Application of modelling by the study of ground water contamination with nitrates under grasslands

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ABSTRACT

At permanent grassland in the foothill regions of the Šumava (545 m a.s.l. subassociation *Trifolio-Festucetum alopecuretosum* Neuhäusl 1972), relations between the use of different doses of N(+PK) and contamination of ground waters with nitrates have been studied with the application of deterministic and probabilistic models with the aim of elaborating a theoretical basis and new methodological approaches for polycriterial optimisation of fertilisation of grass stands. Mutual relations between the use of doses N(+PK), build-up of primary production and perlocations of NO_3^- into ground waters, expressed by that of unit and marginal values of both these processes showed a mirror-like inversion course with a remarkable co-incidence of reverse local extremes. Within the range of doses from 0 to 100 kg N(+PK)/ha P helps, at the ratio of the applied doses P:N ≈ 1:1.5–2.5, to a considerable decrease in the concentration of NO_3^- in ground waters. Specification of suitable doses of N(+PK) to ecologically and phytocenologically similar stands is discussed.

Keywords: grasslands; ground waters; nitrates; fertilisation; deterministic and probabilistic models

Permanent grasslands contribute to effective protection of ground waters from their contamination by mineral nutrients. This protective function of permanent grasslands is much more higher in comparison with crops grown on arable land (Mrkvička 1998, Nagy 2002). A special attention should be paid to the positive effect of grasslands in relation to the protection of ground waters from the contamination by nitrates. If water leaks through grass stands into their rhizosphere nitrates are drained from the water very quickly (Seifert 1972). On the other hand, it has been found that, under nitrification's favourable conditions, permanent grasslands may become the reverse of its original function – a nitrates consumer becomes their significant producer (Ulrich and Seifert 1979). From this point of view, it seems necessary to seek such methods of management that would utilise well permanent grasslands functioning as an efficient biological filter. To solve these problems, it seems necessary to deepen the theoretical approaches to the study of the relations between nutrients doses (especially N) including their mutual interactions (especially N and P) and the process of nitrate perlocation into ground waters. It seems essential to link the theoretical solution to the outlined problems using deterministic and probabilistic models with the production function of N as another important variable in the relations of inputs and outputs of N in grass ecosystems (Klimeš 1990, 1999).

MATERIAL AND METHODS

From 1979 to 1981, at location in the Šumava foothills (Kaplice, South Bohemia), the effect of graded doses of N and P at constant dose of K (Table 1) was studied in relation to the changes in the content of NO_3^- in ground waters in permanent grassland which can be included in the domain of subassociation *Trifolio-Festucetum alopecuretosum* Neuhäusel 1972. Examinations were repeated four times. The used kinds of dressing were as following: nitro chalk with limestone (27.5% N), superphosphate (18% P_2O_5) and potash salt (60% K_2O). Doses of P and K were applied every year in spring. N was applied up to the total dose of 100 kg/ha in a once in spring. Higher doses of N were applied separately in spring and after the first mowing [200 N (150 + 50), 300 N (200 + 100)]. The stands were moved two times per year.

The examined grassland is in the altitude of 545 m a.s.l., the average air temperature is 6.3°C, and the average annual rainfall is 675 millimetres. The geological background material is granite; the

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Table 1. List of studied variants

Variant	Dose of pure nutrients (kg/ha)		
	N	P	K
1	0	0	0
2	0	0	100
3	50	0	100
4	100	0	100
5	200	0	100
6	300	0	100
7	0	20	100
8	50	20	100
9	100	20	100
10	200	20	100
11	300	20	100
12	0	40	100
13	50	40	100
14	100	40	100
15	200	40	100
16	300	40	100

soil type is acid cambisoil, sandy loam, pH_{KCl} 6.5. The content of main nutrients in the soil (mg/kg): 8 P, 47 K, 110 Mg.

The content of NO_3^- in lyzimetric water was monitored in the examined grass stands in the course of the vegetation period in ten days periods. Lyzimetres with horizontal detention area (0.5 × 0.5 m) were used for sampling of the water in the depth of 0.5 m below the surface (Klimeš 1999). The content of NO_3^- in lyzimetric waters was determined by means of a nitrate ion-selection electrode.

The present work analyses the changes in the concentration of NO_3^- in lyzimetric waters in relation to doses of N, or N and P using deterministic and probabilistic models. These changes are also examined in relation to the production process, which was analysed with production functions and their derivative characteristics (marginal production and unit production). For analytical functions describing the mutual relation between the doses of N, or N and P (+K), and the concentration of NO_3^- in lyzimetric waters, their derivative characteristics (marginal concentration and unit concentration) were proposed and specified as analog values of the production functions characteristics. In all the original as well as derivatized deterministic models, their course was investigated using mathematical analysis and their local extreme and critical points were determined (Černý 2002). To keep the principle *ceteris paribus* variants from 2 to 16 for models creation were applied.

Within the framework of the specification of probabilistic models describing the distribution probabilities in the values of the concentration of NO_3^- in lyzimetric waters in the examined doses of N, a suitable type of a model was tested. Also an asymmetry was determined in the distribution of the values of the concentration of NO_3^- in ground waters, in relation to the average by means of three central moments. For the individual levels of dressing by N, probabilistic characteristics of the concentration of NO_3^- in ground waters were determined: the probability of reaching subcritical values standard for drinking water (50 mg NO_3^-/l) and for suckling water (15 mg NO_3^-/l) and also 95%, 99% and 999‰ 100P% of fractiles.

The relations between the dressing of grass stands, production process and the concentration of NO_3^- in ground waters are studied in this work in their mutual interactions with the aim of elaborating theoretical basis and new methodological approaches for polycriterial optimisation of fertilisation of grass stands.

RESULTS AND DISCUSSION

In the course of the experiment period, the dynamics of the stand structure in the examined grassland in relation to their dressing showed quite standard tendency characteristic for similar plant community (Turek and Klimeš 1981, Klimeš 1990, 1999).

The most effective form of explanation and predicting the dependence of dry matter yield (y in t/ha) on a dose of N (x in kg/ha) seems to be the following production function (Figure 1a):

$$y' = 4.330 + 0.016x + 0.000\,090x^2 - 0.000\,000\,350x^3 \quad [I_{yx} = 0.983^{**}] \qquad (1)$$

The above presented production function shows convex-concave course with the inflection at the dose of 86 kg N(+PK)/ha. The production maximum is (8.5 t dry matter/ha) at the dose of 236 kg N(+PK)/ha. The marginal production (mP in kg dry matter/kg N) derived from the above mentioned production function (1) as its first derivative (Figure 1b):

$$mP' = dy'/dx = 16 + 0.180x - 0.001\,050x^2 \qquad (2)$$

Shows concave course with its maximum at 24 kg dry matter/kg N at the dose of 86 kg N(+PK)/ha.

The unit production (jP in kg dry matter/kg N):

$$jP' = (y' - \bar{y}')/x = 16(x - \bar{x}) + 0.090(x^2 - \bar{x}^2) - 0.000\,350(x^3 - \bar{x}^3) \quad (3)$$

derived from the production function (1) after its following transformation (Heady and Dillon 1964):

$$y - \bar{y} = b(x - \bar{x}) + c(x^2 - \bar{x}^2) + d(x^3 - \bar{x}^3) \quad (4)$$

reached its maximum at the dose of 202 kg N(+PK)/ha (Figure 1b).

On the basis of a complex assessment of phytocenological, production and qualitative parameters, the value of the inflexion point seems to be the beginning of biologically rational stage of the production function (1). The value of the maximum unit production seems to be the limit of this stage of the production function (1) (Klimeš 1990, 1999). It is possible to determine a biologically rational stage for phytocenologically and ecologically similar stands within the interval from 86 to 202 kg N(+PK)/ha.

It is necessary to consider, during the optimising of dressing of grass growths, the effect of the supplied nutrients on the quality of ground waters as well (Seifert 1972, Mrkvička 1998). As the most effective form of explanation and predicting the dependance on the concentration of NO_3^- in ground waters (K in mg/l) on the dose of N (x in kg/ha) for the examined collection of variants (Table 1) was determined the following regression function (Figure 1c):

$$K' = 0.983 + 0.086x - 0.000\,678x^2 + 0.000\,001\,765x^3 \quad [I_{Kx} = 0.575^{**}] \quad (5)$$

The curve shows, in relation to the x axis, concave-convex course with its inflexion at 128 kg N(+PK)/ha. In the region of the inflexion point two hardly noticeable local extremes were noticed: maximum at x = 115 and minimum at x = 140. There is a phase of a slight depression between these extremes in the content of NO_3^- in ground waters. At the dose of 165 kg N(+PK)/ha the content of NO_3^- in ground waters returns to the value of the above local maximum. The interval of doses between 115–165 kg N(+PK)/ha thus appears to be a stagnation phase in the content of NO_3^- in ground waters. The margin of ± 0.1 mg NO_3^-/l shifts the stagnation interval to between 83 and 173 kg N(+PK)/ha. The absolute term of function (5) with its value of 0.983 mg NO_3^-/l is the closest to the average value of completely undressed stand (variant 1) where the average NO_3^- content in ground waters during the studied period was 1.071 mg/l

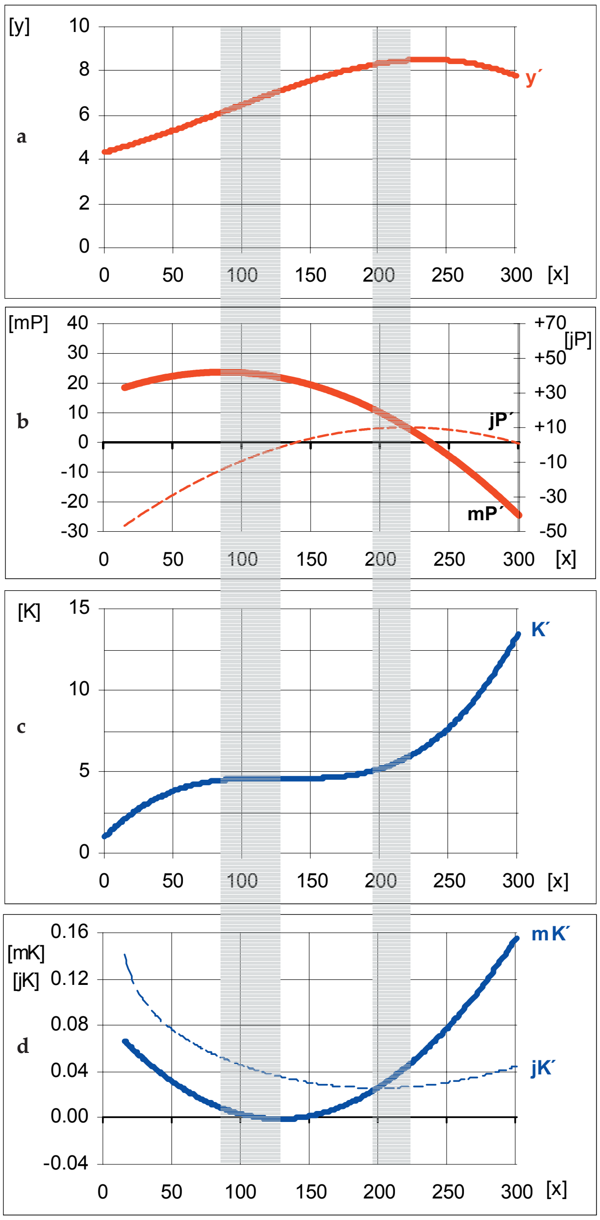

Figure 1. Deterministic model of the dependance of primary production (Figure1a) and the concentration of NO_3^- in ground waters (Figure 1c) on the dose of N(+PK) with the derived characteristics of these models (marginal and unit production – Figure 1b, marginal and unit concentration of NO_3^- – Figure 1d)

x = dose of N(+PK) (kg/ha)
y = primary production of dry matter (t/ha)
mP = marginal production (kg of dry matter/kg N)
uK = unit production (kg of dry matter/kg N)
K = concentration of NO_3^- in ground waters (mg/l)
mK = marginal concentration of NO_3^- in ground waters (mg/l/kg N)
uK = unit concentration of NO_3^- in ground waters (mg/l/kg N)
Vertical bands designate coincidences of local extremes and inflexion points

(0–1.5 mg NO_3^-/l in individual samplings) and it was also close to the value of the stand dressed

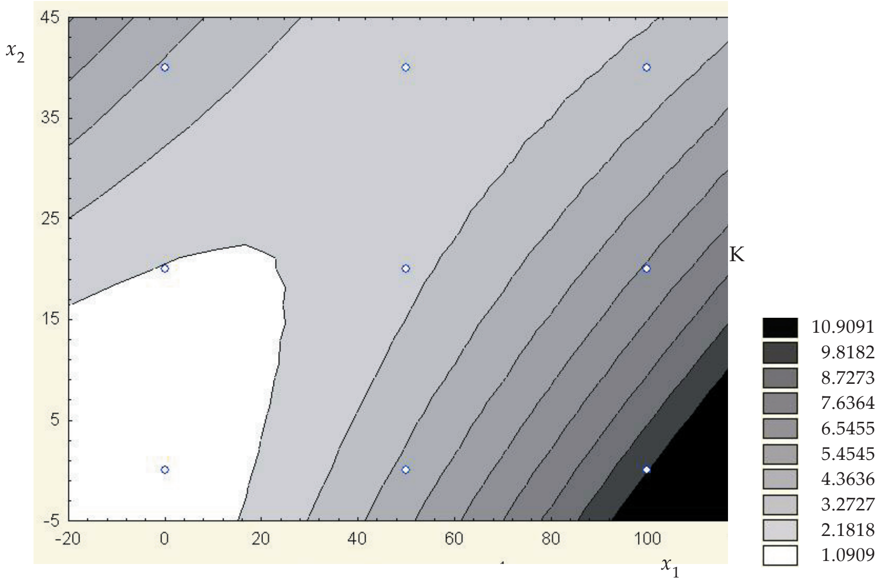

Figure 2. Deterministic model of the dependance of the concentration of NO_3^- in ground waters on the dose of N and P(+K)

x_1 = dose of N (kg/ha)
x_2 = dose of P (kg/ha)
K = concentration of NO_3^- in ground waters (mg/l)

only with potassium (variant 2) where the average NO_3^- content in underground waters was 0.857 mg NO_3^-/l (0–2 mg NO_3^-/l). Both the mentioned variants showed a fast decrease in the number of valuable grass species (the same as in other variants in which N was not applied) and an opening in the stand was also noticed in the variants dressed with the dose of 50 kg N(+PK)/ha. The danger of degradation of species structure with early entrance of *Nardetum* stand type occurs in such areas with insufficiently fertilised or nonfertilised grasslands. This stand type shows 15–20-times lower infiltration ability for water than overwhelming majority of grasslands (Klimeš 1999).

Comparing the functional relations (1) and (5) (Figures 1a, c) there seems to be a certain analogy which can also be found in the relations between production and cost functions (Heady and Dillon 1964, Samuelson and Nordhaus 1989). Drawing on the Bohr principle of complementarity (Vaníček 1982) during assessment of this analogy, the increase in the concentration of NO_3^- in ground waters with the increasing doses of N seems to be a certain price to be paid for lowering the entropy in the grass ecosystem itself by increasing the entropy in its surroundings.

The outlined aspects then seem to propose that it is pragmatic to derive analogical values from the relation (5) as in the production functions. The analogical value for the marginal production (mP) seems to be the value of the nitrate marginal concentration (mK) and the nitrate unit concentration (jK) is the analogical characteristic for the unit production (jP).

The marginal concentration (mK in mg NO_3^-/l/kg N) derived as the first derivation of the function (5) is for the examined collection (Figure 1d):

$$mK' = 0.086 - 0.001\,356x + 0.000\,005\,295x^2 \qquad (6)$$

The unit concentration (jK in mg NO_3^-/l/kg N), during whose derivation it is not necessary to carry out a transformation as is the case of the function (1) due to mutual relations of the parameters in the function (5), can be expressed as follows (Figure 1d):

$$jK' = K'/x = 0.983x^{-1} + 0.086 - 0.000\,678x + 0.000\,001\,765x^2 \qquad (7)$$

Both of the derived characteristics (mK, jK) show a convex course with the minimal values of mK at x = 128 kg N(+PK)/ha and of jK at x = 197 kg N(+PK)/ha.

The mutual comparison of the course of the production characteristics (Figures 1a, b) and the course of the concentration of NO_3^- in ground waters (Figures 1c, d) in relation to the doses of N(+PK) clearly shows some significant coincidences affirming a close link between the use of N for the build-up of production and N perlocation into ground waters in the form of NO_3^-. In the vicinity of the dose of 100 (86–128) kg N(+PK)/ha the shape of the production function changes and its course transforms from a convex to concave one. It reaches the maximum marginal production of 1 kg N and, at the same time, the course of the relation between a dose of N(+PK) and the concentration of NO_3^- in ground waters changes: a phase of stagnation of the concentration of NO_3^- in ground waters begins here, the curve of the concentration of NO_3^- in ground waters shows inflexion and minimal values of marginal NO_3^- concentration in ground waters are reached here (Figures 1a–d). The prominence of the mutual inner link between the unit production

Table 2. Statistical and probabilistic characteristics of NO_3^- concentrations in ground water for various doses of N(+PK)

Dose of N [kg/ha (+PK)]	$\bar{K}$	$\hat{K}$	K_{min}	K_{max}	$m_{K,3}$	Comparison of values K_{max} with levels of 95%, 99% and 999‰ 100P% fractiles
0	1.474	1.500	0.000	7.000	+2.815	$K_{0.95} < K_{max} < K_{0.99}$
50	2.250	1.500	0.000	6.500	+1.355	$K_{max.} < K_{0.95}$
100	4.795	2.000	1.000	28.000	+2.246	$K_{0.99} < K_{max} < K_{0.999}$
200	4.630	2.000	1.000	36.500	+3.227	$K_{0.99} < K_{max} < K_{0.999}$
300	11.950	3.000	0.000	138.000	+3.559	$K_{0.95} < K_{max}\ K_{0.99}$

$\bar{K}$ = average of NO_3^- concentration (mg/l) in ground waters
$\hat{K}$ = the most frequented value (modus) of NO_3^- concentration (mg/l) in ground waters
K_{min} = minimum of NO_3^- concentration (mg/l) in ground waters
K_{max} = maximum of NO_3^- concentration (mg/l) in ground waters
$m_{K,3}$ = assymetry of distribution of values of NO_3^- concentrations in ground waters (3rd central moment of the distribution – skewness of the distribution)

and the unit concentration of NO_3^- in ground waters is also well visible from their inversion course. The same applies to the mutual relations between the course of marginal production and the marginal concentration of NO_3^- in ground waters (Figures 1b, d) and it shows that the NO_3^- perlocation process into ground waters is, apart from a dose of N(+PK) itself, significantly affected by the use of N for production purposes.

At the same time, it seems that the dose of about 200 kg N(+PK)/ha, when the highest unit production of 1 kg N and minimal unit concentration of NO_3^- in ground waters were reached, together with phytocenological and qualitative characteristics thus indicates the uttermost limit of biologically as well as economically rational range of doses of N(+PK) for examined and phytocenologically and ecologically similar grass stands (Heady and Dillon 1964, Samuelson and Nordhaus 1989, Klimeš 1990, 1999). The low limit of biologically as well as economically rational intervals can be determined, considering the full integration of the stand, stabilization of valuable grass species, and utilization of particular stands, at the value of the inflexion point of the production function, i.e. about 80 kg N(+PK).

The following regression function (Figure 2) seems to be suitable as the most effective form

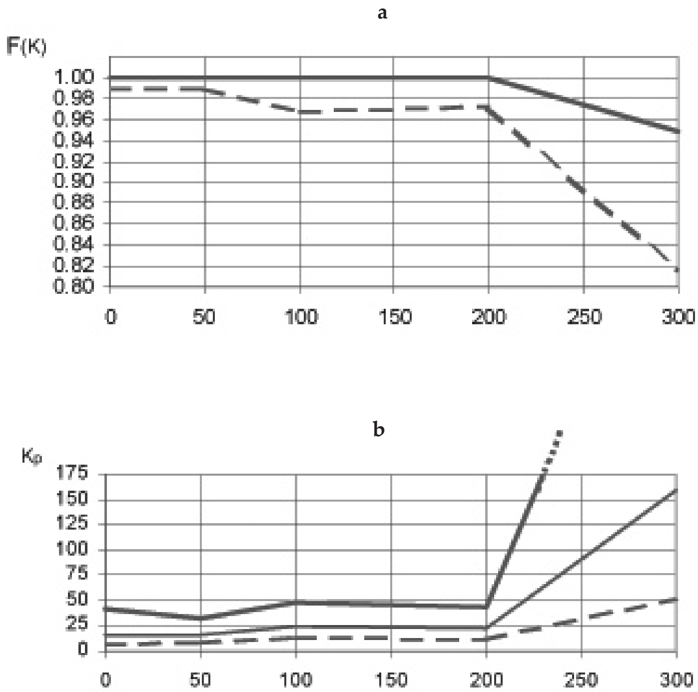

Figure 3. Probabilistic model of the concentration of NO_3^- in ground waters at different doses of N(+PK), expressed by the form of probabilities of reaching subcritical values (Figure 3a) and by the form of 100P% of fractiles (Figure 3b)

x = dose of N [kg/ha (+PK)]
K = concentration of NO_3^- in ground waters (mg/l)
$F_{(K)}$ = probability of reaching subcritical values of the NO_3^- concentration in ground waters:
——— $K \leq 50$ ------- $K \leq 15$

K_P = 100P% of fractiles of the values of the NO_3^- concentration in ground waters (mg/l):
------- $K_{0.95}$ ——— $K_{0.99}$ ▬▬ $K_{0.999}$

of explanation and prediction of the influence of the doses of N (x_1 in kg/ha) and P (x_2 in kg/ha) at a constant level of the doses of potassium on the content of NO_3^- in ground waters (K in mg/l):

$$K' = 0.195 + 0.038x_1 + 0.012x_2 + 0.000573x_1^2 + 0.002x_2^2 - 0.003x_1x_2 \qquad (8)$$

$$\begin{bmatrix} IKx_1x_2 = 0.806^{**} \\ IKx_{1}.x_2 = 0.769^{**} \\ IKx_{2}.x_1 = 0.411^{**} \end{bmatrix}$$

The validity of the above model was verified for the values $0 \leq x_1 \leq 100$ and for $0 \leq x_2 \leq 40$. The concentration of NO_3^- in ground waters is determined by 65% by N and P fertilization in the stated interval. The effect of N is from the view approximately 3.5-time higher than the effect of P same point.

Using the methods of marginal analysis (Heady and Dillon 1964, Klimeš 1999), an optimal combination of the doses of N (x_1) and P (x_2) for the range of relevance were determined at which the lowest concentration of NO_3^- in ground waters is reached. The relations are as follows:

$$x_1 = 2.500x_2 \qquad (9)$$

$$x_1 = 4 + 1.333x_2 \qquad (10)$$

These relations mark the area with the lowest values of the concentration of NO_3^- in ground waters.

The analysis of the asymmetry in the distribution of the values of the concentration of NO_3^- in ground waters in relation to the average, and for individual levels of dressing by N(+PK) using a moment measure of asymmetry ($m_{K,3}$). Showed that for the reasons of strong asymmetry it is not possible to accept normal distribution for the approximation of probability distribution (Table 2). A more detailed analysis lead to a conclusion that the empirical values of the NO_3^- concentration show a logarithmic-normal distribution [LN(μ, σ^2)]. Using the logarithmic-normal distribution, the values of probability of reaching subcritical values [$F_{(K)}$] for $K \leq 15$ mg NO_3^-/l (the standard for suckling water) and for $K \leq 50$ mg NO_3^-/l (the standard for drinking water) and also 95%, 99% and 999‰ 100P% of fractiles of the NO_3^- concentration in ground waters values have been generated. Graphical representations of the outputs of these probabilistic models are presented in Figures 3a, b. It seems that, for the doses up to 200 kg N(+PK)/ha, the probability of reaching lower values of the concentration of NO_3^- in ground waters below 50 mg/l is very high [$F_{(K)} > 0.999$] at 95% 100P% of fractiles 12.028 mg NO_3^-/l (Figure 3b), i.e. less than declares the standard for suckling water. When increasing the doses of N above 200 kg/ha (+PK), the probability of reaching subcritical values of the concentration of NO_3^- in ground waters decreases significantly (Figure 3a) and the relevant fractiles markedly increase (Figure 3b). For practical applications, it is suitable to lower this limit by about 20% because practical dressing is not carried out with such precision which is applied in experimental grassland science.

It appears that probabilistic models verify the biologically rational interval of the doses of N(+PK) derived by means of deterministic models. At the same time, it is confirmed that the combination of both approaches to the model construction is suitable (Dvořák et al. 1982, Devlin 1996).

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ABSTRAKT

Uplatnění modelování při studiu kontaminace podzemních vod nitráty pod travními porosty

U trvalého travního porostu v podhorské oblasti Šumavy (545 m n. m., subasociace *Trifolio-Festucetum alopecuretosum* Neuhäusel 1972) byly při použití deterministických a pravděpodobnostních modelů studovány vztahy mezi různými dávkami N(+PK) a kontaminací podzemních vod nitráty se záměrem vypracovat teoretickou základnu a nové metodologické přístupy pro polykriteriální optimalizaci hnojení travních porostů. Vzájemné relace mezi dávkami N(+PK), tvorbou primární produkce a perkolací nitrátů do podzemních vod, vyjádřené pomocí jednotkových a mezních hodnot obou těchto procesů, vykazují vzájemný zrcadlově inverzní průběh s patrnou koincidencí opačných lokálních extrémů. V rozmezí dávek 0 až 100 kg N(+PK)/ha napomáhá fosfor při poměru aplikovaných dávek P : N ≈ 1 : 1,5–2,5 k výraznému snižování koncentrace NO_3^- v podzemních vodách. Je diskutována otázka volby vhodných dávek N(+PK) k ekologicky a fytocenologicky podobným porostům.

Klíčová slova: travní porosty; podzemní vody; nitráty; hnojení; deterministické a pravděpodobnostní modely

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