About “Non-metallic inclusions” software

It is evident that molten steel and liquid oxide inclusions are in equilibrium state or in a motion to equilibrium. At the same time each procedure during secondary steelmaking (e. g. changing of steel composition by adding of ferroalloys, deoxidizers, slag-making additions, or changing of temperature and pressure over the melt) drifts an equilibrium point of “steel – inclusions” system. Because that the transformation of non-metallic inclusions takes place during secondary steelmaking.

“Non-metallic inclusions” software is designed for simulation of liquid oxide inclusions transformation which follows after change of oxidation level, chemistry, or temperature of liquid steel. Herein, transformation means a change of inclusions mass and chemistry. The program gives clear understanding of the internal dependencies in liquid steel – oxide inclusions system and the effect of some parameters on transformation processes.

The simulation of the ex-solution of solid phases into liquid inclusions and the change of its aggregative state is not provided in the current program version. This obstacle can be compensated by complex analysis of computation results and appropriate phase diagrams.

The model doesn’t take into account influence of slag on metal chemistry, but it is possible to calculate it by means of “Slag – steel” software on www.steelmaker.ru .

The model assumes that liquid metal initially contains some quantity of oxide inclusions (entrapped slag is a main cause of its origin). Three types of initial inclusions can be used in the current program version:

Composition of inclusions (wt. pct.)

Type	FeO	Cr_2O_3	MnO	SiO_2	TiO_2	Al_2O_3	CaO	MgO
1	33	0.5	5	10	0.5	2	39	10
2	0.5	0.5	1	26	1	8	55	8
3	0.5	0.5	1	8	1	26	55	8

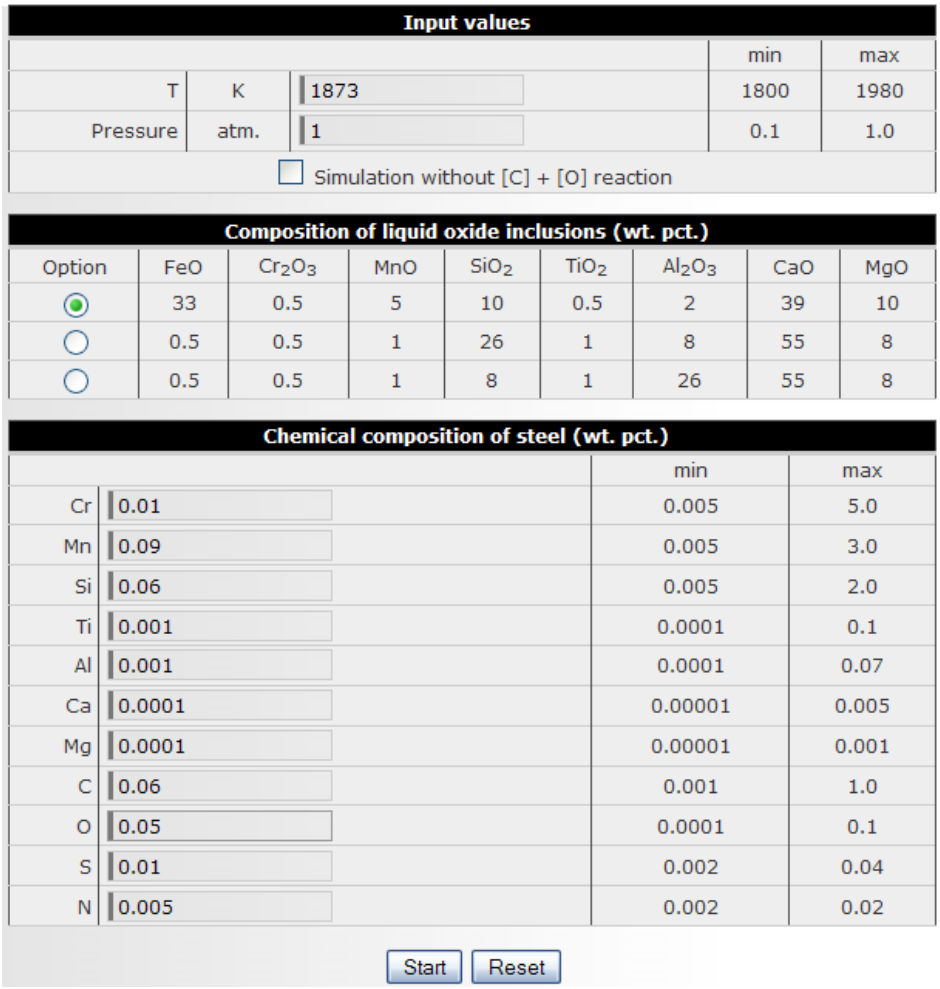
The variation intervals for other initial parameters:

a) temperature is from 1800 to 1980 K;
b) pressure is from 0.1 to 1.0 atm.;
c) elements amounts in the melt are (wt. pct.):

	Cr	Mn	Si	Ti	Al	Ca	Mg	C	O	S	N
Interval	0.005-5.0	0.005-3.0	0.005-2.0	0.0001-0.1	0.0001-0.07	0.00001-0.005	0.00001-0.001	0.001-1.0	0.0001-0.1	0.002-0.04	0.002-0.02

After input of initial parameters, the program computes repartition of elements between inclusions and liquid steel in direction to equilibrium state of the system. If the system doesn’t reach enough to the equilibrium for one cycle (3500 iteration steps) it is possible to continue simulation by pushing “Start”.

Example: *Let’s input some values of parameters: temperature, pressure, type of initial oxide inclusions and metal composition (**fig. 1**).*



Input values

			min	max
T	K	1873	1800	1980
Pressure	atm.	1	0.1	1.0

☐ Simulation without [C] + [O] reaction

Composition of liquid oxide inclusions (wt. pct.)

Option	FeO	Cr_2O_3	MnO	SiO_2	TiO_2	Al_2O_3	CaO	MgO
◉	33	0.5	5	10	0.5	2	39	10
○	0.5	0.5	1	26	1	8	55	8
○	0.5	0.5	1	8	1	26	55	8

Chemical composition of steel (wt. pct.)

		min	max
Cr	0.01	0.005	5.0
Mn	0.09	0.005	3.0
Si	0.06	0.005	2.0
Ti	0.001	0.0001	0.1
Al	0.001	0.0001	0.07
Ca	0.0001	0.00001	0.005
Mg	0.0001	0.00001	0.001
C	0.06	0.001	1.0
O	0.05	0.0001	0.1
S	0.01	0.002	0.04
N	0.005	0.002	0.02

Start Reset

Fig. 1. *The initial parameters values of "steel – inclusions" system.*

The program will compute a repartition of elements between inclusions and liquid steel after pushing on button "Start" and show results: a) finite metal and inclusions compositions ***(fig. 2)****, b) plots of changing of: inclusions composition* ***(fig. 3)****, steel composition* ***(fig. 4)****, mass of inclusions and gas* ***(fig. 5)****.*

The software has an additional operation mode. This is simulation without taking into account a reaction between soluble oxygen and carbon. It can be useful in some cases because in real metallurgical processes this reaction is essentially restricted. It appears in considerable higher values of real [%C]·[%O] in comparison with equilibrium ones. It is known that this phenomenon is caused by ferrostatic pressure and additional energy of boundary metal-gas creation. This operation mode simulation can be realized by mark "Simulation without [C] + [O] reaction". After that the program computes without taking into account reaction between soluble oxygen and carbon (before pushing "Reset" or exit from the program).

Input values

			min	max
T	K	1873	1800	1980
Pressure	atm.	1	0.1	1.0

Simulation without [C] + [O] reaction

Composition of liquid oxide inclusions (wt. pct.)

FeO	Cr_2O_3	MnO	SiO_2	TiO_2	Al_2O_3	CaO	MgO
5.46	0.12	1.19	73.6	3.65	4.03	9.20	2.64

Chemical composition of steel (wt. pct.)

		min	max
Cr	0.01	0.005	5.0
Mn	0.09003	0.005	3.0
Si	0.04545	0.005	2.0
Ti	7.348e-05	0.0001	0.1
Al	0.0001746	0.0001	0.07
Ca	1.431e-05	0.00001	0.005
Mg	7.242e-06	0.00001	0.001
C	0.05371	0.001	1.0
O	0.02348	0.0001	0.1
S	0.01	0.002	0.04
N	0.005002	0.002	0.02

Fig. 2. The finite composition of steel and inclusions.

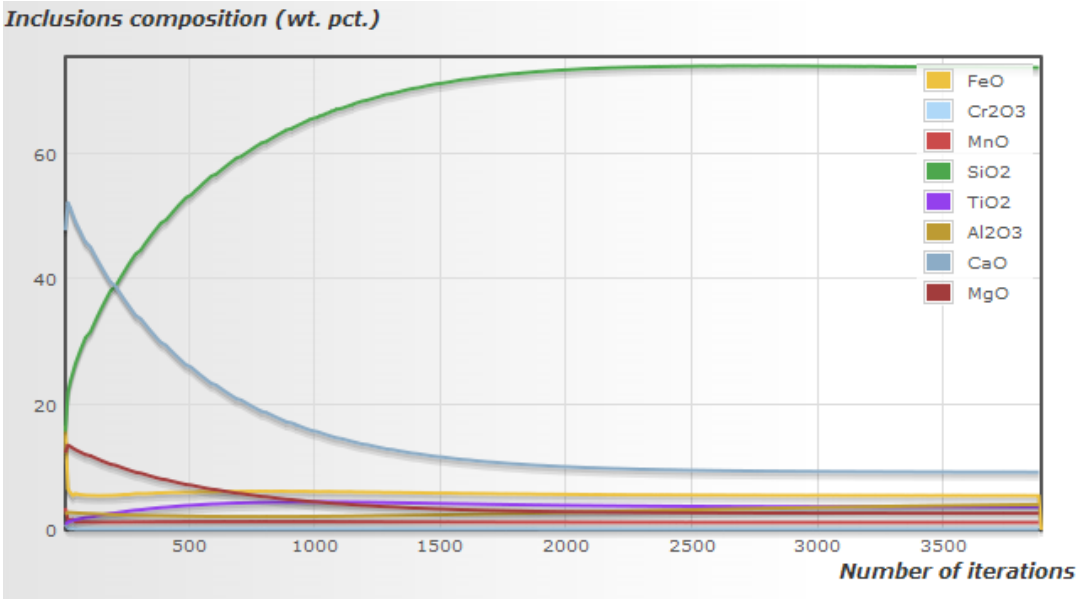


Fig. 3. Transformation of inclusions composition.

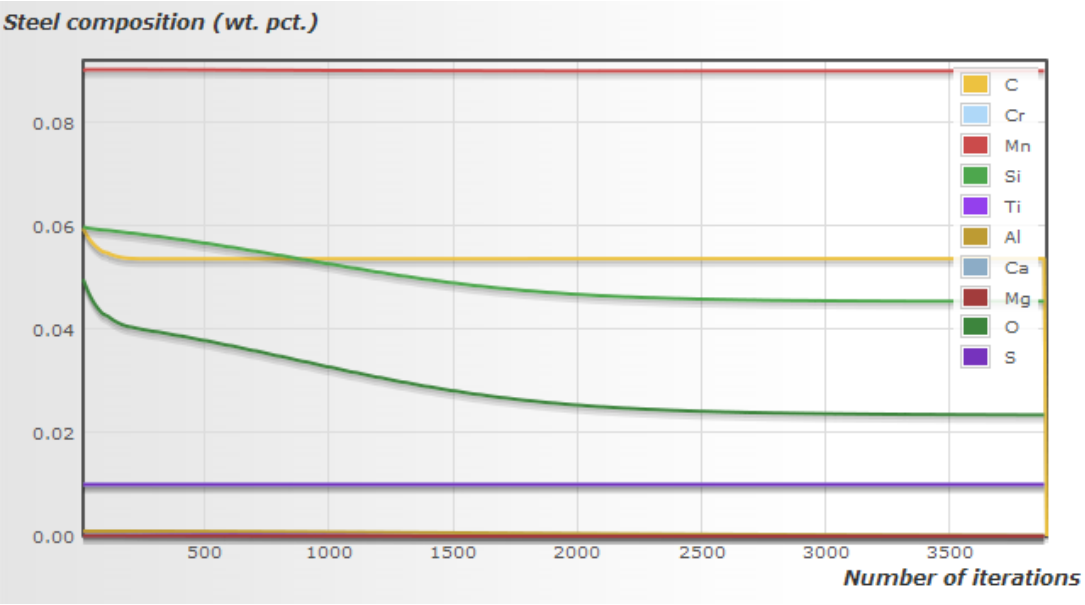


Fig. 4. Changing of steel composition.

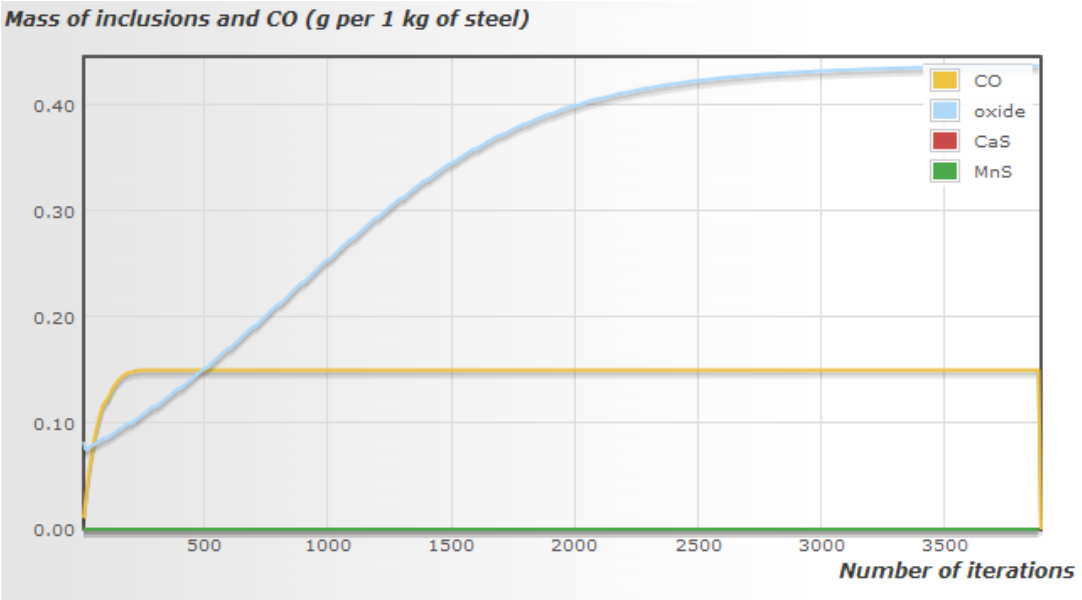


Fig. 5. Changing of mass of inclusions and gas.

About the model

Model assumptions:

1) all elements are evenly located in melt volume;
2) inclusions are still in the metal and spherical;
3) rate-limiting step of inclusions growth or resolution is diffusion of elements in the melt to or from reaction front on the boundary of metal-inclusion.

The driving force of non-metallic inclusions transformation is difference between concentrations of elements in the melt volume and on the boundary of metal-inclusion.

The increase or decrease of components rates in the inclusion is in proportion to components flows:

$$J_R = 4\pi r D_{[R]}([R]^v - [R]^b), \quad (1)$$

where J_R – flow of component R,
r – inclusion radius,
$D_{[R]}$ – diffusion coefficient of element R in liquid steel,
$[R]^v$, $[R]^b$ – concentrations of element R in the melt volume and on the boundary of metal-inclusion.

The concentrations of elements on the boundary of metal-inclusion $[R]^b$ are assumed as equilibrium with inclusions, at each step of iteration.

Each component has its own value of the difference between its concentration in the melt volume $[R]^v$ and on the boundary of metal-inclusion $[R]^b$. The value $[R]^v$ is depended on initial metal chemistry and following step by step changing of this component amount in the metal. This changing is computed by the program on the base of mass balance of the system.

The value $[R]^b$ can be found on each iteration step from expression:

$$a_{[R]^b} = \frac{K_{(R_nO_m)}^{1/n} a_{(R_nO_m)}^{1/n}}{a_{[O]^b}^{m/n}}, \quad (2)$$

if oxygen activity on boundary of metal-inclusion $a_{[O]^b}$ is known.

The oxygen activity $a_{[O]^b}$ is uniquely defined at each moment by condition of quasi-steady character of the mass transfer. It means maintenance of balance of all components flows [1], including soluble oxygen flow, under the condition that expression (2) is realized for all components. In formalized form it can be formulated as:

$$\begin{cases} a_{[R_1]^b} = \dfrac{K_1^{1/n_1} a_{(R_1)}}{a_{[O]^b}^{m_1/n_1}} \\ a_{[R_2]^b} = \dfrac{K_2^{1/n_2} a_{(R_2)}}{a_{[O]^b}^{m_2/n_2}} \\ \cdots\cdots\cdots\cdots\cdots\cdots \\ a_{[R_i]^b} = \dfrac{K_i^{1/n_i} a_{(R_i)}}{a_{[O]^b}^{m_i/n_i}} \\ \sum n_i J_{R_i} = \overline{m} J_O \end{cases} \quad (3)$$

The discrete increases of components mass in inclusions are computed on each iteration step. After that amounts of components in metal are also corrected on the base of mass balance maintenance. The quantity of iteration steps of the simulation is defined by goal of approaching level to equilibrium state.

The software computes the system of 11 components: Fe, Mn, Cr, Si, Ti, Al, Ca, Mg, C, O, and S. The nitrogen influence on elements activities is taken into account also. The temperature influence on values of equilibrium constants and activity coefficients of components in slag and metal is considered. 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 [2 – 5]

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 [5] was used for consideration of temperature influence on interaction parameters:

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

The elements activities are calculated in oxide phase (inclusions) on the base of collectivized electron theory of A.G. Ponomarenko [5], and in steel — by Wagner model.

1. D. A. Frank-Kamenetskii “Diffusion and heat transfer at chemical kinetics”. Moscow. Nauka. 1967. 492 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].
5. V.A. Grigoryan, L.N. Belyanchikov, A.Ya. Stomahin “Theoretical base of electro-steel melting processes”. – Moscow: Metallurgiya. 1987. 272 p. [Rus].

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