Modelling of Dry Matter and Nutrient Accumulation by Winter Wheat

G. BICZÓK, B. LÁSZTITY, A. BÉKÉSSY and M. RUDA

Ecological and Botanical Research Institute of the Hungarian Academy of Sciences, Vácrátót; Research Institute for Soil Science and Agricultural Chemistry of the Hungarian Academy of Sciences, Budapest and Computer and Automation Institute of the Hungarian Academy of Sciences, Budapest

Analysis of agroecological systems

The soil subsystem and plant subsystem within the soil-plant system are investigated in order to identify successive and simultaneous processes on each of the hierarchical levels essential from the point of view of fertilization practice and system theory. Three hierarchical levels are taken into account:

- the phenomenological /soil-plant substance transfer dynamical/ level,
- the agrochemical, more exactly: nutrient element overall kinetic level,
- the level of biochemical and soil chemical mechanisms.

By investigating these levels, the decisive, essential and at the same time necessary and sufficient characteristics of the agroecological systems can be abstracted to attain the objective of developing a simulation algorithm for fertilization recommendations with optimum costs.

On the basis of the system analysis a simple biomathematical model was developed and verified. The non-linear regression problem of model fitting was solved by the Marquardt variant of the Newton method. Special numerical processes were developed for taking a number of plant physiological, genetic and agroclimatic conditions into consideration.

The data on which efforts to develop a practicable biomathematical model were based were mainly the results of several years of systematic observations covering all the major agroecological regions in Hungary. This holds true in the overwhelming majority of cases, and only a few field experiments are included in this work.

Considering the budget available for these investigations, the number of agroecological subunits observed was too great for the fresh and dry phytomass and the concentrations of N, P, K, Na, Ca, Mg, Fe, Mn, Zn, Cu, B and Mo in the plant to be measured more than five times on each occasion and in more than five phenophases of the vegetation period, not to mention the expensive soil analysis and subsequent data processing. Hence, the number of observation dates was restricted.

In this way it became possible to present and analyse a suitably representative set of samples for combinations of 15 basic soil types and the 17 most important annual arable crops cultivated in 32 agroecological regions of plant production significance in Hungary /Fig. 1/.

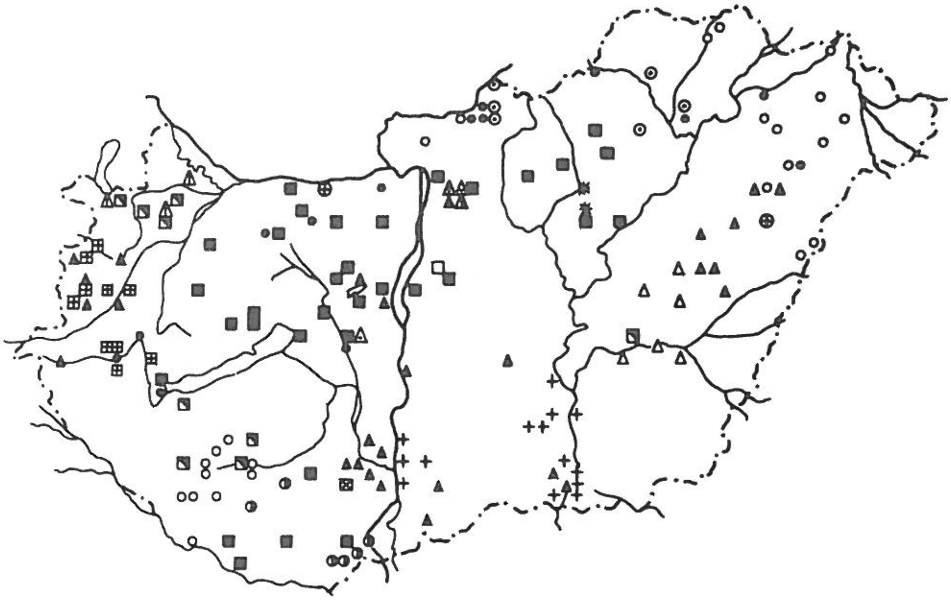


Fig. 1

Distribution of sampling sites in Hungary
Cereals: ▲ winter wheat /Triticum aestivum L./; ▲ rye /Secale cereale L./; △ winter barley /Hordeum vulgare L./; ▲ spring barley /Hordeum vulgare L./; △ rice /Oryza sativa L./. Industrial crops: ■ maize /Zea mays L./; ▧ sugarbeet /Beta vulgaris L. var. saccharifera/; ⊠ sunflower /Helianthus annum L./ ⊞ rape /Brassica napus L. var. oleracea/; □ sorghum /Sorghum bicolor L./. Legumes: ⊙ pea /Pisum sativum L./; ◑ soybean /Glycine soya M./; ⊕ alfalfa /Medicago sativa L./; ○ lupin /Lupinus albus L./. Field vegetables /Solanaceae/: + pepper /Capsicum annum L./; ✱ tomato /Lycopersicum esculentum L./; ● potato /Solanum tuberosum L./

On the other hand, a difficult dual problem arose with respect to the modelling. All the processes of a complex agroecological system or subsystem cannot be quantitatively described in detail by a model based on a data set of this type.

One convenient and rational mathematical way of summarizing this large quantity of data in terms of a few parameters would be the use of an empirical time function /e.g. equation of the whole plant growth curve/. This involves the risk of failing to achieve a real understanding of how the agroecological system works.

What can be done in order to develop a model with few parameters which are also physically interpretable? How many parameters of a simple phenomenological model will be identifiable with the generally accepted characteristics of plant nutritional dynamics /KASAWNEH, 1971; MENGEL, 1972/?

A reasonable aim would be to create a model in which the plant itself could be used as the best indicator of dynamic soil characteristics which could not be satisfactorily estimated by the best routine physico-chemical methods /KASAWNEH, 1971; NÉMETH, 1971/.

When introducing system analysis as a tool for the achievement of this objective, the first and most important step is to develop a simulation algorithm for a fertilizing recommendation with optimum costs.

The cycle of nutrient elements in the soil-plant system consists of consecutive and simultaneous processes /THORNLEY, 1976; GILMANOV, 1975/ /See Table 1/. The high complexity of these processes /BICZÓK, 1980/ usually leads to models containing many parameters, the verification of which turns out to be rather expensive both from the experimental and computational points of view /DE WIT et al., 1970; GILMANOV, 1975; THORNLEY, 1976/. On these ground, and considering the classical results of the biological growth theory /e.g. BERTALANFFY, 1960; VERHULST, 1944 /, a two subcompartment type model /ATKINS, 1969/ is attempted, which could be the first subsystem in a computer-aided fertilizer recommendation system giving optimum inclusion of results in the field of plant nutrition, in the sense that the model can be fitted well even if the number of data measured is relatively small and that it can be used in widely diverse ecological and agrotechnological environments. Also, it has only minimum general restrictions and contains the lowest possible number of parameters, which are nevertheless interpretable. Moreover, it has no phenomenological inconsistency with recent results in biological growth modelling /THORNLEY, 1976; ZELAWSKI and LECH, 1980/.

Table 1

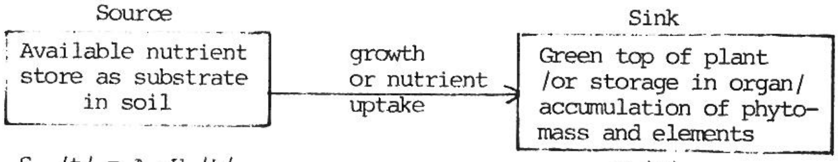
Some important natural process types in the cycle of nutrient elements in the soil-plant system

Type of process	Reference
1. Transport	
1.1 In the soil	
- mass flow	BARBER et al., 1963
- diffusion /slow, fast/	NYE and TINKER, 1977
- interception ...	RAMAMOORTHY and LEPPARD, 1977
1.2 In the plant	
- uptake /organic, inorganic/	NISSEN, 1974
- transport to the xylem	PITMAN, 1977
- transport within the xylem	EPSTEIN, 1972
- transport within the phloem	MINCHIN and TROUGHTON, 1980
2. Transformation	
2.1 Soil chemical	BOLT and BRUGGENWERT, 1976, LINDSAY, 1979
- fixation, release, ageing, weathering, ion-pair formation ...	
2.2 Plant biochemical - photosynthesis, - respiration	EPSTEIN, 1972; KUPERMAN and KHITROVO, 1977; HESS, 1976
2.3 Soil microbiological - mineralization - humification	WALKER, 1975
3. Autocatalytic analogues	TITLYANOVA, 1977

Analysis of the functional subunits in the agroecological system

The following three hierarchical levels are taken into account from the point of view of fertilization practice. On the phenomenological level the interest is primarily in quantitatively describing the mass transfer within a closed system from source to sink. In this case the country is divided into well-defined agroecological regions and districts, and the nutrient cycle is observed within each district on a fixed soil type with a particular plant species.

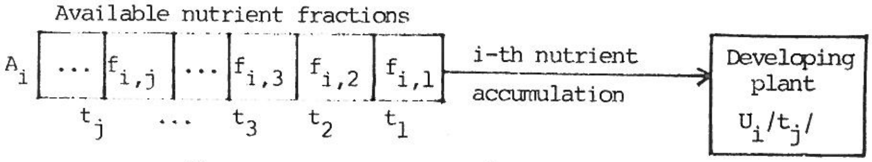
This simplest model describes a closed system consisting of only two compartments:



$S_i\ /t/ = A_i - U_i/t/$ $\qquad$ $U_i/t/$

If it is assumed that the accumulation rate is proportional to the product of the i-th substrate level $S_i/t/$ and to the accumulation of the i-th component $U_i/t/$, and supposing a constancy of all the other environmental variables, this model can predict the sigmoid autocatalytic dynamics for one half of the nutrient cycle: the ascending part of it.

Agrochemists are well aware of the importance of the availability of nutrient elements, and of the fact that senescent plant organs drop onto the soil.

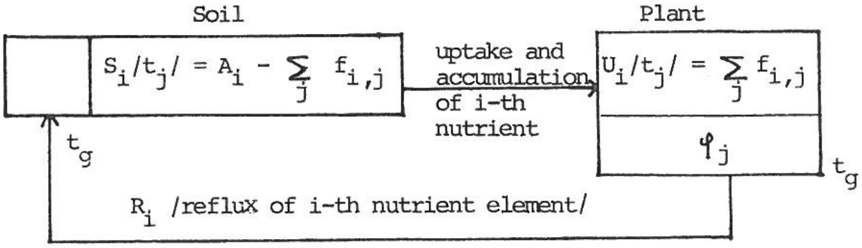


$$S_i/t_j/ = A_i - \sum_j f_{i,j}, \qquad U_i/t_j/ = \sum_j f_{i,j}$$

$f_{i,j}$ represents the available nutrient element fraction which will be quantitatively exhausted by the time t_j. Thus, the plant accumulates the i-th nutrient element more and more slowly because the fractions remaining in the soil are less and less available as time passes from t_1 to t_j. If j approaches a large number, $A_i - U_i/t_j/$ converges on zero, and the accumulation stops.

Another practical observation made by agrochemists indicates that there is a reflux or relocation of nutrients back to the available store in the soil.

At the beginning of the generative phenophase $/t_g/$ the plant may lose the φ_j fractions of nutrient elements because of certain physiological changes. However, this loss of nutrient elements can be taken into account as the available f_j nutrient fraction during the next vegetation season.



Two important conclusions of the system analysis: Without going into the details of the plant nutrition mechanism, a phenomenological model can be presented in the same form for the accumulation both of different nutrient elements and of fresh or dry matter. Considering the processes quoted in Table 2 as senescent processes and reflux processes, it can be assumed that the intensity of reflux is proportional to both the quantity of stored nutrients still remaining from the total possible reflux, and the quantity of substances already relocated to the environment /generally to the soil, except for C, H, O, N/.

Table 2

Some important components of the reflux /loss of the plant/

Reflux components	References
1. Dead plant parts	TITLYANOVA, 1977
- fall,	SHATOKHINA, 1979
- leaching of nutrient elements /depending on the type of chemical bond/	CLARCSON and HANSON, 1980
- decreasing accumulation in the vegetative organs	HESS, 1976
- accelerating respiration /proportional to the substrate quantity remaining in the organ/	KUPERMAN and KHITROVO, 1977
2. Generative period	
- from the beginning: leaching, relocation	MENGEL et al., 1969
- from the period of crop formation: translocation /from the vegetative organs/	HESS, 1976
3. Ripening	
- accelerating respiration, climacteric respiration, regression combinations,	KUPERMAN and KHITROVO, 1977
- product repression	HESS, 1976

Phenomenological modelling of a functional subunit in the agroecological system

According to the generally accepted concept, the nutrient element fractions in the soil /while being in dynamic contacts/ are available at different rates. If the more readily available portion of the nutrient elements enters the plant first, as time t passes after sowing, i.e. as the plant grows, the nutrient element fractions remaining in the soil become less and less available. Consequently, the supply rate for the mineral nutrient is determined by the quantity of its soil reserves /$A-U_1$/. On the other hand, nutrient uptake depends on the phenophase, which means that it is a function of the quantity of the nutrient element already accumulated in the plant /U_1/. Assuming the simplest proportionality, the overall process of nutrient accumulation in the plant can be described by the first subcompartment as follows:

$$\frac{dU_1}{dt} = k \cdot U_1 \cdot /A-U_1/ \qquad /1/$$

where k is a constant characteristic of the given soil-plant system. Integrating the equation /1/ leads to

$$U_1 = \frac{A}{1 + e^{-b/t-t_g/}} \qquad /2/$$

Parameter A /quantity of available nutrient element/ is the limit of the accumulation. The parameter b /nutrient element buffer capacity/ is the deceleration of the nutrient element supplying process in the generative period, and it is proportional to k. t_g represents the time-point of the maximum accumulation rate /i.e. the inflection point which marks the beginning of the generative plant growth phase/.

The logistic curve derived in this way can properly describe the slow growth of the seedling, the extremely high rate of nutrient element accumulation near the inflection point and then the steady state of soil-plant nutrient element transfer for the fully-grown crop.

The saturation period is limited in time. The second subcompartment which describes the nutrient element reflux /U_2/ becomes more and more dominant at higher t values. The loss at the highest rate of fertilizer application takes place at time t_s. It is assumed that the reflux has the same general form as the growth:

$$U_2 = - \frac{R}{1 + e^{-s/t-t_s/}} \qquad /3/$$

where R is the total reflux /the total loss by the plant/, s is the buffer capacity of the plant which decelerates the senescent loss and t_s is the inflection point for the reflux caused by senescence.

Considering the reflux process, good approximative proportionality was assumed between the velocity of the process and $R-U_2$, the mass still remaining from the total reflux R, and between the velocity and the nutrient element quantity U_2 relocated back to the environment /BÉKÉSSY et al. 1982/. This is an acceptable assumption, because senescent plant parts

/i.e. when U_2 increases/ decompose at a higher rate. Thus the next equation is similar to the first one:

$$\frac{dU_2}{dt} = k_r \cdot U_2 \cdot /R-U_2/ \qquad /4/$$

Integrating /4/, equation /3/ follows.

Furthermore, the independence of growth and reflux is assumed, although these processes overlap to a significant degree. Their resultant, however, can be expressed as a sum:

$$U = \frac{A}{1 + e^{-b/t-t_g/}} - \frac{R}{1 + e^{-s/t-t_s/}} \qquad /5/$$

Verification of the model

During the verification of the model /BÉKÉSSY et al., 1982/ certain problems were encountered which will be discussed consecutively in this chapter.

In the majority of the cases analysed so far the number of points measured was only four or five, while there are six model parameters /A, R, b, t_g, s, t_s/. In addition, it was necessary to consider the fact that certain natural restrictions are valid for the parameters:

1. The model parameters are obviously positive.
2. $A > R$, $U > 0$.
3. The derivative of U can only have one local minimum and maximum. This condition can, of course, be satisfied only approximately because of fluctuations during growth or during nutrient element accumulation.

Total model fitting to four or five points was possible because the value A-R could easily be calculated from the data themselves.

The analysis was always performed for fixed A values only. The R values can also be fixed if we know A-R. The lower limit of the real A value has

Table 3

Potential production limits adopted in the model for the arable crops observed

Species	MAY	PMY	PMY/MAY
Winter wheat	4.28	10.0	2.33
Winter barley	3.38	7.5	2.22
Rye	1.75	6.0	3.43
Maize	5.42	14.0	2.58
Potato	16.20	50.0	3.09
Green pepper	11.52	21.0	1.82
Red pepper	6.00	11.0	1.83
Sugar beet	34.35	80.0	2.33
Peas	2.33	6.5	2.79
Lupin	25.00	60.0	2.40

* MAY = maximum average yield measured in Hungary
PMY = practicable maximum yield.

derived from the measured maximum /Y max./. The upper limit was controlled by genetic laws, according to Table 3, where $A < Y_{max} \cdot [PMY/MAY]$. In this interval a sequence of A values was selected and a fitting procedure similar to that for the other parameters, was performed for each fixed A value. For the curve-fitting problem the least squares method was used. The Newton method was applied as modified by MARQUARDT /1963/. The value corresponding to the best approximation was thereafter accepted.

Conditions 2 and 3 mentioned in connection with model parameters control the relationship between growth and the reflux process. The reflux cannot culminate before a saturation in the growth and, in addition, the reflux cannot exceed the growth /$U > 0$/.

If the ascending parts of the curves are replaced by lines corresponding to fixed A, R, t_g and b, then limits for parameters t_s and s can be established /so as to satisfy conditions 2 and 3/.

Sometimes, if the number of data is small, it may happen that the "optimum" curve /in the sense of least squares/ would have unreal b or s parameter values; they turn out to be too large from the point of view of plant

Table 4

Mean length of intensive growth periods

Plant	Phenophase	Day of the vegetation season	Maximum difference of phenophase in Hungary /days/
Winter wheat	Stalk formation /Feekes 6-10/ /Keller-Baggiolini Q-V/	160-193	7
Winter barley	Stalk formation /Feekes 6-10/ /Keller-Baggiolini Q-V/	140-170	4
Rye	Stalk formation /Feekes 6-10/ /Keller-Baggiolini Q-V/	180-200	5
Spring barley	Stalk formation /Feekes 6-10/ /Keller-Baggiolini Q-V/	50-70	4
Maize	Tasselling /Hanway 3-5/ /Keller-Baggiolini D_2-D_8/	60-90	4
Potato	Beginning of flowering	60-90	4
Sugar beet	Root swelling	85-115	5
Green pepper	Flowering	70-90	5
Red pepper	Flowering	70-100	5
Rape	Green bud state	220-240	5
Sorghum	Panicle formation	75-90	-
Pea	Flowering	60-90	7
Lupin	Flowering	70-100	5

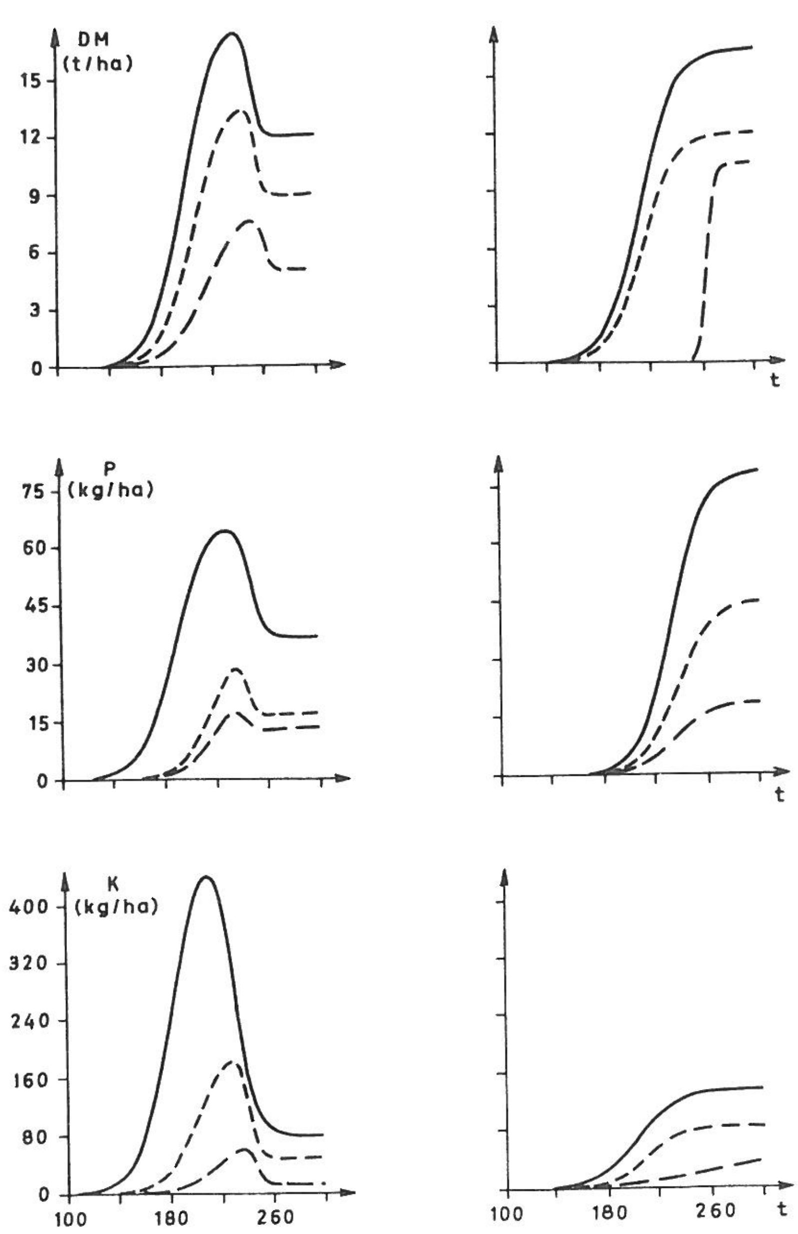


Fig. 2

Range and actual mean of dry matter /DM/ and P, K accumulation dynamics physiology. Fortunately the maximum values of b and s can be estimated utilizing the fact that the phenophases /for wheat, e.g. shooting, ripening, harvest/ which determine the dominant time interval of the growth /accumulation/ can be well fixed, as can the reflux /see Table 4/.

In developing and verifying the model it proved necessary to neglect or simplify several mechanisms of plant growth. However, the aim was not to give a detailed description of these, but to create a simple biomathematic model capable of describing the fresh and dry matter and the mineral nutrient accumulation in the soil-plant systems of annual arable crops cultivated under normal conditions /i.e. if no elemental damage occurs/.

Application of the results

Nowadays agrochemical and computational tools such as the model described here have great importance both for fertilizer recommendation purposes and in environmental science. The model is an equation describing the agrochemical cycle of mineral nutrients in the main phenophases of arable crops. Use of this model enables damage to the environment to be minimized by optimizing agrochemical intervention. The biomathematical model requires only a few data /four or five measurements during the vegetation season/ and is able to give an overall description of events occurring in the soil-plant system, while its accuracy is sufficient for the development of suitable technologies for plant cultivation in farms. If the compartment model is put into practice for making fertilization recommendations it will have the added advantage of modular expandability, allowing it to cover any new plant cultivation technologies devised in the future.

The model has been verified for the most important arable crops in Hungary /Fig. 1/ as well as for the uptake of various essential nutrients and for the fresh and dry matter formed in different years. The model equation always has the same general form /BÉKÉSSY et al., 1982/. Based on these results it is possible to present a good estimation of the nutrient demands at given time points during plant growth for different plant species cultivated on various soil types. In order to provide a concise but convincing picture of the potential latent in the use of the model, simulation curves are presented for winter wheat grown in Hungary /Fig. 2/.

In order to make utilization of the model more complete the next step will be the application of multivariate statistical analysis to establish the relation between model parameters /A, R, .../ and soil characteristics under different climatic and agrometeorological conditions.

Applying equation /5/ as a calibration for the density time series set up using multispectral remote sensing data for the arable crop area /BADHWAR and HENDERSON, 1981/, an up-to-date information base can be created for the purpose of computer-aided fertilizer recommendations. Consequently, it is possible to avoid traditional soil and plant analyses which are both expensive and cumbersome, except when extremely difficult diagnostic problems are faced. This concept can obviously be adapted anywhere.

References

ATKINS, G. L., 1969. Multicompartment models for biological systems. Science Paperbacks, Methuen and Co.

BADHWAR, G. D. and HENDERSON, K. E., 1981. Estimating development stages from spectral data - An initial model. Agronomy Journal. 73. 748-755.

BARBER, S. A., WALKER, J. M. and VASEY, E. H., 1963. Mechanism for the movement of plant nutrients from the soil and fertilizer to the plant root. J. Agr. Food Chem. 11. 204-207.

BERTALANFFY, L. VON., 1960. Principles and theory of growth. In: Fundamental aspects of normal and malignant growth. 137-259. Elsevier. Amsterdam.

BÉKÉSSY, A., BICZÓK, G. and RUDA, M., 1982. Modelling the dynamics of arable crop nutrient uptake. MTA SzTAKI Working Paper IV/21. 1982. Biometria '82 Conference. Toulouse.

BICZÓK, G., 1980. /A quantitative description of the calcium supplying process in the soil-plant system under pot experiment conditions /In Russian/ "Izvestija" Siberian Dept. Acad. Sci. USSR. Series Biol. Sci. 2. 10-20.

BOLT, G. H. and BRUGGENWERT, M. G. M., 1976. Soil chemistry, basic elements. Elsevier. Amsterdam-Oxford.

CLARCSON, D. T. and HANSON, J. B., 1980. The mineral nutrition of higher plants. Ann. Rev. Plant Physiol. 31. 239-298.

DE WIT, C. T., BROUVER, R. and PENNING DE VRIES, F. W. T., 1970. The simulation of photosynthetic systems. In: Prediction and measurement of photosynthetic productivity. /Ed.: SETLIK, J./ 47-70. PUDOC. Wageningen.

EPSTEIN, E., 1972. Mineral nutrition of plants: principles and perspectives. J. Wiley. New York - London.

GILMANOV, T. G., 1975. Plant submodel in the holistic model of biogeochemical cycles in grassland ecosystem. Trans. XIIth Int. Bot. Congr. Nauka. Leningrad. Vol. 1.

HESS, D., 1976. Pflanzenphysiologie, Molekulare und biochemisch-physiologische Grundlagen von Stoffwechsel und Entwicklung. E. Ulmer Co. Stuttgart.

KASAWNEH, F. E., 1971. Solution ion activity and plant growth. Soil Sci. Soc. Amer. Proc. 35. 426-436.

KUPERMAN, J. A. and KHITROVO, E. V., 1977. /Respiratory gas exchange as an element of the plant production process /In Russian/ Publ. Novosibirsk. USSR. Nauka.

LINDSAY, W. L., 1979. Chemical equilibria in soils. J. Wiley.

MARQUARDT, E. W., 1963. An algorithm for least squares estimation of nonlinear parameters. J. Appl. Math. 11. 431-437.

MENGEL, K., 1972. Ernahrung und Stoffwechsel der Pflanze. VEB G. Fischer Verlag. Jena.

MENGEL, K., GRIME, H. and NÉMETH, K., 1969. Potentielle und effektive Verfürbarkeit von Pflanzennahrstoffen im Boden. Landw. Forsch. 23/I. 79.

MINCHIN, P. E. H. and TROUGHTON, J. H., 1980. Quantitative interpretation of phloem translocation data. Ann. Rev. Plant Physiol. 31. 191-215.

NÉMETH, K., 1971. Möglichkeiten zur Bestimmung massgeblicher Faktoren der Bodenfrachbarkeit mittels Electro-Ultrafiltration. Landw. Forsch. Frankfurt a. Main. 26. 192-198.

NISSEN, P., 1974. Uptake mechanisms: Inorganic and organic. Ann. Rev. Plant Physiol. 25. 53-79.

NYE, P. H. and TINKER, P. B., 1977. Solute movement in the soil-root system. Studies in Ecology. Blackwell Sci. Publ. Oxford-London-Melbourne.

PITMAN, M. G., 1977. Ion transport into the xylem. Ann. Rev. Plant Physiol. 28. 71-88.

RAMAMOORTHY, S. and LEPPARD, G. G., 1977. Fibrillar pectin and contact cation exchange at the root surface. J. Theor. Biol. 66. 527-540.

SHATOKHINA, N. G., 1979. /Comparative analysis of the production process in a meadow-steppe phytocenosis and in wheat fields on ordinary chernozems in the Barbara Steppe/ /In Russian/ Pochvovedenie. 2. 96-106.

THORNLEY, J. H. M., 1976. Mathematical models in plant physiology. A quantitative approach to problems in plant and crop physiology. Experimental Botany. Vol. 8. Academic Press. Amsterdam.

TITLYANOVA, A. A., 1977. /Biological cycle of carbon in grassland biogeocenosis/. /In Russian/ Publ. Novosibirsk. USSR. Nauka. 20-23.

VERHULST, P. F., 1944. Recherches mathémathiques sur la loi d'accroissement de la population. Mem. Acad. r. Bruxelles. Vol. 18. 1-58.

WALKER, N., 1975. Soil microbiology. Butterworth and Co. Publ. Ltd. London--Boston.

ZELAWSKI, W. and LECH, A., 1980. Logistic growth functions and their applicability for characterizing dry matter accumulation in plants. Acta Physiol. Plantarum. 2. 187-194.