Macroscopic kinetics of temporal and spatial NDVI variability in conditions of heavy metals contamination of soil

G. P. Glazunov[a], V. M. Gendugov[b], M.V. Evdokimova[a], R.P. Titarev[a], M.V. Shestakova[a]

a Department of Soil Science, Moscow M.V.Lomonosov State University, Moscow, Russia
b Department of Mechanics and Mathematics, Moscow State University, Moscow, Russia

e-mail: glazng@mail.ru

Rates of living cells growth and of substances' concentrations changes

$$\begin{cases} \dfrac{dq}{dt} = F\left(c_{ik}\right) q \\ \dfrac{dc_{ik}}{dt} = m_k\left(\nu'_{ik} - \nu''_{ik}\right)\varepsilon_i \dfrac{1}{\rho} \end{cases}$$

$q -$ **mass of living cells [kg],**

$t -$ **time [s],**

$F\left(c_{ik}\right) -$ **the rate coefficient of a biochemical reaction [1/s],**

$c_{ik} -$ **concentracion of the** $k -$ **th substance [kg/kg] in the** $i -$ **th**

$m_k -$ **molecular weight of the** $k -$ **th** A_{ik} **substance** $[\mathrm{kg/m^3}]$**,**

$\varepsilon_i -$ **the rate of the** $i -$ **th reaction [1/s],**

$\rho -$ **density of the system "living cells-substrate"** $[\text{кг/м}^3]$

The rate coefficient of a biochemical reaction

$$F\left(c_{ik}\right)=\left(-KZ+B\right)\Psi$$

$K-$ **the rate coefficient of a biomass growth,**

$B-$ **the rate coefficient of a biomass decline,**

$$Z=\frac{1}{\sqrt[n]{\prod_{i=1}^{n}\prod_{k=1}^{N_i}c_{ik}^{\mu'_{ik}-\mu''_{ik}}}}$$

$$\Psi=\left(-\frac{1}{n}\right)\left[\sum_{i=1}^{n}\frac{m_k\varepsilon_i}{\rho}\sum_{k=1}^{N_i}\frac{\left(\nu'_{ik}-\nu''_{ik}\right)\left(\mu'_{ik}-\mu''_{ik}\right)}{c_{ik}}\right]$$

Chemical transformations

$$\sum_{k=1}^{N_i}A_{ik}\nu'_{ik}\rightleftarrows\sum_{k=1}^{N_i}A_{ik}\nu''_{ik}$$

$\nu'_{ik},\nu''_{ik}-$ **stoichiometric coefficients of the** $k-$**th substance before and after reaction respectively**

Biochemical transformations

$$\sum_{i=1}^{n}\sum_{k=1}^{N_i}A_{ik}\mu'_{ik}\rightleftarrows\sum_{i=1}^{n}\sum_{k=1}^{N_i}A_{ik}\mu''_{ik}$$

$\mu'_{ik},\mu''_{ik}-$**stoichiometric coefficients of the** $k-$**th substance before and after reaction respectively**

$A_{ik}-$ **chemical symbol of the** $k-$**th substance in the** $i-$**th reaction,** $k=1,...,N_i$**;** $i=1,...,n$

Resulting equations

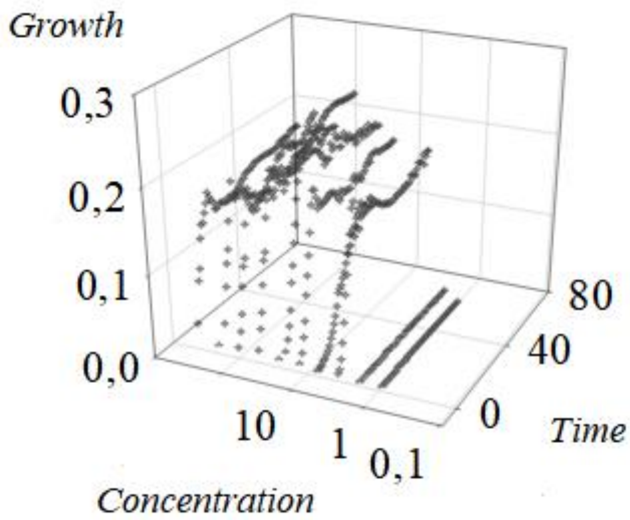
The growth equation (it is derived under the condition of constancy of initial concentrations of substrate components):

$$q = \lambda t^{-B} \exp\left(-\frac{k}{t}\right)$$

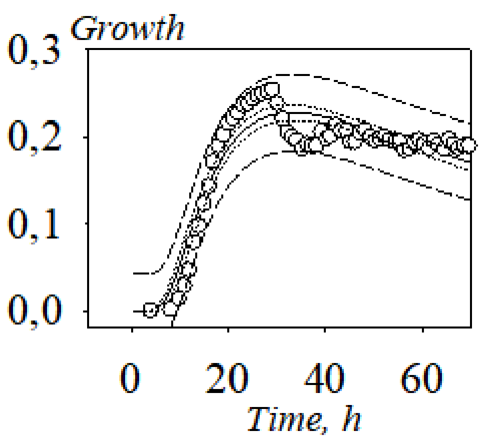
The dose-response equation (it is derived under the condition of constancy of time):

$$q = \Lambda z^{-B} \exp\left(-\frac{K}{z}\right)$$

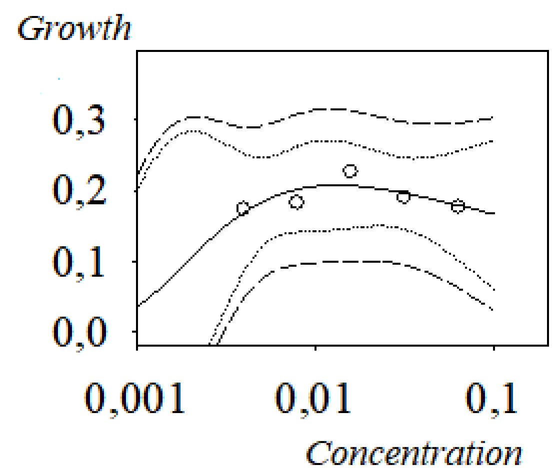
$z = \sqrt[n]{\prod_{i=1}^{n} \left(c_{i1}^{\circ}\right)}$ **– the geometric mean of concentrations of components.**



Modelling of microbial growth and dose-response.

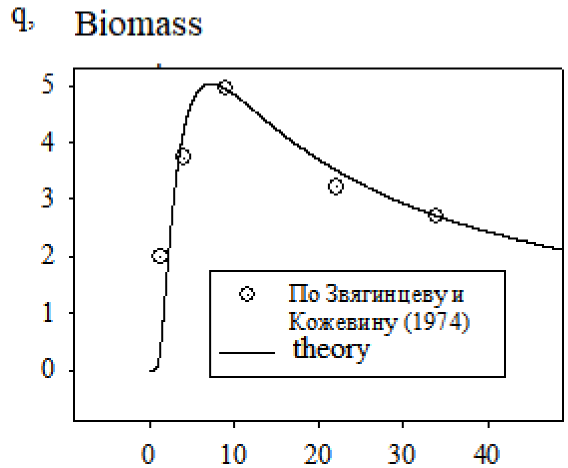


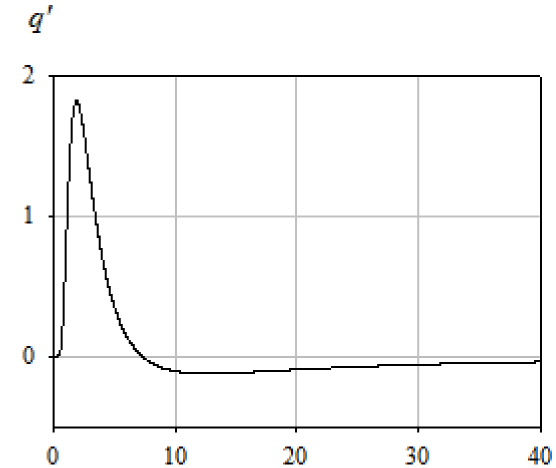
$$q = \lambda t^{-B} \exp\left(-\frac{k}{t}\right)$$

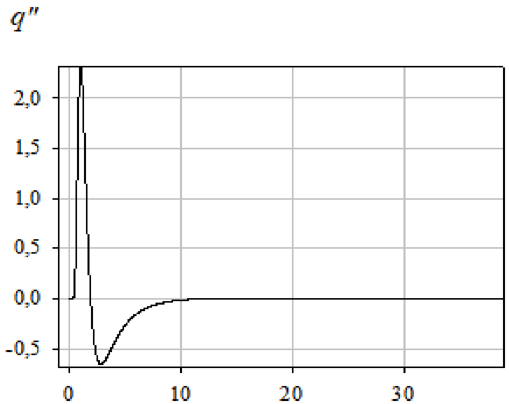


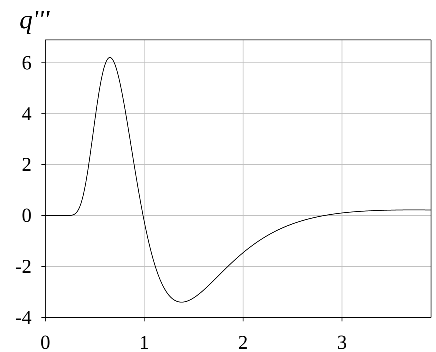
$$q = \Lambda z^{-B} \exp\left(-\frac{K}{z}\right)$$

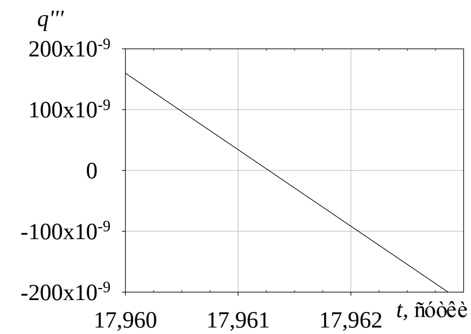
Analyzing singular points.











Singular points

t_0 – **beginning of intensive growth**

t_1 – **concavity to the left of maximum**

t_2 – **nflection to the left of maximum**

t_3 – **convexity to the left of maximum**

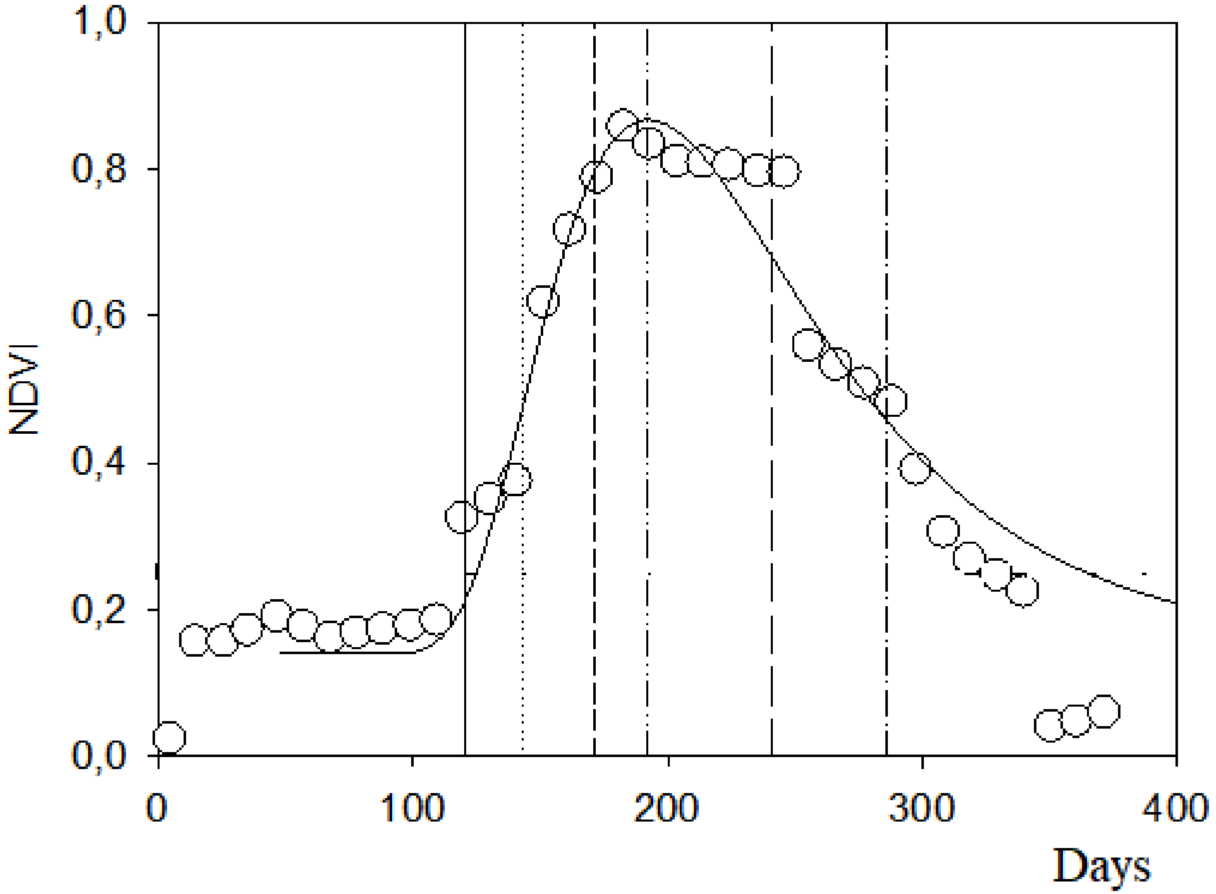
t_4 – **time of maximum biomass**

t_5 – **inflection to the right of maximum**

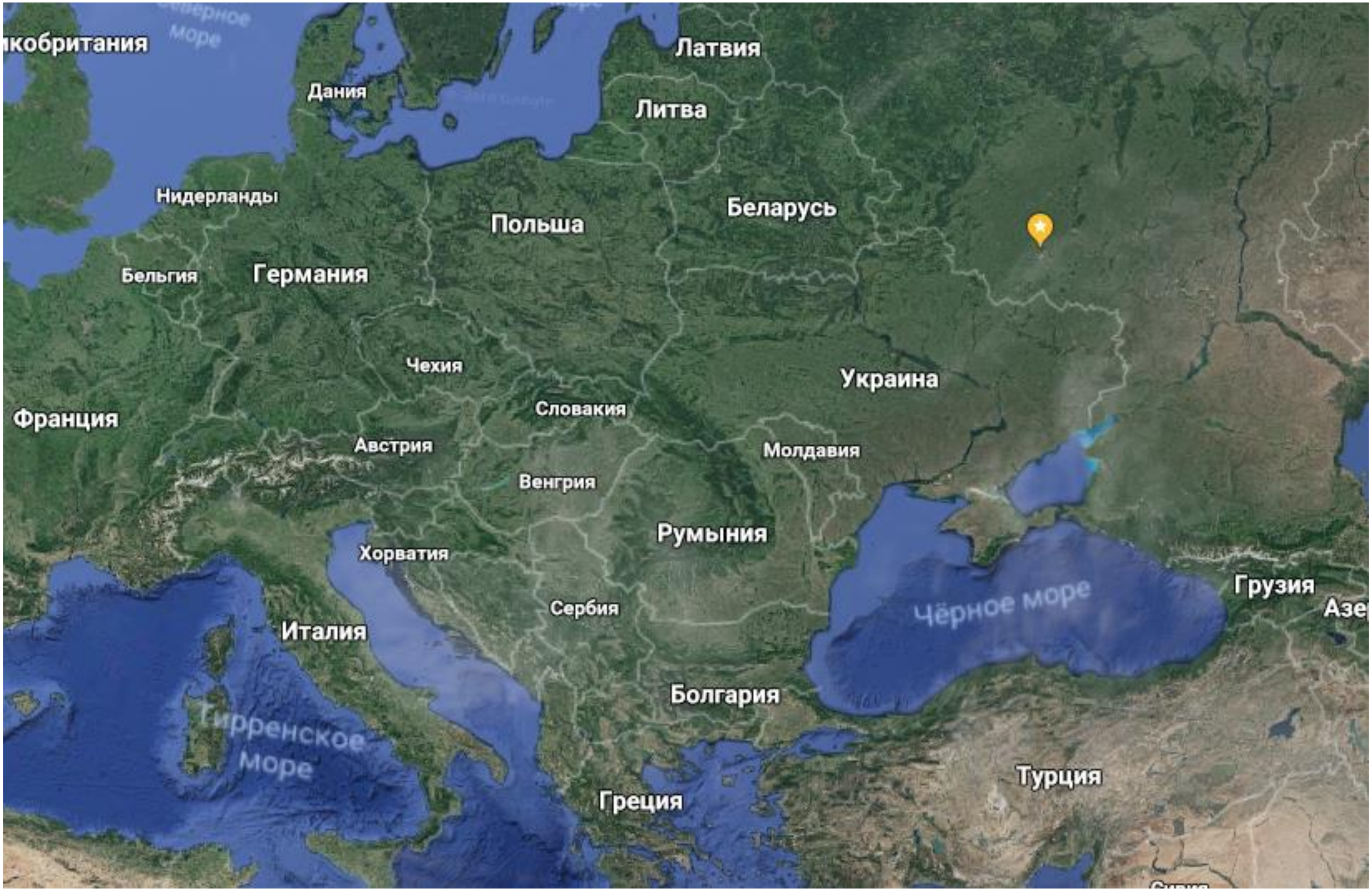
t_6 – **concavity to the right of maximum**

Interval	q	q'	q''
$t_0 < t \le t_1$	+↑	+↑	+↑
$t_1 < t \le t_2$	+↑	+↑	+↓
$t_2 < t \le t_3$	+↑	+↓	–↓
$t_3 < t \le t_4$	+↑	+↓	–↑
$t_4 < t \le t_5$	+↓	–↓	–↑
$t_5 < t \le t_6$	+↓	–↑	+↑
$t_6 < t$	+↓	–↑	+↓

Six singular points separate seven growth phases.



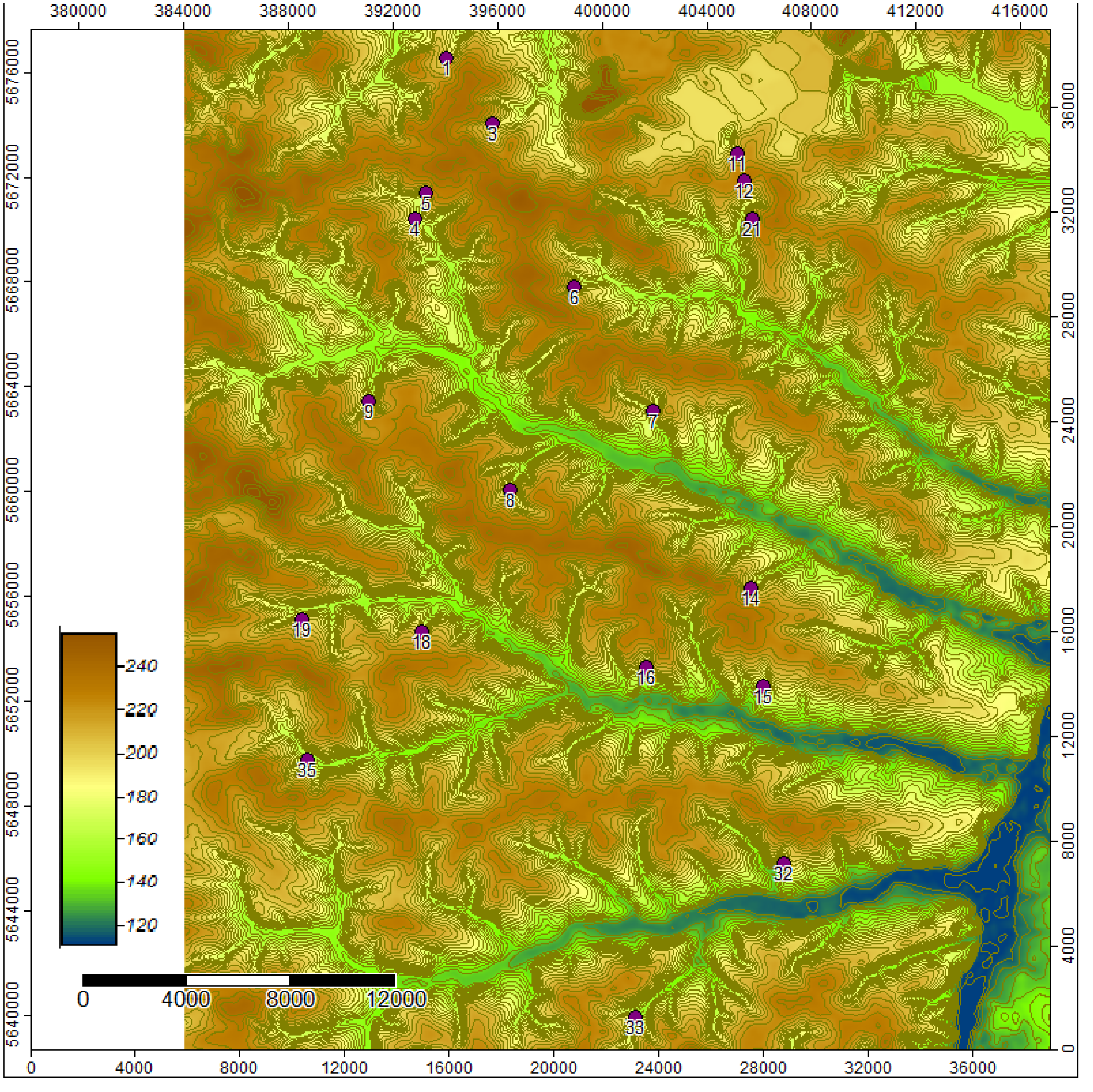
Career on extraction of iron ore near to Gubkin and Stary Oskol in Russian Federation.



Career on extraction of iron ore near to Gubkin and Stary Oskol.

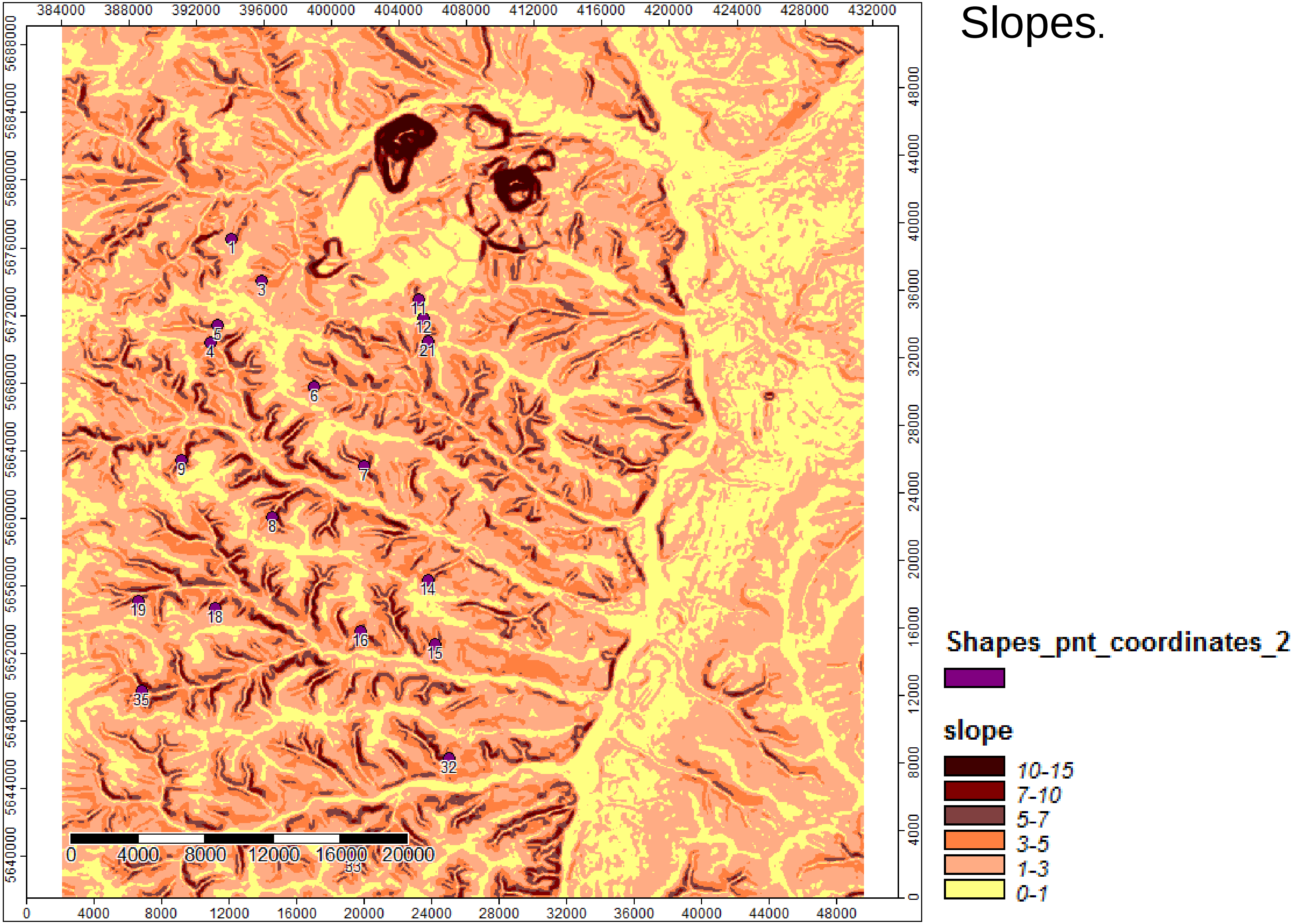
Career on extraction of iron ore near to Gubkin and Stary Oskol.

Relief map.

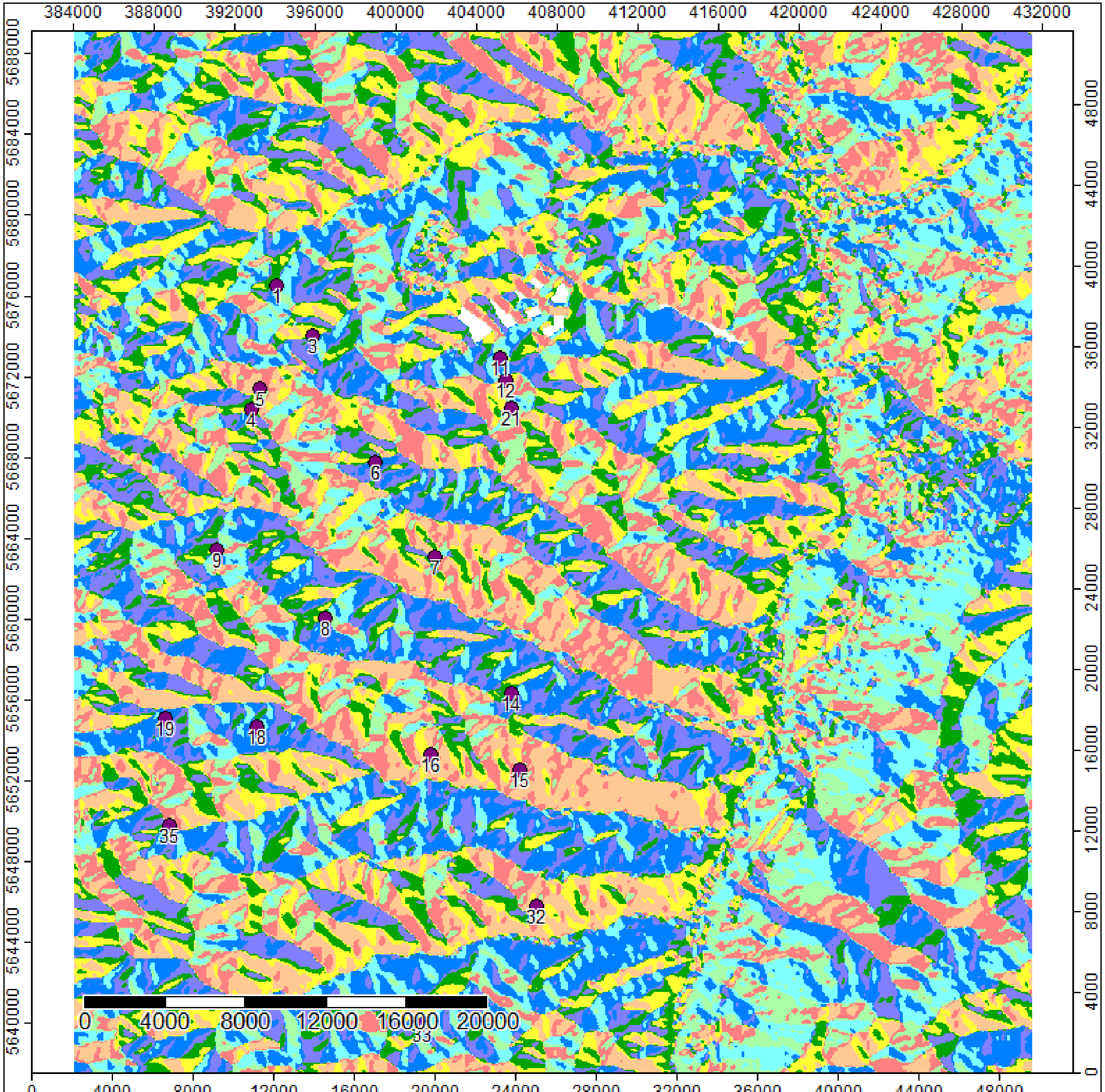


380000
384000
388000
392000
396000
400000
404000
408000
412000
416000
5676000
5672000
5668000
5664000
5660000
5656000
5652000
5648000
5644000
5640000
36000
32000
28000
24000
20000
16000
12000
8000
4000
0
4000
8000
12000
16000
20000
24000
28000
32000
36000
240
220
200
180
160
140
120
0
4000
8000
12000
1
3
11
12
5
4
21
6
9
7
8
14
19
18
16
15
35
32
33

Slopes.


Shapes_pnt_coordinates_2
slope
10-15
7-10
5-7
3-5
1-3
0-1
0 4000 8000 12000 16000 20000

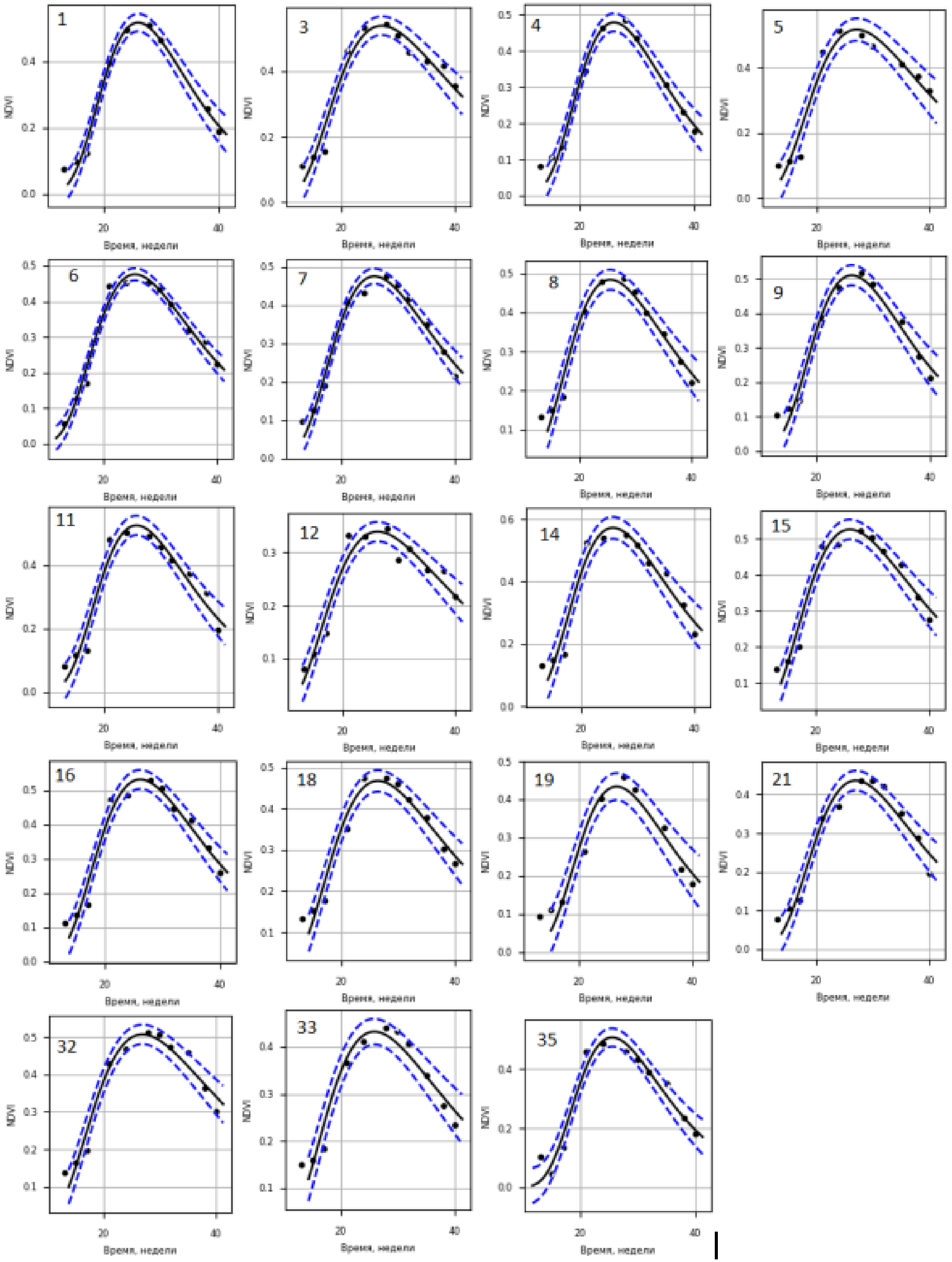
Aspects.



0 4000 8000 12000 16000 20000
Shapes_pnt_coordinates_2
aspect
N
NW
W
SW
S
SE
E
NE
N

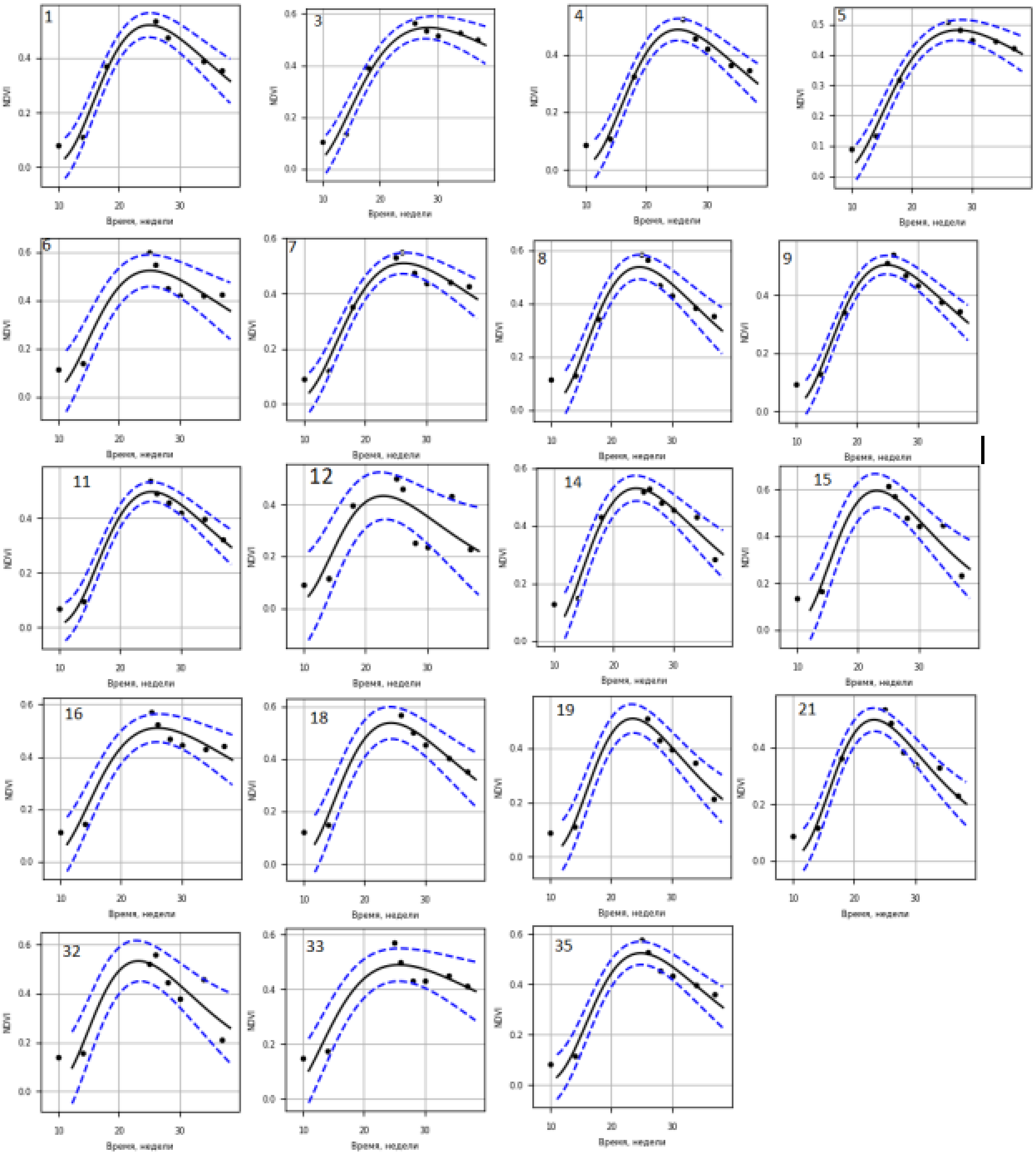
The concentration of components (ppm) in the soil at the monitoring sites (№)

Название н.п.	№ МП	Li	V	Cr	Co	Ni	Cu	Zn	As	Sr	Zr	Mo	Cd	Sn	Sb	Cs	Ba	Pb
Романово	Н1	26.0	110.0	57.0	9.5	32.0	25.0	67.0	6.7	100.0	180.0	1.10	0.36	3.60	2.30	4.0	390.0	24.0
Сенное	Н3	27.0	110.0	54.0	9.5	29.0	18.0	57.0	7.1	91.0	160.0	1.00	0.27	2.50	0.63	4.1	340.0	21.0
Галичи	Н4	29.0	120.0	55.0	11.0	31.0	18.0	63.0	5.7	110.0	160.0	0.85	0.25	2.50	0.54	4.4	360.0	23.0
Кленовенькое	Н5	21.0	120.0	56.0	12.0	32.0	19.0	75.0	7.1	150.0	160.0	1.40	0.33	2.30	0.55	4.2	360.0	24.0
Долгик	Н6	26.0	110.0	50.0	11.0	30.0	20.0	74.0	6.4	100.0	180.0	0.93	0.71	12.00	1.90	3.8	400.0	30.0
Барское	Н7	22.0	110.0	51.0	12.0	31.0	31.0	80.0	4.6	110.0	210.0	1.10	0.58	5.50	0.85	3.6	440.0	27.0
Водяное	Н8	35.0	130.0	59.0	11.0	37.0	21.0	97.0	7.6	93.0	170.0	0.93	0.29	3.50	0.73	4.6	380.0	24.0
Хмелеватое	Н9	27.0	110.0	53.0	9.2	28.0	17.0	54.0	5.7	91.0	180.0	0.78	0.25	2.50	0.57	3.7	350.0	22.0
Днище Суры	Н11	18.0	63.0	71.0	8.3	26.0	26.0	78.0	4.9	110.0	140.0	1.70	0.41	1.90	0.67	3.3	320.0	18.0
Ямская плакор																		
косимая	Н12	26.0	90.0	42.0	8.8	25.0	18.0	47.0	5.1	68.0	110.0	0.81	0.40	2.60	0.54	3.7	310.0	22.0
некосимая	Н13	22.0	90.0	46.0	8.7	25.0	17.0	45.0	5.8	68.0	110.0	0.81	0.32	2.30	0.54	3.5	300.0	21.0
Осинник	Н14	27.0	120.0	54.0	13.0	34.0	20.0	57.0	6.1	110.0	170.0	1.20	0.36	2.70	0.59	4.3	410.0	26.0
Резников Яр	Н15	24.0	110.0	55.0	13.0	35.0	25.0	85.0	6.2	170.0	200.0	0.95	0.54	6.40	1.90	4.1	420.0	28.0
Косино	Н16	22.0	110.0	53.0	13.0	32.0	22.0	61.0	6.0	110.0	210.0	0.97	0.34	2.30	0.57	3.7	420.0	24.0
Воробьево	Н18	29.0	120.0	55.0	11.0	36.0	21.0	63.0	8.4	92.0	140.0	0.93	0.29	2.60	0.66	4.4	330.0	22.0
Вислое	Н19	29.0	120.0	57.0	12.0	34.0	19.0	58.0	7.6	100.0	180.0	0.86	0.29	2.50	0.61	4.3	400.0	24.0
Еремкин лог	Н21	21.0	89.0	94.0	11.0	38.0	34.0	73.0	7.8	110.0	230.0	3.00	0.29	2.50	0.68	3.9	390.0	20.0



Seasonal dynamics of NDVI on monitoring sites of the reserve "Yamskaya steppe" in 2015

Figure in the upper left corner – site code,
points – experiment,
solid line – by growth equation,
dotted – confidence intervals for the model.



Seasonal dynamics of NDVI on monitoring sites of the reserve "Yamskaya steppe" in 2016

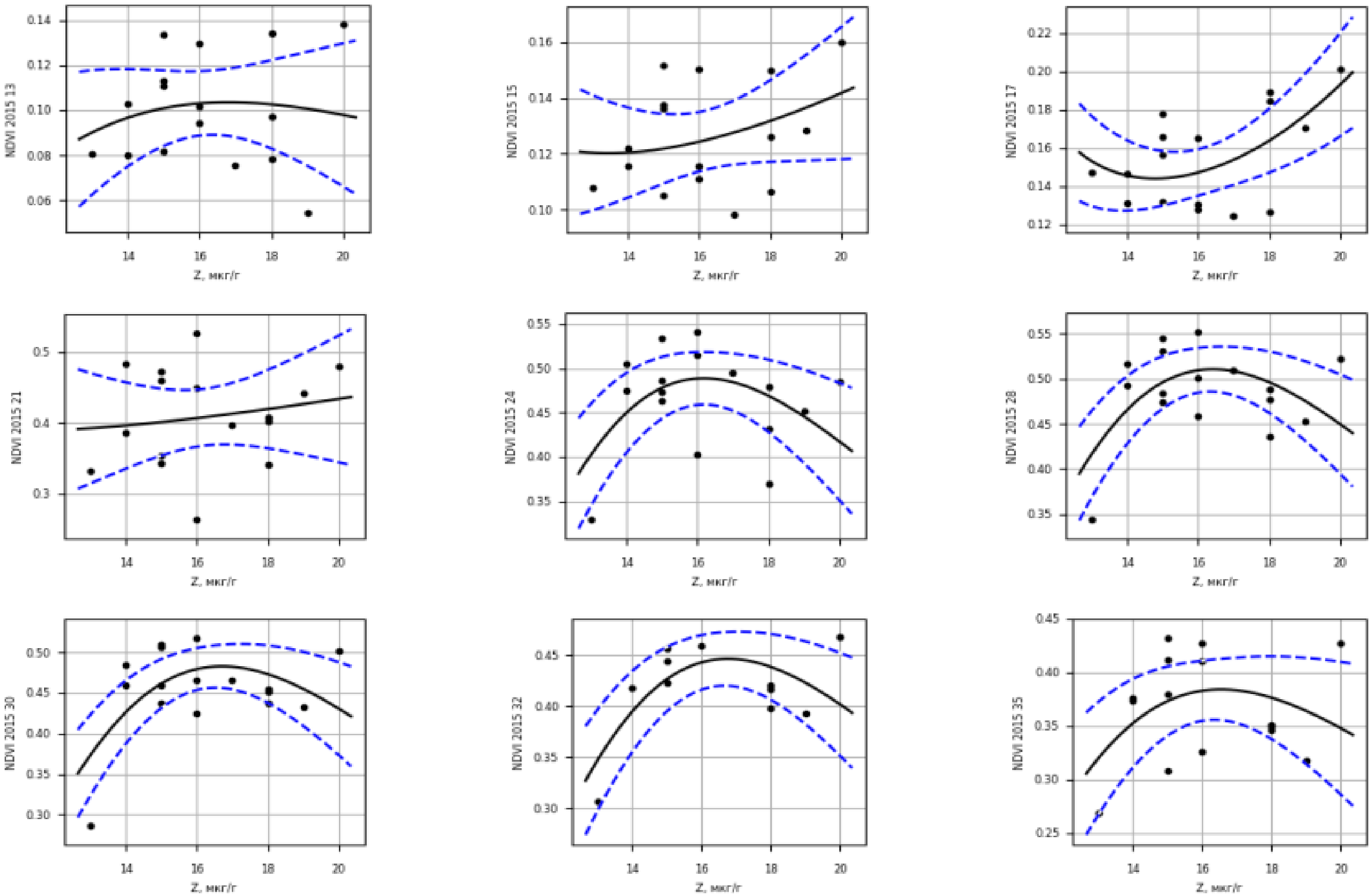
Figure in the upper left corner – site code, points – experiment, solid line – by growth equation, dotted – confidence intervals for the model.

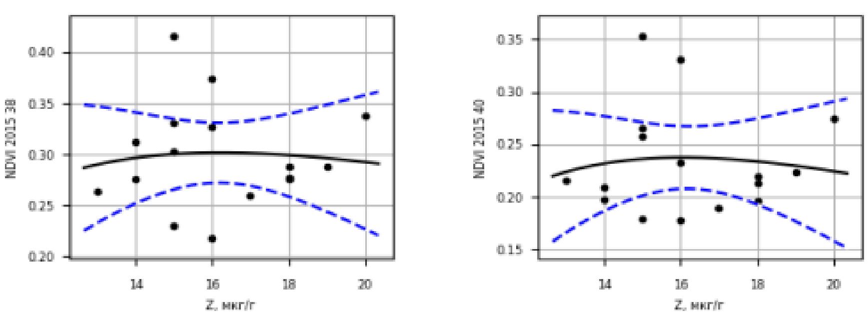
Parameters and special points of the model of seasonal dynamics of NDVI in 2015 for monitoring sites in the reserve " Yamskaya steppe".

Площадка	λ	B	k	t_1	t_2	t_3	t_4	t_5	t_6
1	4,4558E+20	11,3	294,21	15	19	23	26	33	40
3	1,13383E+12	6,6	178,98	13	17	23	27	37	46
4	1,43262E+20	11,1	287,77	15	19	23	26	33	40
5	1,21225E+13	7,2	193,96	13	18	23	27	37	45
6	1,26601E+15	8,4	214,14	13	17	22	26	34	41
7	1,72088E+14	7,9	203,57	13	17	22	26	34	42
8	8,40699E+13	7,7	197,22	13	17	22	25	34	42
9	2,22861E+17	9,5	249,76	14	18	23	26	34	42
11	2,88441E+17	9,6	247,36	14	18	23	26	34	41
12	10300488106	5,7	148,39	12	16	21	26	36	46
14	5,98236E+15	8,7	222,78	13	17	22	26	34	41
15	1,3584E+12	6,7	174,69	12	17	22	26	35	44
16	2,39318E+14	7,9	206,95	13	17	22	26	35	43
18	6,54977E+11	6,5	173,02	12	17	22	26	36	45
19	5,89194E+18	10,3	274,31	15	19	24	27	35	42
21	1,36096E+15	8,3	224,30	14	18	23	27	36	44
32	25598603871	5,7	154,57	12	17	22	27	37	47
33	48121697048	6,0	154,83	12	16	21	26	36	45
35	9,40488E+19	11,0	281,19	14	18	23	26	33	39

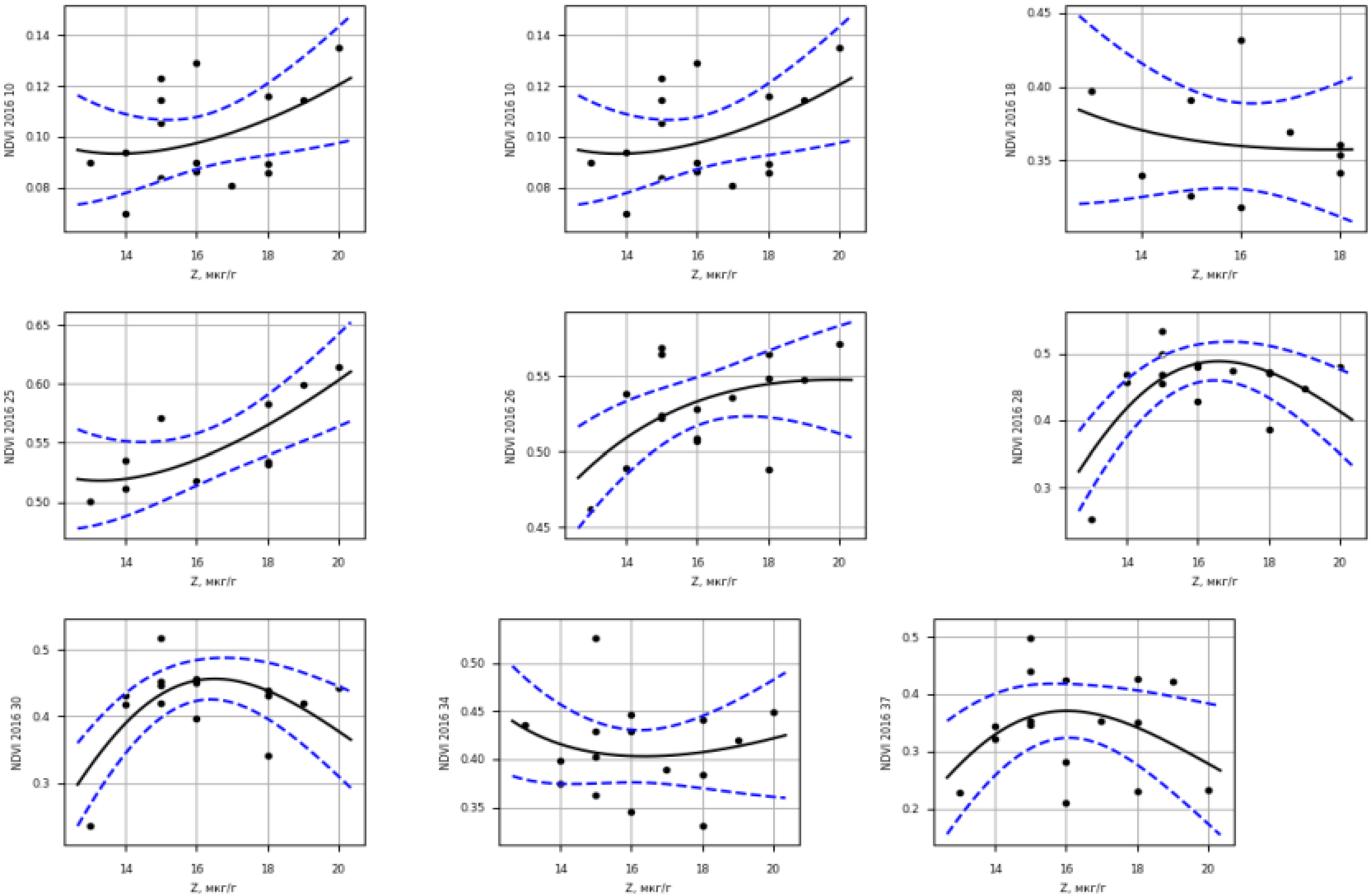
Parameters and special points of the model of seasonal dynamics of NDVI in 2016 for monitoring sites in the reserve " Yamskaya steppe".

Площадка	λ	B	k	t_1	t_2	t_3	t_4	t_5	t_6
1	1,73198E+11	6,3	157,25	12	16	21	25	34	43
3	783228,5986	3,3	92,73	10	15	20	28	42	55
4	1,91265E+11	6,3	159,24	12	16	21	25	35	43
5	5212185,434	3,7	103,89	10	15	21	28	40	52
6	612941042,9	4,9	124,24	11	15	20	25	35	45
7	255097067,1	4,7	123,46	11	15	21	26	37	48
8	2,81212E+12	7,0	171,73	12	16	21	25	33	41
9	1,23954E+11	6,2	154,99	11	16	21	25	34	43
11	1,95226E+12	6,9	173,00	12	16	21	25	34	42
12	27963592219	6,0	137,98	10	14	19	23	32	40
14	18487714512	5,8	138,58	11	15	19	24	33	41
15	2,67229E+13	7,6	175,44	11	15	20	23	31	38
16	23406329,78	4,1	107,91	10	15	20	26	38	48
18	19633438029	5,8	141,48	11	15	20	24	34	42
19	2,01856E+15	8,6	203,79	12	16	20	24	31	38
21	1,26256E+15	8,6	199,09	12	16	20	23	31	38
32	7,36107E+11	6,7	156,61	11	15	19	23	32	39
33	325369,0877	3,2	81,31	9	13	18	26	38	50
35	4,49143E+11	6,5	162,19	12	16	21	25	34	42





Response of NDVI to the concentration of heavy metals Z in soil in 2015.
Date of determination, in weeks, is indicated on the ordinate) (points correspond to the monitoring sites in the reserve "Yamskaya steppe", solid lines – dose dependence, dotted lines – confidence intervals for the model.

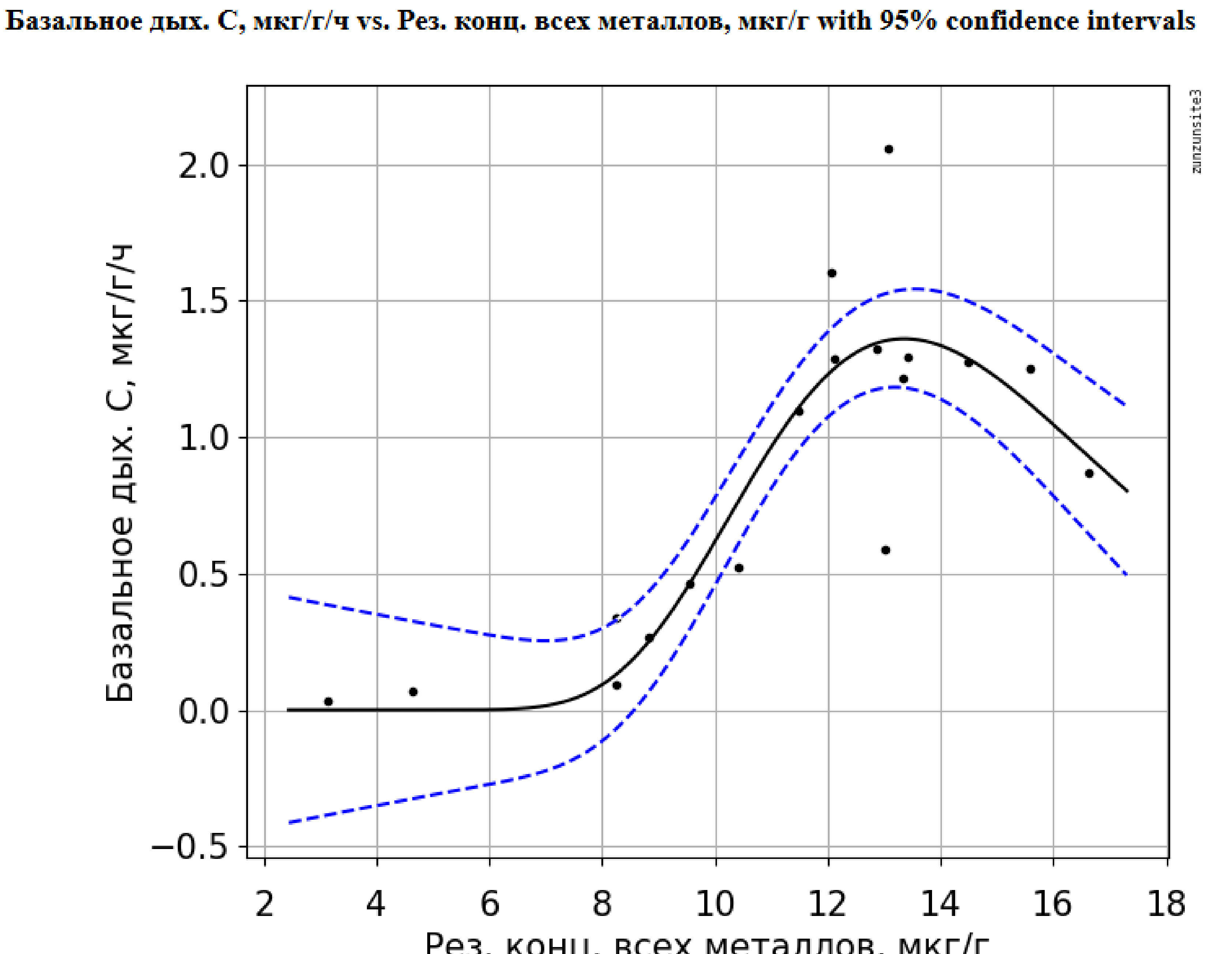


Response of NDVI to the concentration of heavy metals Z in soil in 2016. Date of determination, in weeks, is indicated on the ordinate) (points correspond to the monitoring sites in the reserve "Yamskaya steppe", solid lines – dose dependence, dotted lines – confidence intervals for the model.

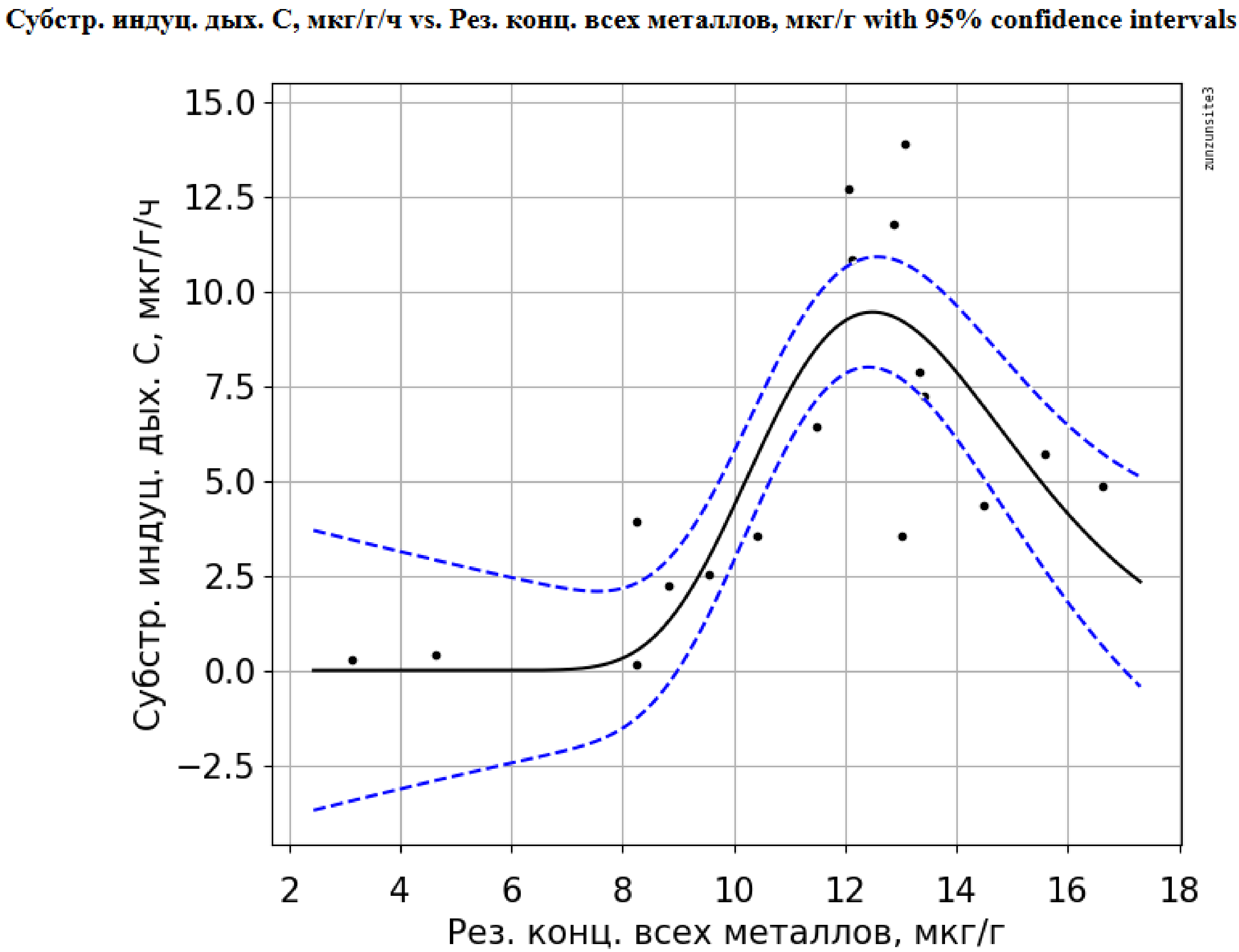
Parameters and singular points of the equation of NDVI response on the resulting concentration of heavy metals Z in the soil for two seasons (2015, 2016) in the reserve "Yamskaya steppe".

Год	Неделя	Λ	B	K	q_4/z_4	z_1	z_2	z_3	z_4	z_5	z_6
2015	13	278218,1	4	65	0,01	6,3	9,2	12,5	16,8	24,4	31,6
2015	24	1,18E+12	8	122	0,03	8,0	10,6	13,8	16,2	21,7	26,8
2015	28	1,37E+11	7	114	0,03	7,9	10,6	13,8	16,4	22,2	27,6
2015	30	1,31E+12	8	125	0,03	8,3	11,0	14,2	16,7	22,4	27,6
2015	32	3,25E+11	7	120	0,03	8,2	10,9	14,1	16,8	22,6	28,0
2015	35	1,71E+09	6	97	0,02	7,4	10,2	13,5	16,5	22,9	28,7
2015	38	86,21018	1	24	0,02	3,4	5,9	8,7	16,2	26,5	36,5
2015	40	3177,799	3	40	0,01	4,8	7,5	10,6	16,0	24,6	32,8
2016	26	36,84956	1	21	0,03	3,3	6,0	9,0	19,9	33,7	47,7
2016	28	2,96E+16	10	168	0,03	9,1	11,6	14,7	16,6	21,6	26,1
2016	30	5,96E+17	11	181	0,03	9,3	11,7	14,7	16,5	21,3	25,4
2016	37	9,59E+19	12	200	0,02	9,3	11,7	14,5	16,0	20,4	24,2

The dependence of basal respiration on the concentration of metals in the soil



The dependence of substrate-induced respiration on the concentration of metals in the soil



Generalization of the dose-response equation

$$x = \frac{z}{z_{\max}} \qquad y = \frac{q}{q_{\max}}$$

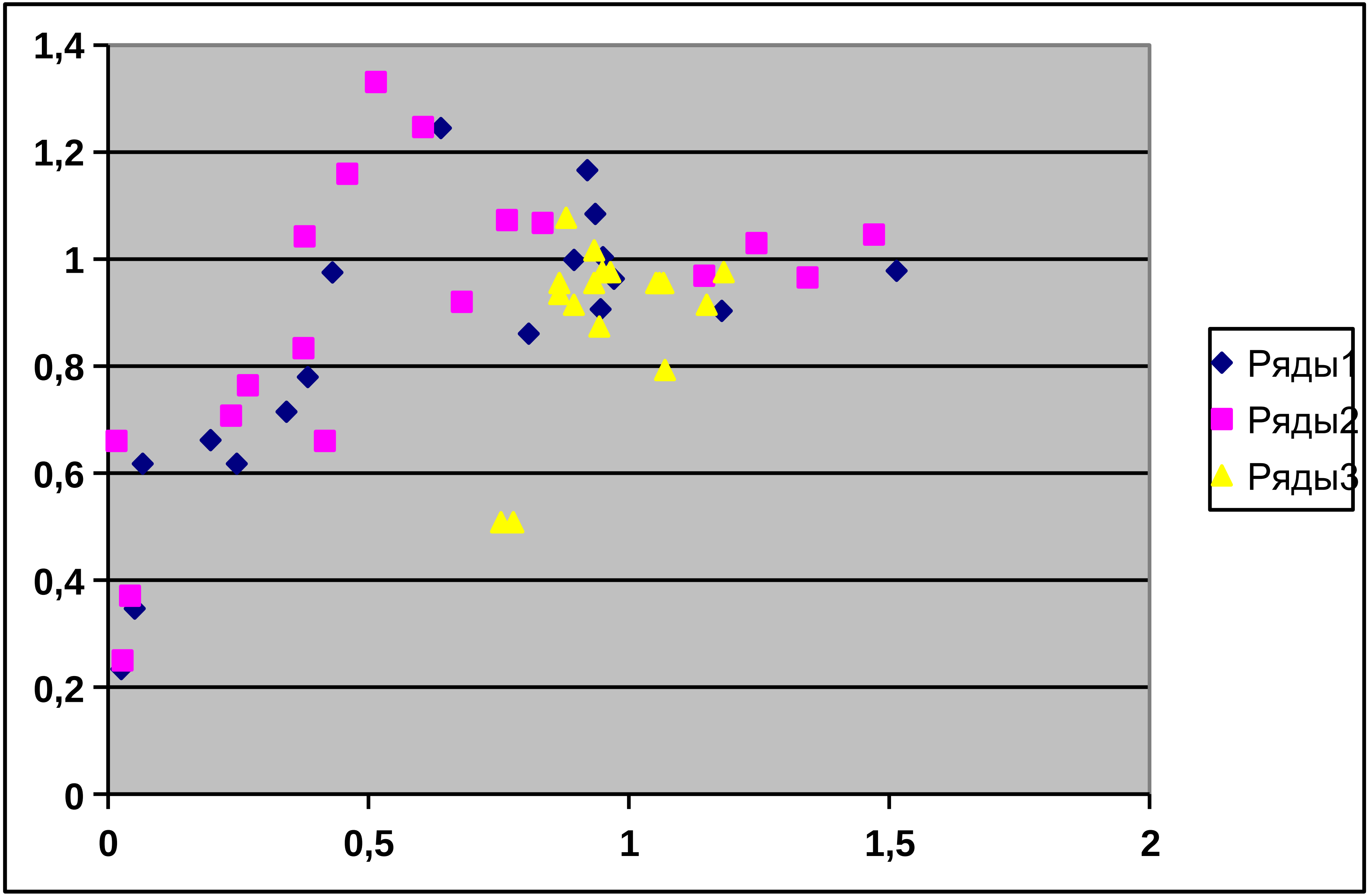
$$y_3 = \frac{NDVI}{NDVI_{\max}}$$

$$y_1 = \frac{basal\,respiration}{basal\,respiration_{\max}}$$

$$y_2 = \frac{substrate\,induced\,respiration}{substrate\,induced\,respiration_{\max}}$$

$$q = \theta\, z^{-\lambda} \exp\left(-\frac{\delta}{z}\right) \rightarrow \quad y = x^{-\lambda} \exp\left(\lambda - \frac{\lambda}{x}\right)$$

Combined graph of NDVI (Row 3), basal respiration (Row 1), and substrate-induced respiration (Row2) versus resultant heavy metal concentrations in soil (in normalized variables)



Results:

1. The growth equation is adequate to experimental data on the seasonal dynamics of the vegetation index NDVI in the vicinity of mine working.

2. The dose-response equation is adequate to the experimental data on the dependence of the vegetation index NDVI at a fixed time on the resulting concentration of substrate components.

3. The dose-response equation is adequate to the experimental data on the dependence of the basal and substrate-induced respiration in soil at a fixed time on the resulting concentration of substrate components.

4. Normalized values of the substrate induced respiration and vegetation index for the same soil samples from the vicinity of mine working are generalized in the framework of the theoretical model.

Conclusion:

1. Seasonal dynamics of the NDVI at all monitoring sites is a subject to the laws of conservation of mechanics and macroscopic kinetics of biological reacting systems. This means that the six singular points of the model separate seven growth phases posessing characteristic features of macroscopic kinetics.

2. This also means that at a fixed time in the phase plane, the dose-effect biological response (in the form of NDVI or microbial soil respiration) to the increasing concentration of the leading components of the substrate first naturally increases, reaching a maximum, and then decreases.

3. Such a natural change in the biological response to the increasing impact makes it possible to identify the threshold concentration of toxicants and to rank soils according to the content of pollutants on the basis of singular points of the model.

Thank you for listening.