Oxygen activity as a function of the composition of mixed fertilizers

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Abstract. The influence of the component composition of mixed mineral fertilizers and soils on the oxygen activity in the composition of mixed nitrogen-containing, phosphorus-containing and potassium-containing mineral fertilizers was studied. The study was performed by the method of physicochemical modeling based on the “Selector” software package. The following system totals were calculated: the isobaric-isothermal potential of the system, the chemical potentials of the respective independent components, the number of components of the solution, the amount of emitted gases, the pH of the solution, the redox potential of the system.

A significant positive effect of limestone and hydrated lime on the chemical activity of oxygen has been revealed. It is shown that clay soils, from the standpoint of chemical thermodynamics, are favorable in terms of increasing the oxygen activity when using nitrogen-containing, phosphorus-containing and potassium-containing fertilizers.

Previously [1], the method of physicochemical modeling was used to investigate the mutual influence of the components of mixed mineral fertilizers. It is revealed that the components of the mixture can have a significant mutual influence, the result of which may be a change in their activity.

As a rule, when discussing the influence of mineral fertilizers on biological indicators of plant growth and development, the ratio of known macronutrients and microelements is taken into account, but the state of oxygen and its chemical potential characterizing the chemical activity of oxygen as an active participant in metabolic processes in a plant are not taken into account.

In this paper, we consider the influence of the components of mixed mineral fertilizers and soil on the chemical activity of oxygen.

The study was carried out by the method of physicochemical modeling based on the “Selector” software package [2-3]. It is known to use the Selector software package to study the processes occurring in soils [4].

The main sources of thermodynamic quantities were the works [5–8].

The main parameters of the simulated systems were determined based on the data presented in [9-10], namely: ammonium nitrate (ammonium nitrate) at the rate of 100 kg/ha N; calcium dihydrogen phosphate (doublesuperphosphate) at the rate of 150 kg/ha P₂O₅; potassium carbonate or potassium chloride at the rate of 120 kg/ha K₂O; CaCO₃ (limestone) at the rate of 6 t/ha.

The following system totals were calculated: the isobaric-isothermal potential of the system, the chemical potentials of the respective independent components, the number of components of the solution, the amount of emitted gases, the pH of the solution, the redox potential of the system.
According to the simulation results, the chemical activity of oxygen in the studied mixtures of substances depends on many factors, including the composition of the mixed fertilizers, the degree of oxidation of the main component of the fertilizer, the nature of the soil.

Figure 1 shows the dependence of the chemical potential, and, consequently, the activity of oxygen on the composition of mixed mineral fertilizers. Various binary combinations of the above mineral fertilizers were investigated. Mixtures with calcium carbonate are of greatest interest.

As it follows from the data presented in figure 1, there is a significant decrease in the chemical potential of oxygen with an increase in the molar amounts of calcium carbonate in mixtures with nitrogen-containing, phosphorus-containing and potassium-containing fertilizers. Therefore, the presence of calcium carbonate in mixed mineral fertilizers has a positive effect on the growth and development of plants, which is consistent with the results of experimental studies [11-13].

The effect of calcium carbonate is approximately the same for all types of binary mixtures. Some difference in the behavior of the system with the participation of calcium dihydrogen phosphate is connected, according to the simulation results, with the formation of hydroxyapatite $3\text{Ca}_3(\text{PO}_4)_2 \cdot \text{Ca(OH)}_2$ in an amount of 0.1 mol.

A comparative characteristic of limestone and hydrated lime as components of mixed mineral fertilizers of different composition was performed. Figure 2 shows the effect of the amounts of these compounds in mixtures with calcium dihydrogen phosphate on the chemical activity of oxygen.

It was revealed that the presence of calcium hydroxide in mixed mineral fertilizers results in a more significant increase in oxygen activity, since the chemical potentials of oxygen in this case are about two times lower than in mixtures with the participation of calcium carbonate. This means that adding equimolar amounts of hydrated lime has a significantly greater effect of increasing the oxygen activity than adding limestone.
Figure 2. The dependence of oxygen activity on the amounts of calcium hydroxide and calcium carbonate in mixtures.

According to the simulation results, the activity of oxygen can depend not only on the type of the main component of the mineral fertilizer, but also on the degree of oxidation of the atoms of this component. Mixtures of phosphorus-containing and nitrogen-containing fertilizers were studied, where nitrogen-containing fertilizers are represented by potassium and ammonium nitrate, urea, and ammonia water (figure 3).

Figure 3. Dependence of oxygen activity on the degree of nitrogen oxidation in nitrogen-containing fertilizers.
As follows from the data shown in figure 3, the oxygen activity is maximum in the case of compounds with the lowest degree of nitrogen oxidation (-3) in urea and ammonia water, the minimum in potassium nitrate, where the degree of nitrogen oxidation is highest (+5), and is intermediate position in ammonium nitrate containing nitrogen in both oxidation states.

The nature of the soil also has a significant impact on the activity of the components of mixed mineral fertilizers, including oxygen activity. Thus, using the method of physicochemical modeling, we studied the effect of one of the main components of clay minerals, namely aluminum oxide, on oxygen activity using nitrogen-containing, phosphorus-containing and potassium-containing mineral fertilizers (figure 4).

**Figure 4.** The dependence of oxygen activity on the content of aluminum oxide in mixtures.

The nature of the curves shown in figure 4 indicates the positive effect of alumina as a component of clay soils on the oxygen activity when using all the above mineral fertilizers. The greatest increase in the activity of oxygen corresponds to phosphorus-containing fertilizer, then to potassium-containing, and, to a somewhat lesser extent, to nitrogen-containing fertilizer.

**Findings:**

- The activity of oxygen as a participant in metabolic processes in a plant depends on the composition of the applied mineral fertilizers and the nature of the soil.
- A significant positive effect of limestone and hydrated lime on the chemical activity of oxygen was revealed.
- Clay soils (disregarding the structure) are favorable with respect to the chemical activity of oxygen.

**References**

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