About the software "Slag – steel"

The software "Slag – steel" is designed for calculating of chemical composition of liquid steel, which is in equilibrium with selected slag. Chemical composition of slag, temperature of metal-slag system, and carbon, nitrogen, sulfur amounts in steel are taken into account by this program. Values of these parameters are set by users.

If the slag – metal equilibrium is realized, for each element *R* is right an expression for *R* activity in metal:

$$a_{[R]} = \frac{K_{(R_nO_m)}^{1/n} a_{(R_nO_m)}^{1/n}}{a_{[O]}^{m/n}},$$

where *K* is equilibrium constant of reaction:

$$(R_nO_m) = n[R] + m[O]. \qquad (1)$$

The elements activities are calculated in oxide phase (slag) on base of collectivized electron theory of A.G. Ponomarenko [1], in steel - by Wagner model.

The software computes the system of 9 components: Fe, Mn, Cr, Si, Ti, Al, Ca, Mg, and O. The carbon, nitrogen, and sulfur influence on elements activities is taken into account supplementarily. The temperature influence on values of equilibrium constants and activity coefficients of components in slag and metal is considered also. Expressions for equilibrium constants are presented in table 1 and for interaction parameters in metal, in table 2.

Table 1

Expressions for equilibrium constants

Reaction	*lgK*	Ref.
(FeO) = [Fe]+[O]	-6320/T + 4,73	[2]
(MnO) = [Mn]+[O]	-12175/T + 5,45	[3]
(Cr_2O_3) = 2[Cr] + 3[O]	-37828/T + 16,51	[2]
(SiO_2) = [Si] + 2[O]	-30225/T +11,56	[2]
(TiO_2) = [Ti] + 2[O]	-30365/T + 10,18	[2]
(Al_2O_3) = 2[Al] + 3[O]	-58320/T + 18,02	[2]
(CaO) = [Ca] + [O]	-34100/T + 12,5	*own*
(MgO) = [Mg] + [O]	-22550/T + 6,54	[4]

Table 2

First order Interaction parameters $e_i^j \cdot 100$ in iron for 1873 K [1 – 4]

i \ j	Mn	Cr	Si	Ti	Al	Ca	Mg	O	C	N	S
Mn			6	-5				-7.2	-7	-9.1	-3.6
Cr		-0.03	-0.43	5.9	2.3			-14	-12	-19	
Si	3		*		5.8	-6.7		-23	*		
Ti	1.7	1.58		1.3	12.9			-112	-64	-154	-11
Al		1,2	0.56	8	*	-4.7		-160	9.1	-53	
Ca		2	-9.7		-7.2			-350	-34		-33.6
Mg		5	-9	-51	-12		-8.5	-301	-24		
O	-2.1	-4.1	-13.3	-37	-96	-141	-198	-17	-45	5.7	-13.3
C	1.2	-2.4	*		4.3			-34	*		
N		-4.6	4.7		*			0.05			
S	-2.1		6.3	-7.2	3.5			-27	11		

* *Appendix to table 2:*

$e_{Si}^{C} = 380/T - 0.023$; $e_{Si}^{Si} = 34.5/T + 0{,}089$; $e_{Al}^{Al} = 63/T + 0.011$; $e_{C}^{C} = 158/T + 0.0581$;

$e_{C}^{Si} = 162/T + 0.008$; $e_{N}^{Al} = 859/T - 0.487$; $e_{N}^{Ti} = -4070/T + 1.643$;

$e_{S}^{Cr} = -94.2/T + 0.0396$; $e_{S}^{S} = 233/T - 0.153$.

The expression from the theory of quasi-regular solutions [1] was used for consideration of temperature influence on interaction parameters:

$$e_{i(T)}^{j} = [(2557/T) - 0{,}365]\ e_{i(1873)}^{j}.$$

Slag and others initial parameters for the software are restricted by the following limits:

Initial parameters	Values limits	
	min	max
(%FeO)	0.1	30
(%MnO)	0.1	10
(%Cr_2O_3)	0.05	5
(%SiO_2)	0.1	40
(%Al_2O_3)	0.1	60
(%CaO)	0.1	65
(%MgO)	0.1	15
[%C]	0.005	1.5
[%N]	0.001	0.02
[%S]	0.001	0.05
T, K	1790	1990

Value ($\%TiO_2$) is calculated by the software as a balance difference: $100 - \sum(\%R_nO_m)$, after user set the rest of slag components.

1. V.A. Grigoryan, L.N. Belyanchikov, A.Ya. Stomahin “Theoretical base of electro-steel melting processes”. – Moscow: Metallurgiya. 1987. 272 p. [Rus].
2. G.G. Mikhailov, D.Ya. Povolotskii “Thermodynamic of steel deoxidizing”. – Moscow: Metallurgiya. 1993. –144 p.[Rus].
3. G.G. Mikhailov, L.A. Chernova “Thermodynamic analysis of calcium and barium deoxidizing of corrosion-resistant Cr18Ni10T steel”/ Izvestiya vuzov. Chernaya metallurgiya. 1991. (12). pp. 37 – 39. [Rus].
4. G.G. Mikhailov “The influence of magnesium on phase transformations in liquid steel” / Electrometallurgiya. 2004. (5). pp. 11 – 18. [Rus].

Alexander Alekseenko