Computer Simulation of Oxide Inclusions Transformation during Secondary Steelmaking and Casting

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Goal

Our goal was to create software for simulation of liquid oxide inclusions transformation.

Herein, transformation means changes of composition and total mass of inclusions.

This simulation is useful for inclusions formation control during secondary steelmaking when each manufacturing procedure affects inclusions composition and its total mass.
Model assumptions

- Molten steel and oxide inclusions tend to equilibrium state.
- All elements are allocated uniformly throughout the melt bulk.
- Inclusions are liquid and spherical.
- The rate determining step of inclusions transformation is mass transfer in metal.
Mass transfer depends on difference in components concentrations in volume and near the inclusion boundary:

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

Those boundary concentrations are completely determined at any moment by the following conditions:

1. They are in equilibrium with inclusions (because chemical reactions don’t control the process).
2. The flows of all components are in balance with oxygen flow (condition of quasi-stationarity of the process).
Model formalization

\[
\begin{align*}
{a}_{[R_1]}^b &= \frac{K_1^{1/n_1}}{a_{[o]}^{m_1/n_1}} a_{(R_1)} \\
{a}_{[R_2]}^b &= \frac{K_2^{1/n_2}}{a_{[o]}^{m_2/n_2}} a_{(R_2)} \\
\sum n_i {J}_{R_i} &= m {J}_{O} \\
{J}_{R_i} &= 4\pi r D_{[R_i]} ([R_i]^n - [R_i]^b)
\end{align*}
\]

The concept may be written as the following equations system.

Solution of the system gives momentary flows of the components.

It allows to compute changes of components shares in inclusions.

Current metal composition is calculated on the basis of material balance conservation in inclusions-metal system.
Inclusions software

Developed software consumes the following input data: temperature, pressure, chemical composition and mass of melt and of inclusions formed before (or slag emulsified).

After reading these input parameters the software iteratively computes redistribution of elements between inclusions and metal in direction to equilibrium. Simultaneously thermodynamic possibility of competitive reactions is tested. And increment of such phases as sulfides and CO is also computed.
When the average inclusions chemical composition is computed, the software finds solid phases in liquid oxide inclusions. To get this effect a database is used which was developed on basis of oxide phases diagrams.
Examples of inclusions transformation simulation

For illustration “how it works” we’ll demonstrate results of the simulation in cases of pressure drop, temperature reduce, and Ti addition.

Initial conditions for these variants were uniform:

- Temperature: 1600°C; pressure: 1 atm;
- Metal composition (wt. pct): 0.160 C, 0.54 Mn, 0.177 Si, 0.00028 Al, 0.0004 Ti, 0.0001 Ca, 0.0001 Mg, 0.004 N, and 0.0120 O_free;
- Inclusions composition (wt. pct): 43 SiO_2, 17 Al_2O_3, 27 CaO, 5 MgO, 1.5 Ti_2O_3, 5 MnO, 1.5 FeO;
- Inclusions mass: 0.1 g per 1 kg of steel.
Vacuum–carbon deoxidation (free oxygen decreased from initial value 120 to 18 ppm) results in a partial dissolving of oxide inclusions. Elements with smaller affinity to oxygen are recovered predominantly.
Simulation of liquid inclusion transformation after temperature dropped to 1550° C

The temperature decrease results in some drift of deoxidation reactions to field of lower equilibrium oxygen, and excessive oxygen is connected by deoxidizers. In case of considered conditions the most of excessive oxygen combines with silicon, and SiO₂ share in oxide phase increases. Inclusions mass grows appreciably.
Simulation of liquid inclusion transformation after Ti addition

The results of simulation after Ti addition up to 0.015 wt. pct. are demonstrated here. We can see that Ti$_2$O$_3$ share in oxide phase rises to 34 wt. pct, and inclusions mass grows 1.5 times.
Testing of the software

- We’ve compared computed results with analyses of real inclusions in steel probes.
- The probes were sampled on different melts from ladles during secondary steelmaking and from tundish during casting.
- Simultaneously oxygen activity in melt and temperature were measured.
- Composition of non-metallic inclusions was analyzed with scanning electron microscope JEOL JSM-646OLV at South Ural State University (Chelyabinsk, Russia).
Computed and SEM-tested inclusions composition (wt. pct)

<table>
<thead>
<tr>
<th>Steel conditions</th>
<th>SEM-tested</th>
<th>Computed</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.07 C, 0.10 Mn, 0.03 Si, $a_{[O]}=140$ ppm, t=1600°C</td>
<td>4-6 Al$_2$O$_3$, 30-35 SiO$_2$</td>
<td>7 Al$_2$O$_3$, 21 SiO$_2$</td>
</tr>
<tr>
<td>LF, after preliminary vacuum-carbon deoxidation of the melt</td>
<td>50-55 CaO, 5-10 MgO</td>
<td>59 CaO, 11 MgO, 0.9 MnO, 1.7 FeO</td>
</tr>
<tr>
<td>0.10 C, 0.45 Mn, 0.11 Si, 0.009 Ti, $a_{[O]}=56$ ppm, t=1590°C</td>
<td>26-37 Ti$_2$O$_3$, 8-13 Al$_2$O$_3$</td>
<td>31 Ti$_2$O$_3$, 15 Al$_2$O$_3$</td>
</tr>
<tr>
<td>LF, after Ti addition. Preliminary the melt was deoxidized by vacuum and slag - by SiC</td>
<td>14-22 SiO$_2$, 32-37 CaO</td>
<td>13 SiO$_2$, 32 CaO</td>
</tr>
<tr>
<td></td>
<td>3-7 MgO, 1 MnO</td>
<td>4 MgO, 1.8 MnO, 0.7 FeO</td>
</tr>
<tr>
<td>0.16 C, 0.54 Mn, 0.18 Si, $a_{[O]}=78$ ppm, t=1620°C</td>
<td>40-45 Al$_2$O$_3$, 25-30 SiO$_2$</td>
<td>44 Al$_2$O$_3$, 31 SiO$_2$</td>
</tr>
<tr>
<td>Ladle, after tapping and argon stirring</td>
<td>10-20 CaO, 10-15 MnO</td>
<td>12 CaO, 6 MgO, 4.5 MnO, 1.2 FeO</td>
</tr>
<tr>
<td>0.17 C, 0.55 Mn, 0.19 Si, 0.025 Al$_{sol}$, 0.0027 Ca, t=1610°C</td>
<td>Calcium aluminates:</td>
<td>Calcium aluminates:</td>
</tr>
<tr>
<td></td>
<td>40 CaO, 60 Al$_2$O$_3$</td>
<td>39 CaO, 61 Al$_2$O$_3$</td>
</tr>
<tr>
<td>Ladle, after Al and Fe-Ca cored wire addition</td>
<td>Heterogen. inclusions:</td>
<td>Heterogen. incl.:</td>
</tr>
<tr>
<td>0.09 C, 1.5 Mn, 0.50 Si, $a_{[O]}=31$ ppm, t=1550°C</td>
<td>1 – alumina,</td>
<td>1 – alumina,</td>
</tr>
<tr>
<td></td>
<td>2 – 44 Al$_2$O$_3$, 25 SiO$_2$,</td>
<td>2–45 Al$_2$O$_3$, 33 SiO$_2$</td>
</tr>
<tr>
<td></td>
<td>17 CaO, 4 MnO, 3 MgO</td>
<td>18 CaO, 4 MnO</td>
</tr>
</tbody>
</table>
About the tests results

- Comparison of the analyses with values computed demonstrates that developed software computes inclusions composition correctly enough.

- Today we are looking for further test and development of the software.

- But already now it is evidently that to get correct results during secondary steelmaking in on-line mode the software should have valid input data.
Determination and control of melt conditions for inclusions formation control

For the purpose of determination and control of current metal conditions during secondary steelmaking we are planning to use our GIBBS® melt control system.
GIBBS® melt control system

The GIBBS® system is based on thermodynamic and kinetic approaches.

The system has demonstrated ability to precisely predict and control of melt chemistry and temperature during secondary steelmaking.

It allows to supply the “Inclusions” software with valid information about current metal conditions.

GIBBS® system also is able to compute inclusions remained or emulsified slag.
Summary and future prospects

- The software for simulation of liquid oxide inclusions transformation was developed and tested.
- More testing is on the way to ensure software correctness for wide group of steel grades.
- Application of the “Inclusions” software in combination with GIBBS® melt control system would allow to facilitate prediction and control of inclusions formed during secondary steelmaking and casting.
Acknowledgements

Authors are greatly grateful to Mr. Dmitry Alexeenko, Ms. Elena Baybekova and Ms. Olga Samoylova for assistance in computer programming, sample preparations and SEM analyses.
Thank you!

Feel free to contact us. We are open to collaboration.

www.steelmaker.ru/en

“Inclusions” software: www.steelmaker.ru/en/software
Appendix. About rate determining step

For detection of limiting step we compare diffusion flows of some component $R$ through oxide inclusion and metal:

$$J_{[R]} = 4\pi D_{[R]} ([R]^v - [R]^b)$$
$$J_{(R)} = 4\pi D_{(R)} ((R^+)^v - (R^+)^b)$$

$$D_{[R]} \approx 5 \cdot 10^{-9} \text{ m}^2/\text{s}; \quad D_{(R)} \approx 5 \cdot 10^{-10} \text{ m}^2/\text{s}$$

$$[R]^v - [R]^b \leftrightarrow [R]^{in} - [R]^{eq} \approx 0.01 \text{ wt. pct} \approx 20 \text{ mole/m}^3$$

$$(R^+)^v - (R^+)^b \leftrightarrow (R^+)^{in} - (R^+)^{eq} \approx 10 \text{ wt. pct.} \approx 1 \cdot 10^4 \text{ mole/m}^3$$

$$\frac{J_{[R]}}{J_{(R)}} = \frac{5 \cdot 10^{-9} \cdot 20}{5 \cdot 10^{-10} \cdot 1 \cdot 10^4} = 1$$
Appendix. Computation of current state of metal–slag–gas–inclusions system

START

**Data gaining from previous step:**
- Melt: mass, composition.
- Slag: mass, composition.
- Inclusions: total mass, composition.
- Temperature.
- Pressure.

**Data gaining about influences on the system during time τ:**
- Slag-forming materials: mass, composition;
- Deoxidizers, alloying and modifying additions: mass, composition;

**Block 1.** Computation of inclusion transformation after addition of deoxidizers, ferroalloys, and modifiers and evaluation of partial inclusions assimilation by slag and slag emulsification into the metal.

**Block 2.** Computation of chemical composition of “metal – slag – gas” system and temperature taking into account added slag-forming materials, applied energy and fuel, and heat losses.

**Block 3.** Computation of inclusions transformation which takes place due to changing of metal composition and temperature computed in Block 2.

**Saving of computed parameters.**

END