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COMPLETE THERMODYNAMIC ANALYSIS OF THE INTERACTION OF IRON PHOSPHATE ($FePO_4$) WITH HYDROGEN (H_2) AND CARBON MONOXIDE (CO)

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Preliminary Note – Prethodno priopćenje

Iron phosphate in the composition of concentrate is a fairly strong chemical compound. However, with the help of gaseous substances, such complex compounds decompose when heated to the required temperature, which contributes to the reduction of not only iron, but also phosphorus. Hydrogen and carbon monoxide were used as gaseous reducing agents. This article describes in detail the thermodynamic analysis of the reduction of phosphorus from iron phosphate, its interaction with hydrogen and carbon monoxide.

Keywords: iron phosphate, thermodynamic analysis, temperature, hydrogen, carbon monoxide.

INTRODUCTION

The problem of phosphorus was from the very beginning of the development of the deposit and for many decades remains unresolved. Over such a long period of time, there have been attempts by scientists and specialists aimed at reducing the phosphorus content in the concentrate and developing a technology for producing a conditioned metal from phosphorus-containing ores [1].

Elevation lisakovsk gravity magnetic concentrate by removing phosphorus today's time is the actual problematic task. The peculiarity of the concentrate is the high content of phosphorus in it at the level of 0,60 – 0,75 %, which is unacceptable in its metallurgical processing.

The improvement of the lisakovsk gravitational magnetic concentrate due to its desphosphorization is an urgent problem today.

RESULTS OF THERMODYNAMIC ANALYSIS

A complete thermodynamic analysis of the interaction of iron phosphate ($FePO_4$) with hydrogen (H_2) and carbon monoxide (CO) was performed by these following reactions:

$$2FePO_4 + 8H_{2(g)} = Fe_2P + 0{,}25P_{4(g)} + 8H_2O_{(g)} \quad (1)$$

$$8FePO_4 + 32CO_{(g)} = 4Fe_2P + P_{4(g)} + 32CO_{2(g)} \quad (2)$$

Thermodynamic analysis was performed using the HSC – 5.1: temperature range: 200 - 1 400 °C; pressure 1 bar; temperature step 100 °C [2]. The influence of temperature on the equilibrium distribution of iron and phosphorus was determined.

Table 1 and Figure 1 (a) shows the primary tabular and graphical data on the quantitative distribution/ kg of the interaction of iron phosphate ($FePO_4$) with hydrogen (H_2), obtained using the HSC - 5.1 software package.

Table 2 and Figure 1 (b) shows the primary tabular and graphical data on the quantitative distribution/ kg of the interaction of iron phosphate ($FePO_4$) with carbon monoxide (CO).

When iron phosphate ($FePO_4$) interacts with hydrogen (H_2) and carbon monoxide (CO), the decomposition of iron phosphate into various iron and phosphorus com-

Table 1 **Influence of temperature on the equilibrium distribution of substances/ kg in the interaction of iron phosphate ($FePO_4$) with hydrogen (H_2)/ temperature range 200 – 1 400 °C**

T/ K	Phase	Units	MW / g/mol	Min	Max			
						1	2	13
Compo-nent	0	C	0,000	200,000	1 400,000	2,00E+02	3,00E+02	1,40E+03
PO_2 / gas	1	kg	62,973	0,000	1,000	6,30E–35	6,03E–28	2,16E–03
FeP_2	3	kg	117,795	0,000	1,000	4,15E–18	2,70E–15	5,85E–06
P_4O_{10} / gas	1	kg	283,889	0,000	0,000	2,84E–34	2,84E–34	7,52E–13
P_4 / gas	1	kg	123,895	0,000	0,000	1,24E–34	1,24E–34	2,58E–16
H_2O / gas	1	kg	18,015	0,607	108,579	6,07E–01	6,61E+00	1,09E+02
P_2O_5 / gas	1	kg	141,945	0,000	0,000	1,42E–34	1,42E–34	4,68E–07
FeH / gas	1	kg	56,855	0,000	1,000	5,69E–35	3,15E–32	6,92E–06
P_2O_3 / gas	1	kg	109,946	0,000	1,000	1,10E–34	2,5E–30	1,03E–04
P_2 / gas	1	kg	61,948	0,000	0,000	6,19E–35	4,03E–32	5,84E–07
FeP	3	kg	86,821	0,000	1,000	2,04E–07	8,88E–06	1,53E–01
H_2 / gas	1	kg	2,016	3,949	16,031	1,60E+01	1,54E+01	3,95E+00
$FePO_4$	2	kg	150,818	0,000	300,310	3,00E+02	2,84E+02	1,51E–34
P_4O_6 / gas	1	kg	219,891	0,411	73,233	4,11E–01	1,47E+00	7,27E+01
P_3O_6 / gas	1	kg	188,918	0,000	0,000	1,89E–34	1,89E–34	2,98E–09
Fe_2P	3	kg	142,668	0,006	1,000	5,73E–03	7,36E–02	5,17E+00
P_2O_4 / gas	1	kg	125,945	0,000	0,000	1,26E–34	7,22E–34	1,78E–06
Fe_3P	3	kg	198,515	0,738	131,407	7,38E–01	8,02E+00	1,28E+02

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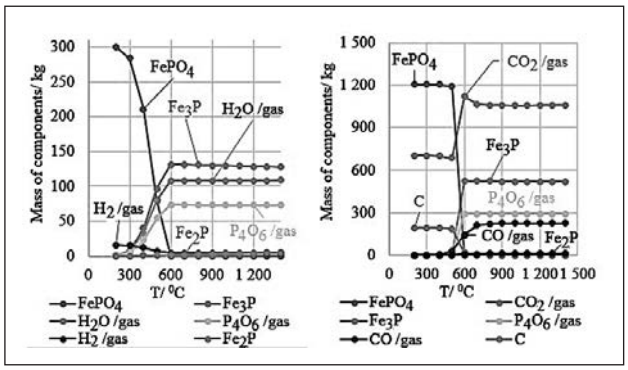


a) b)

Figure 1 Influence of temperature on the equilibrium distribution of substances/ kg in the interaction of iron phosphate ($FePO_4$) with hydrogen (H_2) (a) and carbon monoxide (CO) (b)

Table 2 **Influence of temperature on the equilibrium distribution of substances/ kg in the interaction of iron phosphate ($FePO_4$) with carbon monoxide (CO)/ temperature range 200 – 1 400 °C**

T/ K	Phase	Units	MW / g/mol	Min	Max			
						1	2	13
Compo-nent	0	C	0,000	200,000	1 400,000	2,00E+02	3,00E+02	1,40E+03
$FePO_2$	2	kg	150,818	0,000	1 206,607	1,21E+03	1,2E+02	1,5E–34
CO_2 (g)	1	kg	44,010	687,125	1 121,502	7,04E+02	7,04E+02	1,06E+03
Fe_3P	3	kg	198,515	0,000	523,027	1,99E–34	1,66E–17	5,19E+02
P_4O_6 (g)	1	kg	219,891	0,000	292,324	6,31E–12	2,50E–12	2,92E+02
CO (g)	1	kg	28,010	0,006	222,450	5,59E–03	2,63E–01	2,22E+02
C	3	kg	12,011	0,000	1,000	1,92E+02	1,92E+02	4,32E–04
Fe_2P	3	kg	142,668	0,000	1,000	1,53E–28	27,72E–15	1,14E+01
FeP	3	kg	86,821	0,000	1,000	2,06E–23	5,84E–15	1,84E–01
PO_2 (g)	1	kg	62,973	0,000	1,000	6,30E–35	2,77E–29	1,57E–02
P_2O_3 (g)	1	kg	109,946	0,000	1,000	1,10E–34	1,10E–-34	4,09E–04
P_2O_4 (g)	1	kg	125,945	0,000	1,000	1,26E–34	1,26E–34	2,37E–05
P_2O_5 (g)	1	kg	141,945	0,000	1,000	1,42E–34	1,42E–34	2,07E–05
FeP_2	3	kg	117,795	0,000	0,000	1,18E–34	5,33E–32	1,16E–06
P_3O_6 (g)	1	kg	188,918	0,000	0,000	1,89E–34	1,89E–34	7,25E–08
P_2 (g)	1	kg	61,948	0,000	0,000	6,19E–35	6,19E–35	6,31E–08
P_4O_{10} (g)	1	kg	283,889	0,000	0,000	2,84E–34	2,84E–34	3,17E–10
P_4(g)	1	kg	123,895	0,000	0,000	1,24E–34	1,24E–34	7,58E-19

pounds (Fe_3P, Fe_2P, FeP, FeP_2), as well as into various phosphorus oxides in gas phases (P_4O_6, PO_2, P_2O_3, P_2O_4, P_2O_5, P_3O_6, P_4O_{10}) is considered. Other products of the system, such as compounds with Ca and Mg, were not taken into account, since their content is insignificant [2].

This graph shows that the temperature of the beginning of the decomposition of iron phosphate ($FePO_4$) begins from 200 °C and with a further increase in temperature, the decomposition of iron phosphate ($FePO_4$) is more intense. The same situation occurs with hydrogen (H_2). At a temperature of 600 °C, the initial components of the iron phosphate system ($FePO_4$) and hydrogen (H_2) completely decompose into Fe_3P, H_2O (gas phase), P_4O_6 (gas phase), and Fe_2P.

In the system under consideration, the interaction occurs with the participation of these substances: $FePO_4$, Fe_3P, $H_2O_{(g)}$, P_4O_6, $H_{2(g)}$, Fe_2P, FeP, PO_2, P_2O_3, FeH, FeP_2, P_2O_4, $P_{2(g)}$, P_2O_5, P_3O_6, P_4O_{10} и $P_{4(g)}$.

Then the percentage of iron and phosphorus in the compounds at different temperatures is calculated. The percentage of elements (iron and phosphorus) in the compounds was calculated by dividing the molecular weight of the element in g/mol [3].

Table 3 **Percentage of phosphorus in compounds when iron phosphate ($FePO_4$) reacts with hydrogen (H_2)/ temperature range 200 – 1 400 °C**

T/ °C	200	300	1 200	1 300	1 400
$FePO_4$	0,205	0,205	0,205	0,205	0,205
P_4/gas	1	1	1	1	1
P_4O_{10}/gas	0,436	0,436	0,436	0,436	0,436
P_3O_6 /gas	0,492	0,492	0,492	0,492	0,492
P_2O_5/gas	0,436	0,436	0,436	0,436	0,436
P_2/gas	1	1	1	1	1
P_2O_4/gas	0,492	0,492	0,492	0,492	0,492
FeP_2	0,526	0,526	0,526	0,526	0,526
P_2O_3/gas	0,563	0,563	0,563	0,563	0,563
PO_2/gas	0,492	0,492	0,492	0,492	0,492
FeP	0,357	0,357	0,357	0,357	0,357
Fe_2P	0,217	0,217	0,217	0,217	0,217
P_4O_6/gas	0,563	0,563	0,563	0,563	0,563
Fe_3P	0,156	0,156	0,156	0,156	0,156

Table 4 **Percentage of phosphorus in compounds when iron phosphate ($FePO_4$) reacts with carbon monoxide (CO)/ temperature range 200 – 1 400 °C**

T/ °C	200	300	1 200	1 300	1 400
$FePO_4$	0,205	0,205	0,205	0,205	0,205
Fe_3P	0,156	0,156	0,156	0,156	0,156
P_4O_6/gas	0,563	0,563	0,563	0,563	0,563
Fe_2P	0,217	0,217	0,217	0,217	0,217
FeP	0,357	0,357	0,357	0,357	0,357
PO_2 /gas	0,492	0,492	0,492	0,492	0,492
P_2O_3 /gas	0,563	0,563	0,563	0,563	0,563
P_2O_4/gas	0,492	0,492	0,492	0,492	0,492
P_2O_5 /gas	0,436	0,436	0,436	0,436	0,436
FeP_2	0,526	0,526	0,526	0,526	0,526
P_3O_6 /gas	0,492	0,492	0,492	0,492	0,492
P_2 /gas	2	2	2	2	2
P_4O_{10} /gas	0,436	0,436	0,436	0,436	0,436
P_4 /gas	4	4	4	4	4

Then the mass of iron and phosphorus in the compounds was calculated when iron phosphate ($FePO_4$) interacts with hydrogen (H_2).

Based on Tables 3, 4, the mass of iron in compounds when iron phosphate ($FePO_4$) interacts with hydrogen (H_2) is determined to be 111,8 kg. The mass of iron in the compounds is determined by the interaction of iron phosphate ($FePO_4$) with carbon monoxide (CO) equal to 446,8 kg. The mass of phosphorus in compounds when iron phosphate ($FePO_4$) interacts with hydrogen (H_2) is 62,0 kg. The mass of phosphorus in the compounds by the interaction of iron phosphate ($FePO_4$) with carbon monoxide (CO) is equal 247,8 kg [4].

Then based on the above Tables was calculated the degree of extraction of iron and phosphorus from the compound at different temperatures.

Table 5 **The degree of iron extraction at different temperatures when iron phosphate ($FePO_4$) interacts with hydrogen (H_2)/ temperature range 200 – 1 400 °C**

T/ °C	200	300	1 200	1 300	1 400
$FePO_4$	99,44	93,90	0,00	0,00	0,00
FeP	0,00	0,00	0,04	0,06	0,09
Fe_2P	0,00	0,05	2,94	3,28	3,62
Fe_3P	0,56	6,05	97,03	96,66	96,29

Table 6 **The degree of phosphorus recovery at different temperatures during the interaction of iron phosphate ($FePO_4$) with hydrogen (H_2)/ temperature range 200 – 1 400 °C**

T/ °C	200	300	1 200	1 300	1 400
$FePO_4$	99,44	93,90	0,00	0,00	0,00
FeP	0,00	0,00	0,04	0,06	0,09
Fe_2P	0,00	0,03	1,47	1,64	1,81
P_4O_6/gas	0,37	4,06	66,15	66,08	66,00
Fe_3P	0,19	2,02	32,34	32,22	32,10

Table 7 **The degree of iron recovery at different temperatures when iron phosphate ($FePO_4$) reacts with carbon coxide (CO)/ temperature range 200 – 1 400°C**

T/ °C	200	300	1 200	1 300	1 400
$FePO_4$	100,01	100,01	0,00	0,00	0,00
Fe_3P	0,00	0,00	98,12	98,05	97,98
FeP	0,00	0,00	0,02	0,02	0,03

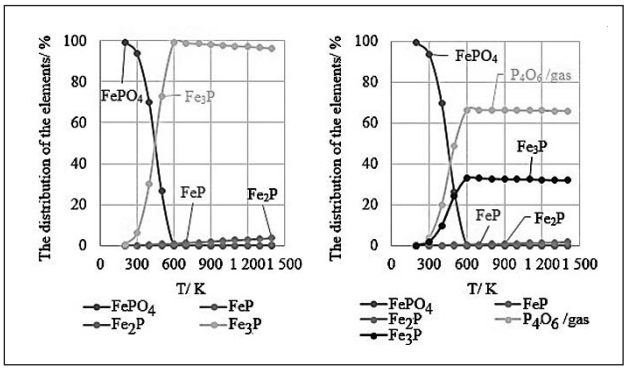
Table 8 **The degree of phosphorus recovery at different temperatures during the interaction of iron phosphate ($FePO_4$) with carbon monoxide (CO)/ temperature range 200 – 1 400 °C**

T/ °C	200	300	1 200	1 300	1 400
$FePO_4$	100,01	100,01	0,00	0,00	0,00
Fe_3P	0,00	0,00	32,71	32,68	32,66
P_4O_6/gas	0,00	0,00	66,35	66,34	66,32
Fe_2P	0,00	0,00	0,93	0,97	1,00
FeP	0,00	0,00	0,02	0,02	0,03

CONCLUSION

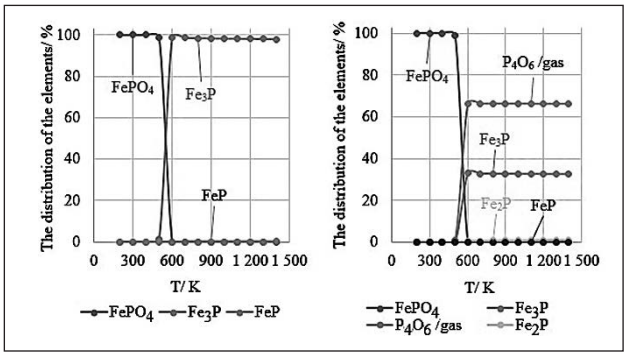
The Tables 5, 6, 7, 8 above shows that when iron phosphate ($FePO_4$) interacts with hydrogen (H_2) and carbon monoxide (CO) at initial temperatures of 200 - 400 °C, it partially decomposes into P_4O_6 and Fe_3P, when the temperature rises to 500 °C, $FePO_4$ begins to appear other compounds like Fe_2P, and at maximum temperatures of 1 100 °C and above, $FePO_4$ completely decomposes into FeP, Fe_2P, $P_4O_{6(g)}$ and Fe_3P. This phenomenon can be depicted on graphs.

Comparing Figures 2, 3, it can be also concluded that the interaction of iron phosphate ($FePO_4$) with hydrogen (H_2) already at the initial temperatures of 300 - 400 °C appears a compound of iron with phosphorus Fe_2P, and the interaction of iron phosphate ($FePO_4$) with carbon monoxide (CO) iron phosphate decomposes only to Fe_3P and FeP. At maximum temperatures of 1 300 - 1 400 °C, iron is almost completely (96 - 97 %) converted to Fe_3P. When iron phosphate ($FePO_4$) reacts with hydrogen (H_2) during the decomposition of iron phosphate, phosphorus in the form of gaseous oxide P_4O_6 begins to appear at 200



a) b)

Figure 2 Influence of temperature on the equilibrium degree of distribution of iron in compounds during the interaction of iron phosphate with hydrogen (a) and carbon monoxide (b)



a) b)

Figure 3 Influence of temperature on the equilibrium degree of phosphorus distribution in compounds during the interaction of iron phosphate with hydrogen (a) and carbon monoxide (b)

°C, and when iron phosphate reacts with carbon monoxide (CO) – at 500 °C. This suggests that phosphorus passes into the oxide compound better when iron phosphate ($FePO_4$) interacts with hydrogen (H_2). When iron phosphate ($FePO_4$) interacts with hydrogen (H_2), a compound of iron and phosphorus Fe_2P appears at the initial temperatures of 300 - 400 °C. At maximum temperatures of 1 300 - 1 400 °C, iron is almost completely (96 - 97 %) converted to Fe_3P.

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Note: The responsible for English language is translator from Temirtau Dana Ybrai, Temirtau, Kazakhstan