

CALCULATION OF KINETICS OF RADIATION-CHEMICAL DECOMPOSITION OF HEPTANE ADMIXTURES IN THE WATER MEDIUM

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In the previous papers [1-2] we adduced the results of experimental researches of radiation-chemical transformations of heptan in the water medium. The regularities of formation of gases H_2 , CO and hydrocarbons C_1-C_6 , and also decomposition of C_7H_{16} are studied at initial concentration of heptane 0,1-0,001 %, temperatures 40-400C and the absorbed doses up to 260 kGy.

On the basis of the carried out experimental researches and the analysis of the literature data the kinetic scheme of proceeding reactions is created. There are 4 groups of reactions: radiolytic generation of active particles, recombination of active particles, reaction of detachment, decomposition of macro radicals .At first in the scheme have been included more than 100 chemical reactions of atoms, radicals and the ions, arising under action of radiation in the system heptan-water. As a result of the comparative analysis of rate of reactions in the conditions of experiments in the scheme only 25 reactions are left. In these reactions participate 9 active atoms and radicals and 22 neutral molecules. In case of presence of oxygen the number of such reactions reaches 34. On the basis of the offered kinetic scheme of proceeding reactions calculations of kinetics of formations gases H_2 , CO and hydrocarbons C_1-C_6 are carried out.

The numerical modulation of kinetics carried out by use of Program GEPASI for homogeneous chemical and biochemical systems . As a method of numerical integration the method of Gear is used.

In result of calculations the kinetic curves of accumulation of the specified gases and decomposition initial heptane are received. Comparisons of results shows that in case of gases H_2 ,

C_1 - C_4 the good consent turns out, and hydrocarbons C_5 - C_6 is observed small deviations.

In the report the substantiation of the choice of reaction constants in detail described. The reasons for differences of calculation and experimental values of concentration of some products are considered.

Reference

1. I. Mustafaev, A. Yermakov, R. Rzayev, N. Guliyeva. Kinetics of radiation-thermal conversions of heptane admixtures in the water medium. Workshop «Environmental impact of oil transportation», 22-25 November, 2005. Baku, Azerbaijan, p.47-48
2. I. Mustafaev, R. Rzayev and N. Guliyeva. Radiation-thermal purification of wastewater from oil pollution. M.K. Zaidi (ed.), Wastewater Reuse-Risk Assessment, Decision-Making and Environmental Security, 315-322. © 2007 Springer.