

THERMODYNAMIC INTERACTION OF CONCENTRATE, SLUDGE AND MILL SCALE FROM CARBON

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Due to the gradual depletion of reserves of a number of natural minerals, on the one hand, and the accumulation of a huge amount of waste containing valuable useful components, on the other, the problem of developing so-called man-made deposits is becoming increasingly urgent. Of particular interest are currently man-made deposits formed or being formed on the territory of the objects of placement of man-made waste of the metallurgical complex, including the preparation of raw materials (mining, processing, agglomeration, etc.), directly metallurgical processing and related production. The downward trend in iron ore reserves makes it particularly relevant to process man-made waste from ferrous metallurgy in order to obtain man-made iron ore raw materials.

Keywords: thermodynamic modeling, Gibbs energy, calculation, iron oxides, carbon

INTRODUCTION

Two-stage technology - is the main technology for processing iron ore raw materials and steel production in general. In this production, a lot of emissions are released as gases and waste, which are stored in dumps and slime storage facilities. Therefore, further development of iron and steel metallurgy should be directed to the transition to a single-stage continuous steel production technology.

The purpose of this work is to obtain high-quality metalized ore-coal pellets that will meet the requirements of a single-stage continuous steel production technology in the future.

The effects of temperature on the change in the Gibbs free energy in the interaction of iron oxides with carbon are considered.

THE METHODOLOGY OF THE STUDY

Thermodynamic modeling of the interaction of concentrate, sludge, and rolled scale with carbon was performed using the HSC-5.1 software package, the reaction Equations subroutine of Which allows calculating enthalpy (ΔH), entropy (ΔS), Gibbs energy (ΔG), reactions [1, 2], and the Equilibrium Compositions subroutine allows simulating the interaction in the system under study with an equilibrium quantitative distribution of substances in the system under study. The calculation of equilibrium by the HSC-5.1 Outokumpu complex is based on the principle of minimum Gibbs energy, taking into account the activities of substances based on the following expression:

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$$G(x) = \sum_{a=1}^f * \sum_{j=1}^{ia} X_j (C_j + \ln \left(\frac{X_j}{X_a} \right) + \ln \gamma_j) \rightarrow G(x) \min \quad (1)$$

under restrictions in the form of a system of linear equations of the mass balance of a substance:

$$\sum_{j=1}^m a_{ij} X_j = b_i \quad (2)$$

and the normalization condition:

$$\sum_{j=1}^{La} X_j = X_a \quad (3)$$

where f - is the total number of the phases; i - is the total number of independent component in the system; a_{ij} - the weight of numbers representing the i independent components in the phase a and system; b_i - is the number of independent components of the system; γ_j - empirical thermodynamic function; X_j - the total number of moles of phase a in the system; X_a - dependent mole fraction of component in phase a ; γ_j - the activity coefficient of the component. The equilibrium parameters of a thermodynamic system are determined by solving the mathematical problem of finding the extremum, taking into account all restrictions, using Langrange functions and the method of successive approximations of Newton.

When working with the HSC - 5.1 complex, the initial information is presented in the form of the quantitative/ kg distribution of substances in the system under study. Then, in accordance with the algorithm developed by us [3], the equilibrium degree of element distribution (α_{el} / %) over the interaction products was calculated.

INFLUENCE OF TEMPERATURE ON THE CHANGE IN THE GIBBS FREE ENERGY IN THE INTERACTION OF IRON OXIDES WITH CARBON

Thermodynamic interaction of iron oxides (Fe_2O_3 , Fe_3O_4 , FeO) with carbon (C). Research results:

Table 1 Thermodynamic parameters per 1 g/mol of iron oxide Fe₂O₃ when interacting with solid carbon

T/ K	ΔH/ kJ	ΔS/ J/K	ΔG/ kJ
100	14,31286	944,7412	6,440013
200	7,417983	297,5431	2,45893
300	6,875786	268,266	0,169135
400	7,035119	273,7096	-2,08853
500	7,132286	276,3631	-4,38284
600	7,220132	278,2487	-6,6923
700	7,586655	284,9207	-9,03372
800	8,601325	301,0314	-11,4674
900	9,196188	309,9063	-14,0468
1 000	8,342234	298,9675	-16,5717
1 100	8,293599	298,4074	-19,0604

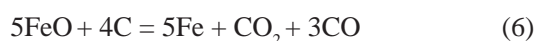
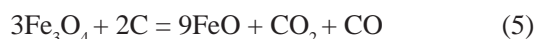
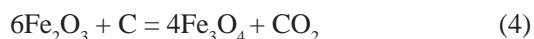
Table 2 Thermodynamic parameters per 1 g / mol of iron oxide Fe₃O₄ when interacting with solid carbon

T/ K	ΔH/ kJ	ΔS/ J/K	ΔG/ kJ
100	34,000	-475,195	39,280
200	46,714	408,032	37,646
300	48,568	480,103	32,564
400	48,606	481,545	27,204
500	48,227	474,017	21,892
600	47,555	463,089	16,682
700	46,340	446,357	11,623
800	44,182	420,579	6,797
900	42,001	397,172	2,284
1000	41,250	390,012	-2,084
1100	40,935	387,278	-6,399

Table 3 Thermodynamic parameters per 1 g/mol of iron oxide FeO when interacting with solid carbon

T/ K	ΔH/ kJ	ΔS/ J/K	ΔG/ kJ
100	123,053	650,355	110,046
200	122,828	643,990	97,069
300	122,231	632,020	84,310
400	121,463	621,019	71,782
500	120,595	611,347	59,461
600	119,704	603,220	47,318
700	118,898	596,995	35,319
800	118,295	592,950	23,423
900	118,060	591,538	11,583
1 000	118,441	593,506	-0,260
1 100	119,020	596,323	-12,171

The following reactions were considered:



When the temperature increases from 100 K to 1 200 K Gibbs energy (ΔG), the processes change from positive to negative values.

Reaction 1, the temperature of the beginning of the reduction of Fe₂O₃ by solid carbon begins (according to ΔG = 0) at a temperature of 307,5 K.

Reaction 2, the temperature of the beginning of the reduction of Fe₃O₄ by solid carbon begins (according to ΔG = 0) at a temperature of 952,1 K.

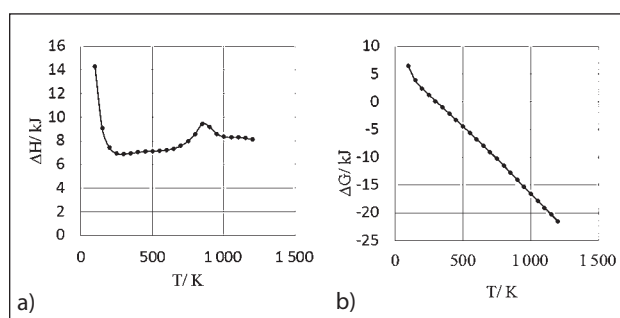


Figure 1 Effect of temperature on the change in the enthalpy of ΔH (a), in the Gibbs energy (ΔG) (b) by 1 g/mol of Fe₂O₃ when interacting with solid carbon (C)

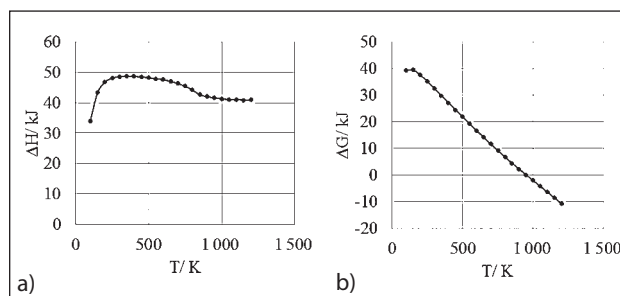


Figure 2 Effect of temperature on the change in the enthalpy of ΔH (a), in the Gibbs energy (ΔG) (b) by 1 g/mol of Fe₃O₄ when interacting with solid carbon (C)

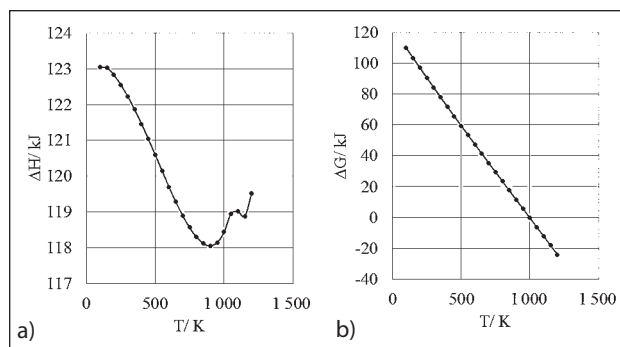


Figure 3 Effect of temperature on the change in the enthalpy of ΔH (a), in the Gibbs energy (ΔG) (b) by 1 g/mol FeO when interacting with solid carbon (C)

Reaction 3, the temperature of the beginning of the reduction of FeO by solid carbon begins (according to ΔG = 0) at a temperature of 997,8 K.

Thus, as the temperature increases, Fe₂O₃ is initially restored to Fe₃O₄, then Fe₃O₄ to FeO, then FeO to Fe.

To reduce the thermodynamic parameters to 1 mol of the substance, 1 mol of the initial oxide, Fe₂O₃, was selected. Tables 1, 2, 3 show the thermodynamic parameters of reactions per 1 g/mol of the initial Fe₂O₃, Fe₃O₄, and FeO oxides in the interaction of iron oxides with carbon, respectively figures 1, 2, 3 the effect of temperature on changes in the enthalpy of (ΔH) and the Gibbs energy (ΔG).

CONCLUSION

This paper presents the results of thermodynamic modeling of the interaction of concentrate, sludge and

rolled scale with carbon using the HSC-5.1 software package.

The following conclusions were identified:

(1) The initial reduction temperatures from Fe_2O_3 to Fe were determined from the above three reactions.

At a real process temperature of 900 – 1 000 K, based on the above figures, the reduction of iron from Fe_2O_3 is characterized with the highest thermodynamic probability, then from Fe_3O_4 , respectively, iron oxide FeO has the lowest thermodynamic probability of iron reduction.

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