 24. Menu of saving results

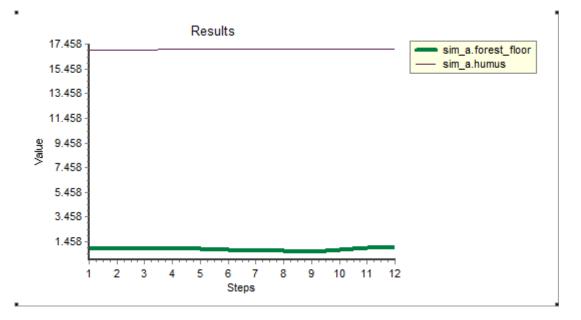


Figure 25. Example of graph kept as "Bitmap" and further inserted into this text

9. For an exit of the program press button \mathbb{P} in a command line, or choose in the *File* $\rightarrow Exit$ menu; it is also possible to use the standard Windows command \blacksquare .

3.2. Work with own data

You need perform the following to replace the test files by the files with your own data:

1. Preparation the files with own data. The information how to prepare files with own data is in the section 2. 'Preparation of Input Files for the ROMUL'.

Note. Replace files only with files of the same structure! Do not move files to another folder and do not change file structure.

2. If the program was already started with the test data, -please close the program (\mathbf{P}) and start it again (prShellGUILes_user.exe file).

3. Add the project scheme as it is described in sections 1 and 2 of part 3 (see above): press the

button i, then the button mear the Model Scheme window and choose file scheme modSoil_v7_0_2_users file; then test files with input data are automatically loaded: InitValues_users.txt, Climat.csv, LitterFall.csv (Fig. 26).

4. Replace test files with your data files. For this procedure, please call for files catalog by pressing button $\boxed{\hdotset{ or corresponding}}$ and select by cursor a necessary file, clicking by mouse at corresponding line (Fig. 26). Confirm choice of files by $\boxed{\hdotset{ ok}}$.

A DLES 1.0.1				X		
File Simulation Tools Display + [1] [] [] []						
New Project						
Project Name	Pre	efix				
sim_c	c					
Project Description						
12:54:02 23.01.	2013	*				
Model Scheme	Model Scheme					
D:\DLES_user\data\ROMULS\modSoil_v7_0_2_users.dlessch						
Input Data:						
Data type	Input File					
InitValues	D:\DLES_user\data\ROMULS\InitValues_users_1.txt					
Climate	D:\DLES_user\data\ROMULS\climate_1.csv					
LitterFall	D:\DLES_user\Data\ROMULS\LitterFall.csv	•				
	OK Cance	el				

Figure 26. Replacement of test files by files with own data

If necessary, edit the project name. For this purpose, please mark out the already written down name of the project by the cursor, and write down your file name . The name of the project has to be written down without blanks (the underscore is admissible), do not begin name with number. The name should contain no more than 223 symbols. Whenever possible, please award a short name as the long one creates inconveniences at a transfer of results to graph or to printing. By default projects, the names are called as "sim_a, sim_b", etc. (Fig. 26).

If necessary, you can add the project description in the section "Project Description". By default, this field contains time and date of opening of the project. Any letters can be used in the description, the number of symbols isn't practically limited (to 70000 signs) (Fig. 26).

References

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Hierarchy: From Molecules to the Ecosphere". Eds F.Jordan and S.E. Jorgensen. Developments in Environmental Modelling Series , V.25, Elsevier Science, pp. 331-354.

- Chertov, O.G. Komarov, A.S., Nadporozhskaya, M.A., Bykhovets, S.A., Zudin, S.L. 2001. ROMUL a model of forest soil organic matter dynamics as a substantial tool for forest ecosystem modelling. Ecological Modelling 138 (1-3): 289-308.
- Komarov, A.S., Chertov O.G., et al. 2007. Modelling of organic matter dynamics in forest ecosystems. V.N.Kudeyarov (Ed.). Moscow. Nauka. 380 p. (In Russian).
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Plant material	Ash, %	C. %	N. %	C/N
Clover (Trifolium pratense)	7.6	34.22	2.31	15.6
Arrhenatherum elatius	9.0	41.58	1.67	24.9
Fern (Athyrium filix-femina)	11	34.61	2.38	14.8
Birch, leaves (Betula pendula)	4.6	37.58	2.15	17.6
Oak, leaves (Quercus robur)	5.4	39.36	2.01	20.8
Spruce, needles	5.7	41.28	1.10	37.3
Bearberry, leaves (Arctostaphylos uva-ursi)	3.0	42.59	1.17	36.4
Cowberry, leaves (Vaccinium vitis-idaea)	3,2	38,05	0,73	52,1
Green mosses*	4.2	34.19	1.53	23.8
Sphagnum sp.	2.7	35.27	1.59	23
Oak cork (Quercus robur)	5.0	35.15	0.79	44.6
Spruce (Picea abies)sawdust	0.8	45.30	0.32	141.6
Fern (Matteuccia aspleniaceae)	9.3	37.14	0.68	54.62
Fern (Gymnocarpium dryopteris)	10.3	37.38	0.89	42.00
Alder, leaves	4.9	42.12	1.72	24.49
Mountain ash, leaves	6.4	40.14	2.40	16.73
Aspen, leaves	8.3	39.16	1.35	29.01
Pine, needles	2.7	45.36	1.23	36.88
Nettle, leaves	20	32.45	1.97	16.47
Nettle, stems	5.4	39.04	1.41	27.69
Lime-tree, leaves	7.5	40.76	2.26	18.04
Colts-foot	21	33.52	1.57	21.35
Horse-tail (Equisetum arvense)	18.4	31.76	1.19	26.69
StJohn's wort (Hypericum perforatum)	3.1	41.34	1.61	25.68
Camomile (Chamomilla suaveolens)	13.4	37.24	1.55	24.03

Appendix 1. Ash, C, N, , C/N in different plants (OMRISK, ..., 2008)

Appendix 2. The main commands for work with the Romul model

Main menu	Toolbar	Description
Editor		Edition of properties of the chart
Add experimental points		Opens the menu for addition of experimental points on the chart
Save as		Choice of a way of saving results
Copy to clipboard		Copy results to clipboard for inserting in other documents
Simulation→Add project	+	Opens the menu for addition of the new project
Simulation→Init all project	<u>ت</u>	Initializes the open project
	1	Window for input of number of modeling steps
Simulation→Step all project	>	Makes active the number of modeling steps
Tools→Project properties		Opens the panel of properties of the project
Tools \rightarrow Selecting data	6	Opens the barl of a choice of data for visualization
Tools→Log		Field for information on system mistakes
Tools→Close all toolboxes		Closes all panels, except a toolbar
Displays→Windows		Choice of mode of display charts and tables
Displays→Series Chart		Displays the chosen data in the form of the diagram
Displays→Table	⊞	Displays chosen data as a table
Displays→Close all		Closes all windows with charts and tables
File→Exit	P	Closes the program
The additional menu (is acti	vated by pressing	g of the right button of a mouse)
Editor		Edition of properties of the chart
Add experimental points		Opens the menu of addition of experimental points on the chart
Save as		Choice of a way of saving results
Copy to clipboard		Choice of a way of copying results for inserting in other documents

Variable name in the program list	Description		
1	Organic matter in the L horizon		
f	Organic matter in the F horizon		
h	Organic matter in the H horizon		
forest_floor	Total organic matter in a forest floor		
labile_humus	Labile organic matter of the mineral horizons		
stable_humus	Stable organic matter of the mineral horizons		
humus	Sum of labile and stable organic matter		
n_l	Nitrogen in organic matter in the L horizon		
n_f	Nitrogen in organic matter in the F horizon		
n_h	Nitrogen in organic matter in the H horizon		
n_forest_floor	Total pool of nitrogen in a forest floor		
n_labile_humus	Nitrogen in labile organic matter of the mineral horizons		
n_stable_humus	Nitrogen in stable organic matter of the mineral horizons		
n_humus	Total nitrogen in organic matter of the mineral horizons		
cn_l	C/N ratio in L horizon		
f	C/N ratio in F horizon		
h	C/N ratio in H horizon		
cn_forest_floor	C/N ratio in forest floor		
cn_labile_humus	C/N ratio in labile organic matter of the mineral horizons		
cn_stabile_humus	C/N ratio in stable organic matter of the mineral horizons		
cn_humus	C/N ratio in mineral soil		
co2_l	CO2 emission from L horizon		
co2_f	CO2 emission from F horizon		
h	CO2 emission from H horizon		
co2_forest_floor	CO2 emission from forest floor		
co2_labile_humus	CO2 emission from labile organic matter of the mineral horizons		
co2_stable_humus	CO2 emission from stable organic matter of the mineral horizons		
co2_humus	CO2 emission from mineral horizons		
l_fall	Total litter flow on the soil		
n_available	Mineral nitrogen available to plants		

Appendix 3. Description of variables in the Romul program