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Prediction of the formation of low-molecular components, particles, and condensed phases during thermal destruction of oil-contaminated soil

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ABSTRACT

In this study, thermodynamic modelling of the process of thermal destruction of oil-contaminated soil of Ozenmunaigas JSC, which includes compounds such as carbon, silicon, aluminum, iron, calcium, magnesium, sodium, potassium, chromium, phosphorus, manganese, copper, titanium, molybdenum, nickel, vanadium, and water, was carried out. The physicochemical and thermodynamic parameters of the complex system were calculated at P=0.1 MPa, T=598-3000 K. The concentration distribution of components, particles, and condensed phases in the gas phase has been established. In the process of thermal destruction of oil-contaminated soil, the formation of condensed phases was as follows: SiO_2(c), Al_2O_3(c), AlO_3H_3(c), Cu(c), Cu_2O(c), FeO(c), Fe_2O_3(c), Fe_3O_4(c), Fe_2SiO_4(c), NiO(c), MnO(c), Mn_3O_4(c), MnO_2H_2(c), Cr_2O_3(c), MoO_2(c), V_2O_3(c), V_2O_4(c), TiO_2(c), $MgSiO_3$(c), Mg_2SiO_4(c), $MgTi_2O_5$(c), $Ca_3P_2O_8$(c), Mg_2SiO_4(c), $MgTi_2O_5$(c), $Ca_3P_2O_8$(c), $CaCO_3$(c), $CaSiO_3$(c), $CaTiO_3$(c), $Na_2Si_2O_5$(c), $K_2Si_4O_9$(c). At the same time, the amount of condensed calcium silicate $CaSiO_3$(c) was significant and amounted to 3.2 mol/kg, which is due to the initial standard content of oxides of the type (g/kg): SiO_2-473,7, CaO-181,5 in oil-contaminated soil. The formation of various types of condensed phases (from 10^{-30} to 10^{-4} mol/kg) during thermal degradation can help reduce the synergism and toxicity of metal particles in oil-contaminated soils. In the process of thermal destruction of oil-contaminated soil, its carbon-containing components (mg/kg: C_{12}-6,27; C_{13}-10,98; C_{14}-15,69; C_{15}-18,82; C_{16}-23,52; C_{17}-31,37; C_{18}-27,80; C_{19}-17,25; C_{20}-29,80) were mainly converted into oxide, carbon dioxide, and water, and thereby neutralized the organic mass of the soil.

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1. Introduction

In the process of production, pumping, and storage of oil, operation of treatment facilities, a significant amount of oil sludge, oil-contaminated soils, and asphalt-resin-paraffin deposits are formed, which leads to environmental pollution. In this regard, the problem of developing and applying technologies adapted to specific conditions remains an urgent task.

When developing technologies for cleaning soils and waters under changing weather conditions, it is necessary to take into account not only the climatic features of the region but also the properties of the oil, such as its hydrocarbon composition, and soil conditions. Therefore, one of the directions for the development of technologies for removing oil from ecosystems is the development of effective approaches that can ensure the removal of hydrocarbons from the environment. [1-17].

According to the above studies, it was noted in the works that the mechanism of ecosystem self-healing after oil pollution is rather complicated and is limited to decades [10-17]. At the same time, the authors emphasize that sorption methods for processing oily wastes are of great importance. Taking into account these circumstances, new technology has been developed for processing oily waste into useful products using an energy-accumulating substance based on humates, followed by the disposal of oil-contaminated soil. This study is a continuation of the above study [10-17], to predict the formation of low molecular weight components, particles, and condensed phases during the destruction of oil-contaminated soil under the influence of external thermal influences.

2. Material and method

The content of metals in the oil-contaminated soil in the preliminary stages of the study was determined using an AA240 spectrometer. In this case, the decomposition of the sample was carried out with a mixture of nitric, hydrofluoric, and perchloric acids until the sample was completely opened. The fractional composition of oil products present in the waste was determined by gas-liquid chromatography of a hexane extract on a mass-selective detector using an Agilent 6890 chromatograph and on a Fluorat-02 analyzer. The content of oxides of silicon, aluminum, iron, calcium, magnesium, potassium, sodium, chromium, and phosphorus was determined using a Lambda-35 spectrophotometer. Metals were determined by the decomposition of a sample and its fusion with sodium carbonate or with a mixture of sodium and potassium carbonates [16, 17].

Based on the obtained experimental data [16], the chemical matrix of oil-contaminated soil was compiled taking into account its organic and inorganic parts, as well as water. Using the chemical matrix of oil-contaminated soil, thermodynamic modeling of a complex system at the maximum entropy was carried out based on the “Terra” software package [18]. According to this program, the methodological basis of the calculation algorithm of the program allows for calculating formation in the equilibrium of gaseous, condensed substances, electrically neutral and ionized components, pure phases, and their solutions in the system under consideration. In computational experiments, the phase and elemental composition of oil-contaminated soil were calculated per 1 kg of a carrier (mol/kg). [17, 19], as well as the value of the limits of pressure and temperature of the destruction of the solid phase was in the range from 593 to 3000K (with a step of 500K).

3. Results and discussion

Oil-contaminated soil of “Ozenmunaigas” JSC consists of organic and inorganic components (mg/kg) such as C_{12}-6,27; C_{13}-10,98; C_{14}-15,69; C_{15}-18,82; C_{16}-23,52; C_{17}-31,37; C_{18}-27,80; C_{19}-17,25; C_{20}-29,80; SiO_2-473700; Al_2O_3-29400; Fe_2O_3-143100; CaO-181500; MgO-46500; Na_2O-20100; K_2O-46700; CrO-35200; P_2O_5-14700; Mn-5; Cu-12; Ti-23; Mo-12; Ni-1; V-5; H_2O-2,2 and the soil belong to substances of the 3rd hazard class. Acetylene fractions are the main danger in oil-contaminated soil [16, 17]. At the same time, the toxicity of the neutralized soil decreases due to the transfer of low-boiling acetylene oil fractions to high-boiling ones [17]. In this regard, it was of scientific interest to study the process of thermal destruction of oil-contaminated soil to predict the formation and concentration distribution of components, particles, and condensed phases, where the formation of a condensed phase promotes the transfer of toxic substances from the gas-liquid phase to the solid.

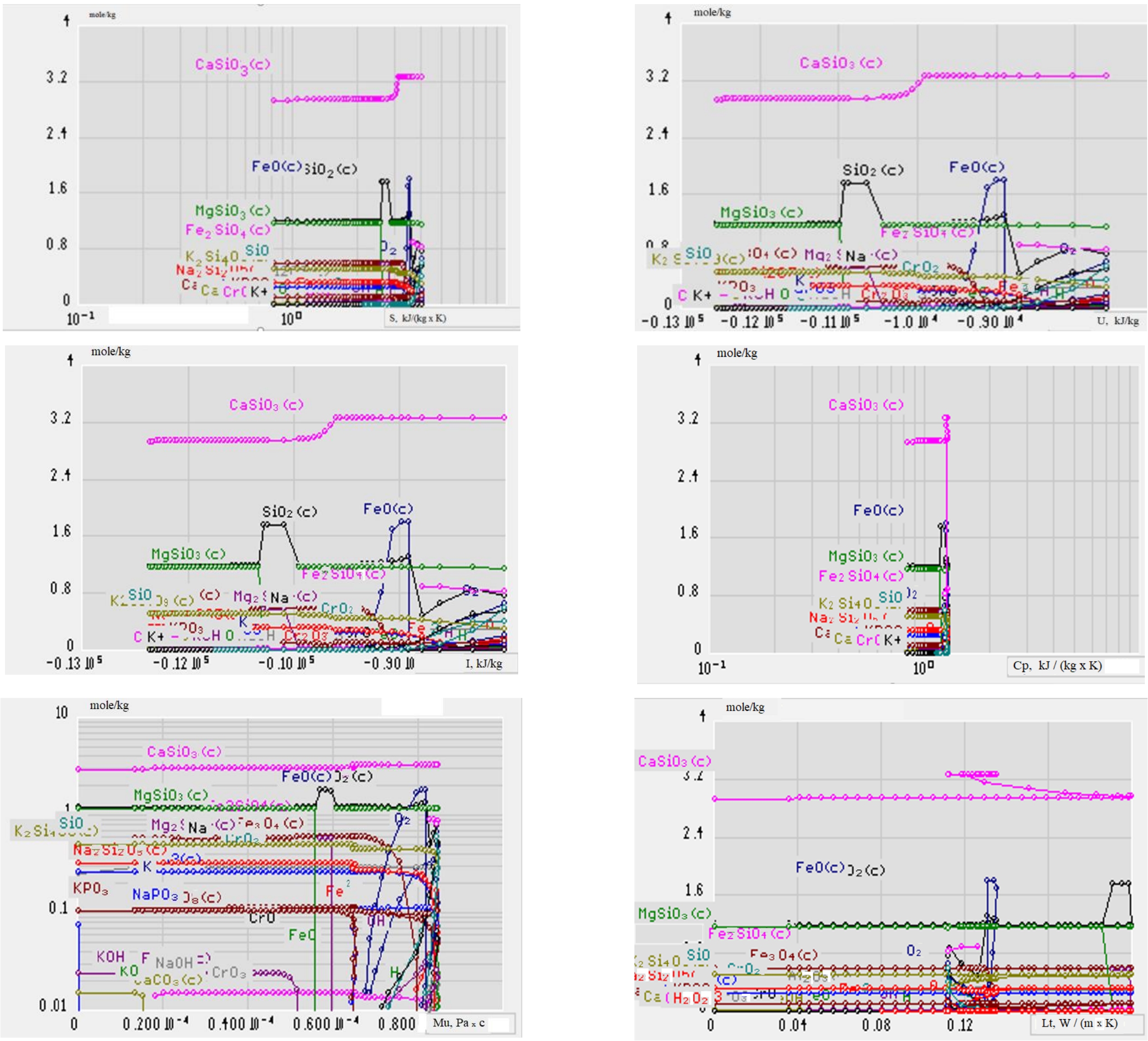
The following thermodynamic parameters were calculated: (entropy S, kJ/(kg K); enthalpy I, kJ/kg); internal energy (U, kJ/kg) and physical and chemical parameters (dynamic viscosity Mu, Pa s); heat capacity Cp, kJ/(kg K); thermal conductivity Lt, W/(m K); dimensionless Prandtl number, Pr; mass fraction of condensed phases, h) oil-contaminated soil in the temperature range T=298-3000 K at P=0.1 MPa. The values of enthalpy and internal energy (I and U) of the oil-contaminated soil were negative (Table 1, Fig. 1), which indicated the direction and course of the process of destruction of the initial mixture of complex chemical composition (mg/kg): C_{12}-6,27; C_{13}-10,98; C_{14}-15,69; C_{15}-18,82; C_{16}-23,52; C_{17}-31,37; C_{18}-27,80; C_{19}-17,25; C_{20}-29,80; SiO_2-473700; Al_2O_3-29400; Fe_2O_3-143100; CaO-181500; MgO-46500; Na_2O-20100; K_2O-46700; CrO-35200; P_2O_5-14700; Mn-5; Cu-12; Ti-23; Mo-12; Ni-1; V-5; H_2O-2,2 [12, 13].

The destruction of the oil-contaminated soil proceeded mainly with the formation of silicon-containing metal compounds (Fe, Na, Ca, Mg, K) (Fig. 1). Changes in thermodynamic (S, U, I) and physicochemical (Cp, Mu, Lt, Pr, z) parameters of oil-contaminated soil components during its thermal destruction within the temperature range of 293-3000K at P=0.1 MPa, showed the formation of a significant amount of condensed calcium silicate $CaSiO_3$(c) -3.2 mol/kg (Fig. 1).

Table 1. *Thermodynamic parameters of oil-contaminated soil at P=0.1 MPa*

T	S	I	U	Mu 10^5	Cp	Lt	Pr	z
293	0,69	-12590,3	-12590,3	-	0,77	-	-	1,00
593	1,34	-12310,7	-12311,0	2,19	1,00	0,06	0,69	1,00
1093	2,03	-11740,1	-11741,0	3,86	1,13	0,12	0,69	1,00
1593	2,49	-11124,8	-11126,2	5,3	1,16	0,17	0,69	1,00
2093	3,03	-10144,2	-10146,8	6,52	1,27	0,17	0,59	0,99
2593	3,35	-9377,9	-9386,6	7,33	1,27	0,13	0,63	0,97
2993	4,01	-7522,5	-7599,6	8,45	1,24	0,11	0,68	0,84

This amount of $CaSiO_3$(c) is due to the initial standard content of oxides of the type (mg/kg): SiO_2-473700, CaO-181500 in oil-contaminated soil. In addition to CaSiO3(c), other condensed phases were formed, as well as various components and particles (Table 2, Fig. 3).



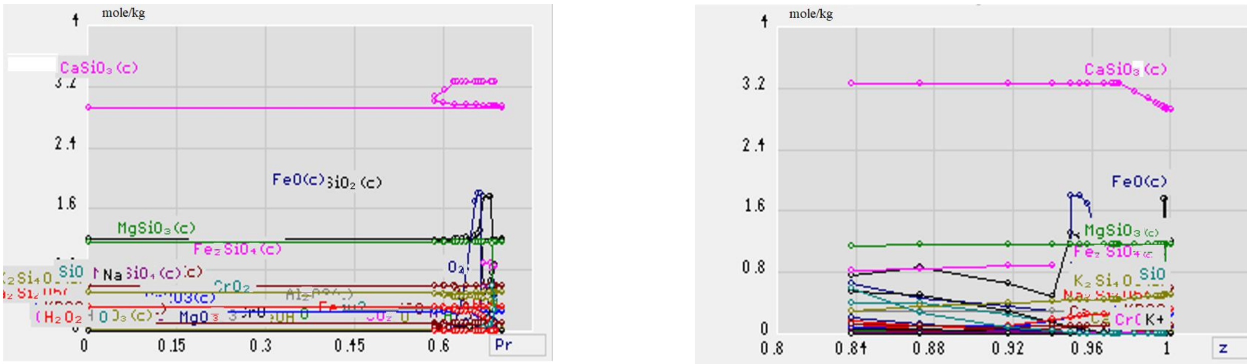


Figure.1. *Changes in thermodynamic (S, U, I) and physicochemical (Cp, Mu, Lt, Pr, z) parameters of oil-contaminated soil components during its thermal destruction within the temperature range of 593-3000K at P=0.1 MPa*

In general, the condensed phases have the following range of compounds (Fig. 2-4, Tables 2 and 3): SiO_2(c), Al_2O_3(c), AlO_3H_3(c), Cu(c), Cu_2O(c), FeO(c), Fe_2O_3(c), Fe_3O_4(c) Fe_2SiO_4(c), NiO(c), MnO(c), Mn_3O_4(c), MnO_2H_2(c), Cr_2O_3(c), MoO_2(c), V_2O_3(c), V_2O_4(c), TiO_2(c), $MgSiO_3$(c), Mg_2SiO_4(c), MgTi2O5(c), $Ca_3P_2O_8$(c), Mg_2SiO_4(c), $MgTi_2O_5$(c), $Ca_3P_2O_8$(c), $CaCO_3$(c), $CaSiO_3$(c), $CaTiO_3$(c), $Na_2Si_2O_5$(c), $K_2Si_4O_9$(c).

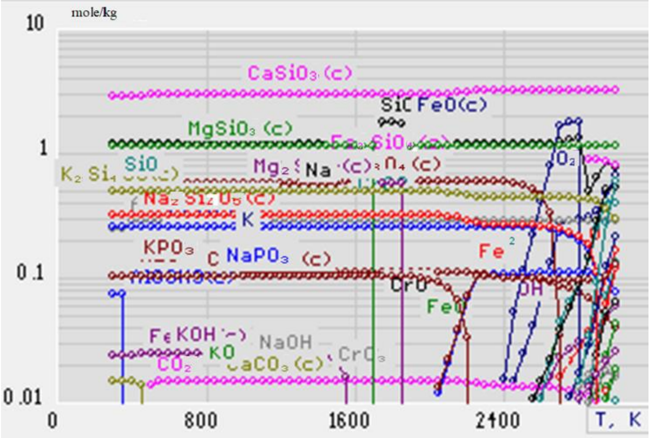


Figure 2. *Components, particles, and condensed phases formed during the destruction of oil-contaminated soil (mol/kg) depending on temperature. P=0.1 MPa.*

Table 2. *Change in the concentration of phosphorus, chromium, magnesium, iron, calcium, sodium, potassium, aluminum containing substances during the destruction of oil-contaminated soil (mol/ kg) depending on temperature. P=0.1 MPa.*

T	P	P_2	PO	PO_2	P_2O_3	P_2O_4	P_2O_5	PH	PH_2	HPO
593	1,9e-22	1,9e-22	1,9e-22	1,9e-22	1,9e-22	1,9e-22	1,9e-22	1,9e-22	1,9e-22	1,9e-22
1093	1,9e-22	1,9e-22	1,9e-22	5,1e-20	1,9e-22	1,9e-22	1,9e-22	1,9e-22	1,9e-22	1,9e-22
1593	1,9e-22	1,9e-22	1,1e-15	5,6e-12	6,1e-22	8,6e-20	1,4e-16	1,9e-22	1,9e-22	5,7e-20
2093	1,0e-13	1,0e-19	2,5e-08	1,1e-06	3,1e-12	4,9e-12	2,7e-10	7,7e-15	3,4e-16	6,3e-12
2593	1,7e-09	3,9e-14	2,1e-05	1,5e-04	2,7e-09	7,9e-10	1,6e-08	6,7e-11	1,2e-12	5,6e-09
2993	6,6e-07	3,4e-11	1,0e-03	1,6e-03	2,2e-08	1,6e-09	1,2e-08	7,1e-09	3,0e-11	1,0e-07

T	Cr	CrO	CrO2	CrO3	Cr2O3(c)	Cr2O3	CrO2H2	CrO3H3	CrO4H4
593	1,9e-22	1,9e-22	1,9e-22	1,9e-22	2,6e-01	1,9e-22	1,9e-22	1,9e-22	1,9e-22
1093	1,9e-22	1,9e-22	2,2e-17	1,5e-16	2,6e-01	1,9e-22	1,2e-16	2,6e-15	1,3e-18
1593	7,8e-18	9,2e-14	7,2e-09	1,5e-07	2,6e-01	4,7e-15	2,3e-11	6,8e-11	9,7e-14
2093	3,0e-10	6,6e-08	2,3e-05	1,0e-05	2,6e-01	7,4e-09	1,1e-07	1,2e-08	2,9e-12
2593	5,7e-06	2,9e-04	1,0e-02	1,3e-03	2,5e-01	8,4e-05	1,1e-05	1,7e-07	1,5e-11
2993	4,3e-03	6,3e-02	4,0e-01	1,6e-02	1,0e-30	8,6e-03	2,8e-05	3,9e-08	5,2e-13

T	Mg	MgO	MgH	MgOH	MgO_2H_2	$MgSiO_3$(c)	Mg_2SiO_4(c)	$MgTi_2O_5$(c)
593	1,9e-22	1,9e-22	1,9e-22	1,9e-22	1,9e-22	1,1e+00	1,0e-30	1,0e-30

1093	1,9e-22	1,9e-22	1,9e-22	3,4e-20	4,6e-14	1,1e+00	1,0e-30	1,0e-30
1593	4,2e-15	6,9e-14	2,7e-21	7,2e-13	5,3e-09	1,1e+00	1,0e-30	1,0e-30
2093	4,1e-09	1,0e-08	1,0e-13	2,7e-08	1,3e-06	1,1e+00	1,0e-30	2,4e-04
2593	9,1e-06	1,9e-05	8,0e-10	9,0e-06	2,3e-05	1,1e+00	1,0e-30	1,6e-04
2993	4,3e-03	5,8e-03	3,0e-07	3,7e-04	4,9e-05	1,1e+00	1,0e-30	1,0e-30

T	**Fe**	**FeO(c)**	**FeO**	**FeO_2**	**Fe_2O_3(c)**	**Fe_3O_4(c)**	**FeOH**	**FeO_2H_2**	**Fe_2SiO_4(c)**
593	1,9e-22	1,0e-30	1,9e-22	1,9e-22	2,4e-02	5,8e-01	1,9e-22	1,9e-19	1,0e-30
1093	7,6e-20	1,0e-30	6,8e-20	5,5e-20	2,4e-02	5,8e-01	1,5e-13	1,5e-10	1,0e-30
1593	3,1e-13	1,0e-30	7,7e-12	6,8e-11	1,2e-24	6,0e-01	2,9e-09	2,8e-07	1,0e-30
2093	2,8e-07	1,0e-30	4,4e-07	1,4e-07	1,0e-30	6,0e-01	1,4e-05	4,4e-05	1,0e-30
2593	4,5e-04	4,1e-01	3,6e-04	4,4e-05	1,0e-30	4,6e-01	9,3e-04	4,2e-04	1,0e-30
2993	1,1e-01	1,0e-30	4,2e-02	1,8e-03	1,0e-30	1,0e-30	1,0e-02	4,3e-04	8,1e-01

T	**Ca**	**CaO**	**CaOH**	**CaO_2H_2**	**$Ca_3P_2O_8$(c)**	**$CaCO_3$(c)**	**$CaSiO_3$(c)**	**$CaTiO_3$(c)**
593	1,9e-22	1,9e-22	1,9e-22	1,9e-22	1,0e-01	1,0e-30	2,9e+00	1,0e-30
1093	1,9e-22	1,9e-22	1,9e-22	1,4e-15	1,0e-01	1,0e-30	2,9e+00	1,0e-30
1593	1,3e-19	5,7e-18	2,3e-15	3,7e-10	1,0e-01	1,0e-30	2,9e+00	4,8e-04
2093	8,7e-13	2,8e-12	1,9e-10	1,2e-07	8,2e-02	1,0e-30	3,0e+00	1,0e-30
2593	6,9e-09	1,4e-08	1,1e-07	2,7e-06	1,0e-30	1,0e-30	3,2e+00	1,0e-30
2993	6,7e-06	7,1e-06	6,7e-06	6,5e-06	1,0e-30	1,0e-30	3,2e+00	1,0e-30

T	**Na**	**NaO**	**Na_2O**	**NaOH**	**$Na_2O_2H_2$**	**$NaPO_2$**	**$NaPO_3$**	**$Na_2Si_2O_5$(c)**
593	1,9e-22	1,9e-22	1,9e-22	1,1e-19	1,9e-22	1,9e-22	1,9e-22	3,2e-01
1093	7,6e-12	1,3e-17	1,9e-22	2,1e-09	9,8e-14	3,4e-21	6,1e-10	3,2e-01
1593	1,0e-07	7,4e-10	3,9e-14	5,8e-06	4,8e-10	9,5e-14	5,0e-05	3,2e-01
2093	1,4e-04	9,1e-07	8,0e-10	3,2e-04	2,7e-08	7,1e-08	2,1e-02	3,1e-01
2593	1,5e-02	2,5e-04	7,4e-07	5,2e-03	2,9e-07	1,3e-05	1,1e-01	2,6e-01
2993	5,4e-01	1,0e-02	3,5e-05	1,7e-02	1,2e-07	1,0e-04	7,8e-02	1,0e-30

T	**K**	**K_2O**	**K_2O_2**	**KOH**	**$K_2O_2H_2$**	**KPO_3**	**K_2CO_3**	**$K_2Si_4O_9$(c)**
593	1,93e-22	1,93e-22	1,93e-22	8,90e-18	1,93e-22	1,93e-22	1,93e-22	4,99e-01
1093	2,20e-12	1,93e-22	1,93e-22	1,29e-08	1,27e-13	3,29e-09	4,58e-15	4,99e-01
1593	2,05e-08	6,58e-15	6,53e-16	1,06e-05	1,97e-10	8,93e-05	2,38e-12	4,99e-01
2093	2,49e-05	6,59e-11	8,21e-13	3,44e-04	7,15e-09	2,27e-02	4,61e-11	4,88e-01
2593	2,81e-03	4,94e-08	4,94e-10	4,51e-03	7,52e-08	9,83e-02	3,30e-10	4,46e-01
2993	2,12e-01	8,36e-06	4,85e-08	2,61e-02	1,22e-07	1,27e-01	6,91e-10	3,03e-01

T	**Al_2O_3(c)**	**Al_2O_3**	**HAlO**	**$HAlO_2$**	**AlO_2H_2**	**AlO_3H_3(c)**	**AlO_3H_3**
593	2,9e-01	1,9e-22	1,9e-22	1,9e-22	1,9e-22	1,0e-30	1,9e-22
1093	2,9e-01	1,9e-22	1,9e-22	1,9e-22	1,3e-20	1,0e-30	8,5e-16
1593	2,9e-01	1,9e-22	1,9e-22	8,9e-15	6,3e-14	1,0e-30	1,9e-11
2093	2,9e-01	1,1e-16	3,3e-16	3,9e-10	1,7e-09	1,0e-30	3,2e-09
2593	2,9e-01	2,5e-11	9,7e-12	2,6e-07	3,2e-07	1,0e-30	3,0e-08
2993	2,9e-01	6,4e-08	5,0e-09	1,0e-05	2,6e-06	1,0e-30	1,2e-08

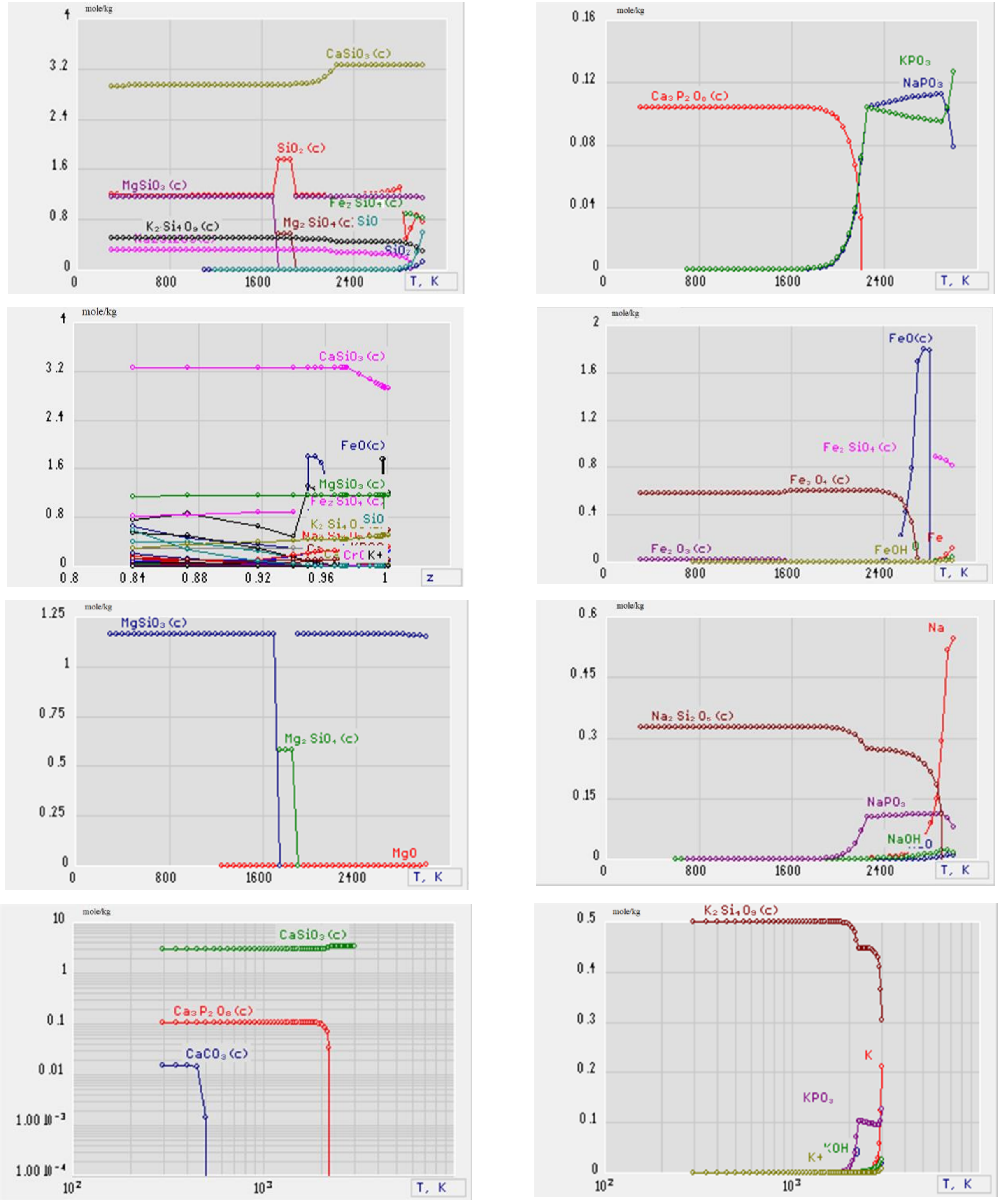


Figure 3. *Concentration change (mol/kg): silicon, iron, phosphorus, magnesium, chromium, sodium, calcium, and potassium-containing substances during the destruction of oil-contaminated soil depending on temperature. P=0.1 MPa.*

Table 3 shows the concentrations of copper, nickel, manganese, molybdenum, vanadium, titanium-containing particles, and components formed during the thermal destruction of oil-contaminated soil depending on temperature (593-2993 K). It is noted that complex redox processes occur and a wide range of substances are formed in small amounts (mol/kg): Cu(c), Cu, Cu_2, CuO, Cu_2O(c), CuH, CuOH; Ni, NiO(c), NiO, NiH, NiOH, NiO_2H_2, Mn, MnO(c), MnO, MnO_2, Mn_3O_4(c), MnH, MnOH, MnO_2H_2(c), Mo, MoO, MoO_2(c), MoO_2, MoO_3, Mo_2O_6, MoO_2H_2, MoO_3H_2, MoO_4H_2, V, VO, VO_2, V_2O_3(c), V_2O_4(c), V_4O_8, V_4O_{10}, Ti, TiO, TiO_2(c), TiO_2, TiOH (Table 3).

Table3. *Change in concentration (mol/kg): copper, nickel, manganese, molybdenum, vanadium, titanium-containing components, particles, and condensed phases during the destruction of oil-contaminated soil depending on temperature. P=0.1 MPa.*

T	Cu(c)	Cu	Cu_2	CuO	Cu_2O(c)	CuH	CuOH
593	1,9e-04	1,9e-22	1,9e-22	1,9e-22	1,0e-30	1,9e-22	1,9e-22
1093	1,9e-04	6,0e-11	8,9e-16	5,7e-16	1,0e-30	6,6e-13	9,4e-12
1593	1,0e-30	1,4e-06	4,8e-10	2,5e-08	9,4e-05	2,9e-09	3,9e-07
2093	1,0e-30	1,8e-04	1,5e-07	1,8e-06	1,0e-30	1,2e-06	5,9e-06
2593	1,0e-30	1,8e-04	6,4e-09	3,6e-06	1,0e-30	1,0e-06	1,7e-06
2993	1,0e-30	1,8e-04	2,4e-10	3,4e-06	1,0e-30	3,7e-07	2,2e-07

T	Ni	NiO(c)	NiO	NiH	NiOH	NiO_2H_2
593	1,93e-22	1,72e-05	1,93e-22	1,93e-22	1,93e-22	1,66e-19
1093	1,21e-16	1,72e-05	6,29e-18	2,41e-17	1,09e-13	6,89e-10
1593	1,88e-10	1,44e-05	5,10e-10	2,02e-12	1,34e-08	2,73e-06
2093	1,83e-06	1,00e-30	4,38e-07	3,70e-08	3,39e-06	1,15e-05
2593	1,18e-05	1,00e-30	1,78e-06	1,42e-07	2,63e-06	7,83e-07
2993	1,56e-05	1,00e-30	1,17e-06	5,69e-08	2,78e-07	5,47e-09

T	Mn	MnO(c)	MnO	MnO_2	Mn_3O_4(c)	MnH	MnOH	MnO_2H_2(c)
593	1,93e-22	9,16e-05	1,93e-22	1,93e-22	1,00e-30	1,93e-22	1,93e-22	1,00e-30
1093	2,25e-18	1,00e-30	4,19e-19	1,63e-20	3,05e-05	5,35e-18	3,73e-17	1,00e-30
1593	2,61e-12	1,00e-30	2,90e-11	4,00e-11	3,05e-05	3,62e-13	2,11e-11	1,00e-30
2093	8,94e-07	8,90e-05	9,33e-07	9,75e-08	1,00e-30	2,37e-07	4,70e-07	1,00e-30
2593	4,64e-05	1,00e-30	3,12e-05	1,93e-06	1,00e-30	7,16e-06	4,90e-06	1,00e-30
2993	6,52e-05	1,00e-30	2,21e-05	6,76e-07	1,00e-30	2,95e-06	7,18e-07	1,00e-30

T	Mo	MoO	MoO_2(c)	MoO_2	MoO_3	Mo_2O_6	MoO_2H_2	MoO_3H_2	MoO_4H_2
593	1,9e-22	1,9e-22	1,2e-04	1,9e-22	1,9e-22	1,9e-22	1,9e-22	1,9e-22	1,6e-14
1093	1,9e-22	1,9e-22	3,3e-05	9,6-18	1,6e-10	1,5e-07	1,9e-22	7,0e-14	2,4e-05
1593	1,9e-22	7,5e-20	1,0e-30	2,4e-12	1,2e-06	7,4e-06	5,0e-21	1,3e-11	6,3e-05
2093	4,6e-17	1,7e-12	1,0e-30	6,1e-08	6,1e-05	9,9e-06	4,7e-15	6,5e-09	4,0e-05
2593	3,7e-13	1,2e-09	1,0e-30	1,8e-06	1,1e-04	1,8e-07	2,0e-13	7,9e-09	2,3e-06
2993	1,2e-10	6,9e-08	1,0e-30	1,1e-05	9,6e-05	1,6e-09	2,4e-13	8,3e-10	2,9e-08

T	V	VO	VO_2	V_2O_3(c)	V_2O_4(c)	V_4O_8	V_4O_{10}
593	1,9e-22	1,9e-22	1,9e-22	4,9e-05	1,0e-30	1,9e-22	1,9e-22
1093	1,9e-22	1,9e-22	1,3e-14	1,0e-30	4,9e-05	2,6e-10	1,0e-12
1593	1,9e-22	7,6e-16	7,3e-08	1,0e-30	1,7e-29	2,0e-05	4,6e-06
2093	3,9e-15	6,0e-10	5,3e-05	1,0e-30	1,0e-30	1,1e-05	3,0e-09
2593	4,9e-12	2,9e-08	9,8e-05	1,0e-30	1,0e-30	1,1e-12	3,7e-17
2993	4,6e-10	2,9e-07	9,8e-05	1,0e-30	1,0e-30	4,4e-19	1,9e-22

T	Ti	TiO	TiO_2(c)	TiO_2	TiOH
593	1,9e-22	1,9e-22	4,8e-04	1,9e-22	1,9e-22
1093	1,9e-22	1,9e-22	4,8e-04	4,8e-21	1,9e-22
1593	1,9e-22	2,4e-19	1,0e-30	4,5e-12	6,6e-22
2093	1,1e-18	9,9e-12	1,0e-30	1,9e-07	3,3e-14
2593	9,2e-13	1,8e-07	1,0e-30	1,5e-04	2,7e-10
2993	3,6e-10	5,4e-06	1,0e-30	4,7e-04	2,0e-09

The content of condensed phases following types: Cu(c), Cu_2O(c), NiO(c), MnO(c), Mn_3O_4(c), MnO_2H_2(c), MoO_2(c), V_2O_3(c), V_2O_4 (c), TiO_2(c) ranges from 10-30 to 10-4 mol per 1 kg of the gas phase. Under real conditions, synergism of these particles can take place in soils; combined effect on the components of the environment [19-22]. In the process of thermal destruction of oil-contaminated soil, the organic phase under the action of water (H_2O-2.2 mg/kg) and metal particles of the soil undergoes oxidation and destruction with the formation of oxygen-containing, hydrogen, and carbon-containing components, particles (Table 4, Fig. 4).

Table 4. *Change in concentration (mol/kg): oxygen, hydrogen, and carbon-containing substances during the destruction of oil-contaminated soil depending on temperature. P=0.1 MPa*.

T	**O**	**O_2**	**H**	**H_2**	**OH**	**HO_2**	**H_2O**	**H_2O_2**	**O_3**
593	1,9e-22	1,9e-22	1,9e-20	3,8e-06	6,2e-21	1,9e-22	1,1e-01	1,9e-22	1,9e-22
1093	1,0e-14	2,1e-10	1,3e-11	3,0e-06	2,1e-09	1,6e-15	1,1e-01	3,9e-14	1,9e-22
1593	3,0e-07	3,9e-03	3,6e-08	3,9e-06	3,9e-05	4,0e-08	1,1e-01	6,8e-09	2,0e-16
2093	3,6e-05	4,1e-03	2,5e-05	4,0e-04	8,1e-04	4,1e-07	1,1e-01	4,3e-08	2,9e-14
2593	4,1e-03	7,2e-02	1,2e-03	2,2e-03	1,1e-02	1,1e-05	9,8e-02	3,3e-07	3,1e-11
2993	1,6e-01	6,6e-01	1,8e-02	3,9e-03	5,9e-02	5,1e-05	4,0e-02	3,0e-07	2,0e-09

T	**CO**	**CO_2**	**CH_4**	**CHO**	**CHO_2**	**CH_2O**	**CH_2O_2**
593	1,6e-08	1,5e-02	1,6e-15	1,9e-22	3,3e-22	4,1e-19	1,6e-13
1093	4,0e-07	1,5e-02	1,9e-22	6,5e-19	4,6e-15	5,2e-18	3,4e-13
1593	1,6e-06	1,5e-02	1,9e-22	5,0e-16	2,3e-12	2,1e-17	6,3e-13
2093	2,6e-04	1,4e-02	1,4e-19	1,1e-11	5,0e-10	2,5e-13	6,2e-11
2593	1,9e-03	1,3e-02	2,8e-18	6,3e-10	4,7e-09	3,9e-12	1,4e-10
2993	6,4e-03	8,7e-03	6,3e-19	2,6e-09	4,5e-09	3,0e-12	2,5e-11

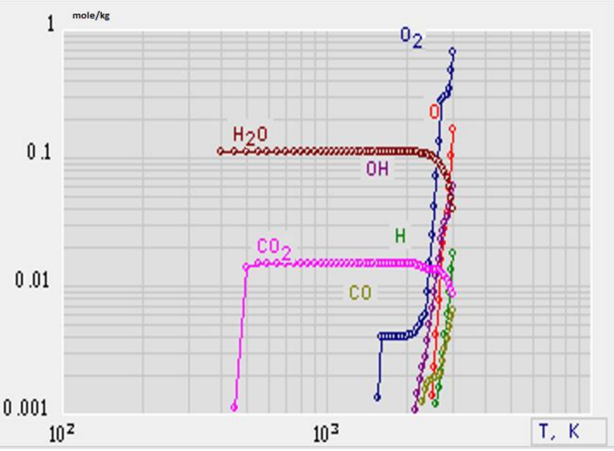


Figure 4. *Change in concentration (mol/kg): oxygen, hydrogen, carbon-containing substances during the destruction of oil-contaminated soil depending on temperature*

The content in the gas phase the concentration of compounds were: molecular oxygen =0.66 mol/kg (at 2993 K), water vapor = 0.01 mol/kg (at 593-2093 K), carbon dioxide =0.015 mol/kg (at 593-1593 K), carbon monoxide =0.0019 mol/kg (at 2593K), atomic oxygen= 0.16 mol/kg (at 2993K), atomic hydrogen= 0.018 mol/kg (at 2993K), hydroxyl = 0.059 mol/kg (at 2993K). Following types of particles: HO_2, H_2O_2, O_3, CH_4, CHO, CHO_2, CH_2O, CH_2O_2 were contained in trace amounts (Fig. 4, Table 4).

Thus, in the process of thermal degradation, the formation of various types of condensed phases can help reduce the toxicity of metal particles in oil-contaminated soils, and its carbon-containing components are mainly converted into oxide, carbon dioxide, water, and thus the neutralization of the organic mass of the soil was shown.

4. Conclusion

1. Thermodynamic modeling of the process of thermal destruction of oil-contaminated soil, consisting of carbon, silicon, aluminum, iron, calcium, magnesium, sodium,

potassium, chromium, phosphorus, manganese, copper, titanium, molybdenum, nickel, vanadium, and water, was carried out.

2. The physicochemical and thermodynamic parameters of the oil-contaminated soil were calculated at P=0.1 MPa, T=598-3000 K. The concentration distribution of components, particles, and condensed phases in the gas phase was established.
3. In the process of thermal destruction of oil-contaminated soil of “Ozenmunaigas” JSC, the formation of various condensed phases were: SiO_2(c), Al_2O_3(c), AlO_3H_3(c), Cu(c), Cu_2O(c), FeO(c), Fe_2O_3(c), Fe_3O_4(c), Fe_2SiO_4(c), NiO(c), MnO(c), Mn_3O_4(c), MnO_2H_2(c), Cr_2O_3(c), MoO_2(c), V_2O_3(c), V_2O_4(c), TiO_2(c), $MgSiO_3$(c), Mg_2SiO_4(c), $MgTi_2O_5$(c), $Ca_3P_2O_8$(c), Mg_2SiO_4(c), $MgTi_2O_5$(c), $Ca_3P_2O_8$(c), $CaCO_3$(c), $CaSiO_3$(c), $CaTiO_3$(c), $Na_2Si_2O_5$(c), $K_2Si_4O_9$(c).
4. Changes in thermodynamic (S, U, I) and physicochemical (Cp, Mu, Lt, Pr, z) parameters of oil-contaminated soil components during its thermal destruction in the temperature range of 593-3000 K and at P=0.1. MPa showed the formation of a significant amount of condensed calcium silicate $CaSiO_3$(c) - 3.2 mol/kg, which is due to the initial content of oxides of the type (mg/kg): SiO_2-473700, CaO-181500 in oil-contaminated soil. The mass fraction of all condensed phases of the system varied within Z=0.84-1.0.
5. The formation of a large number of condensed phases (from 10^{-30} to 10^{-4} mol/kg) was noted, which is very important in the processes of reducing the toxicity of various metal particles.
6. In the process of thermal destruction of oil-contaminated soil, its carbon-containing components (mg/kg): C_{12}-6,27; C_{13}-10,98; C_{14}-15,69; C_{15}-18,82; C_{16}-23,52; C_{17}-31,37; C_{18}-27,80; C_{19}-17,25; C_{20}-29,80 were mainly converted into carbon monoxide and dioxide, water, and thus the neutralization of the organic mass of the soil is achieved.

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