Physical-mathematical simulation in design of technological processes

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The present paper is an attempt to develop a technology of fertilizer production with optimal output of nutrients (humates, macro- and microelements) on the basis of physical-mathematical simulation using vibroaction. An empirical formula relating the basic technological parameters, such as the frequency of vibroaction, time and temperature of the process, has been obtained.

The importance of the method of mathematical simulation in design of complex constructions, units and multicomponent technological processes is well-known. This method often makes it possible to avoid labor-consuming and expensive experiments, creation of a succession of prototypes of systems, the scale and functions of which are similar to the systems being developed by "computational experiments" with mathematical models.

It does not, however, always allow computation of optimal parameter values of the systems under design, because the number of these parameters is very large and (or) the relation between them is complex. In these cases there arises the problem of determination of an efficient combination of the methods of mathematical and physical (natural) simulation and the use of empirical relations as an addition to the physical and mathematical models.

In the present paper, the question of such "hybrid" simulation is considered with reference to design of an economical and ecologically clean technology of production of peat-humin fertilizers.

It was established previously [1, 2] in design of some technological processes (using physical-mathematical simulation) that vibration is an effective factor which influences the activation and structure of substances. Action of vibration on a substance reorganizes, weakens and breaks chemical bonds, destroys adsorption complexes, increasing considerably the chemical activity and reactivity of substances.

The use of vibroaction makes it possible to improve technologies by increasing the output, reduction of energy consumption, improvement of the quality of end products, more efficient utilization of source components.

Combination of the physical-mathematical simulation with the empirical properties of vibroaction in design of technological processes is a factor that allows not only improvement of the existing energy-saving technologies, but also development of some new ones.

The present paper is an attempt to develop a technology of fertilizer production with optimal output of nutrients (humates, macro- and microelements) on the basis of physical-mathematical simulation using vibroaction. An empirical formula relating the basic technological parameters, such as the frequency of vibroaction, time and temperature of the process, has been obtained.

The results of a previous series of experiments to investigate the influence of the time and frequency of vibroaction on the temperature, rate and extraction of nutrients, such as humin acids in the form of potassium humates, macro- and microelements, were used in the development of the technology. The investigations were carried out using an UZG-4 ultrasonic unit in a frequency range of 16–22 kHz.

The empirical relation is as follows:

$$V \approx \left[1 - \nu e^{-\alpha T - kf^{3/2}}\right] \frac{t^2}{c^2 + t^2},$$

where

V is the volume of nutrients on a per-unit basis;

T is the temperature of the process in degrees Celsius;

f is the frequency of vibroaction in Hz;

t is the time of the process in minutes;

 ν is a constant which depends on the properties of the substance (viscosity, density, melting point, boiling point), in this case $0 \le \nu \le 1$;

 α is the index of the temperature T action in the degrees₋₁;

k is a coefficient which reflects the absorbing properties of a substance in $Hz^{-3/2}$;

c is the time constant in minutes.

The empirical relation of the technological parameters makes it possible to calculate their optimal values in a minimal number of control experiments.

Besides, the parameters of the technological process in this formula can be varied and their optimal values can be chosen depending on the quality and composition of the initial components of raw material.

Thus, the optimal values of the technological parameters for lowland peat at maximal volume of extracted nutrients are as follows:

$$\nu = 0.8, \qquad \alpha = 0.3 \times (10^{-2}) \, \mathrm{degree^{-1}},$$
 $V = 98\%, \qquad k = 0.15 \times 10^{-5} \, \mathrm{Hz^{-3/2}},$
 $T = 60^{\circ}\mathrm{C}, \qquad f = 18.5 \cdot 10^{3} \, \mathrm{Hz},$
 $t = 20 \, \mathrm{min}, \qquad t_{\mathrm{max}} = 70 \, \mathrm{min}.$

At these values of technological parameters, 98% of nutrients must be extracted from peat in accordance with the calculations, and 97.2% in experiments. Thus, the deviation of the experimental data from the theoretical data does not exceed 2%, which is within the range of error values of the experimental investigations.

Besides, the experimental data and calculations show that the time of the technological process is reduced by an order of magnitude, and the temperature of extraction of nutrients from peat is decreased by 20°C.

It should be noted that this technology is free from shortcomings typical for present-day technologies for producing fertilizers on the basis of peat [3-6 and others] which are not economically feasible and make the end product expensive, because they are characterized by:

- 1) low output of humin compounds (less than 30% of their total amount in the initial peat);
- 2) introduction of mineral salts into fertilizers to enrich it with macroand microelements;
- 3) low exploitation properties.

Composition of the fertilizer obtained with the help of the technology proposed is as follows:

- 1. Organic fraction (up to 90%): physiologically active substances containing organic nitrogen composed of water-soluble and easily assimilable humates similar in their properties to humus of soils which is the most important measure of their fertility.
- 2. Inorganic fraction (not less than 10%): a complex of water-soluble compounds of macro- and microelements (the number of which is more than 30): N, C, K, P, Ca, Mg, Al, Fe, Si, Mn, Ag, Co, Mo, Cu, B, Zn, V, S, Ni, and others.

The use of the empirical relation of technological parameters makes it possible not only to calculate their optimal values, but also to reduce the number of control experiments (which had to be carried out earlier only at physical simulation) from 87 to 6. The use of vibration and simultaneous action of high temperature on the reaction medium intensifies the process, accelerates mixing, increases the area of contact of reacting compounds, and initiates forced convection. Vibroaction activates circulation in the zone of heating, and thereby contributes to entrainment of large masses of the reaction medium into heat exchange, increases the homogeneity of temperature fields.

This is very important for uniform heating and full extraction of nutrients. In this case the larger is the amplitude of oscillations, the deeper

is the penetration of excitation pulses into the environment and the more active is the circulation of the medium. Intensifying circulation and heat exchange, vibroaction affects the heat transfer coefficient which increases by an order of magnitude. Hence, the amount of heat transferred to the reaction medium by the reactor walls increases considerably.

In conclusion it should be noted that the technology which has been developed with the use of vibroaction and physical-mathematical simulation makes it possible not only to intensify the process of extraction of nutrients (up to 98the temperature of the reactive medium, and to reduce the time of the technological cycle by an order of magnitude. This makes reprocessing of raw material more economical and profitable, improves the quality of the produced fertilizers, increasing considerably its biological activity. The empirical formula obtained can be used in design of the production process of fertilizers. The parameters of the technological process can be varied and their optimal values can be chosen depending on the composition and quality of reactants and the raw material.

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