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REGULAR ARTICLE

Scrap melting model for steel converter founded on interfacial solid/liquid phenomena

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Abstract. The primary goal in steel converter operation is the removal of carbon from the hot metal. This is achieved by blowing oxygen into the melt. The oxidation of carbon produces a lot of heat. To avoid too high temperatures in the melt cold scrap (recycled steel) is charged into the converter. The melting rate is affected by heat and carbon mass transfer. A process model for steel converter is in development. This model is divided into several modules, which are fluid dynamics, heat- and mass-transfer, scrap melting and chemical reactions. This article focuses on the development of the scrap melting module. A numerical model for calculating temperature and carbon concentration in the melt is presented. The melt model is connected with the solid scrap model via solid/liquid interface. The interface model can take into account solidification of iron melt, melting of solidified layer, a situation without such phase changes, and scrap melting. The aim is to predict the melting rate of the scrap including the properties of the hot metal. The model is tested by calculating the melting rates for different scrap thicknesses. All of the stages in the interface model were taking place in the test calculations.

Keywords: steel converter / scrap melting / modeling / heat transfer / mass transfer / numerical method

1 Introduction

Basic oxygen converter process is the primary steelmaking stage in which crude steel is produced by removing carbon from the hot metal. This is achieved by blowing oxygen into the melt. The oxidation of carbon and other components like silicon produces a lot of heat. Recycled steel scrap is used to cool the process temperature, which would rise too high due to the oxidation reactions. Thus, steel converting is an important process for recycling too. Consequently, any model that aims to predict the temperature evolution of the hot metal must take into account the influence of scrap. The hot metal contains initially a high concentration of carbon (4.0–4.5 wt.%). Due to high velocity oxygen gas jet impinging on the hot metal surface carbon as well as other elements are oxidized during the process. The high carbon content in the melt accelerates the melting of the scrap. This occurs because of mass transfer of carbon from the melt to the surface of the scrap containing a low amount of carbon. The carbon at the liquid/solid interface of scrap surface lowers the melting point of the local solid material. The low carbon scrap can then melt even if the hot metal temperature is lower than the melting point of scrap. Thus mass transfer of carbon is very important in the scrap melting process. In addition to scrap melting, hot metal

solidification can take place as well. Initially the scrap is cold and when hot metal is poured on top of it, solidification can happen due to rapid heat transfer from the melt into the scrap.

In the literature several authors [1–5] have developed 1-D scrap melting models. These models have either an analytical or numerical fixed grid approach. These models use constant material parameters for the entire temperature range from room temperature to the melting point. Shukla et al. [6] and Gaye et al. [7,8] have developed a scrap melting model taking into account changing melt properties. Taking into account changing melt temperature and carbon concentration is very important when modeling scrap melting in steel converter.

A 1-D scrap melting model has been developed in the previous article [9]. The model solves enthalpy and carbon concentration equations for solid material. The equations are discretized into moving numerical grid. The scrap shape can be a plate, cylinder or sphere. Previously surrounding melt properties were kept constant. This model is further developed in this paper to consider more realistic behavior between the scrap and the hot metal. Now hot metal temperature and carbon composition solutions are included in the model. The melt model is 0-D, thus the enthalpy and concentration equations represent averaged conditions for the hot metal. This approach assumes ideal mixing in the melt. The interactions between the solid and the melt are taken into

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account with source terms and solid/liquid interface model. Sources include also chemical reactions due to carbon oxidation. Constant rate of carbon oxidation is assumed in the current paper. This paper considers a special situation previously unreported in literature. In this situation a solidified layer forms on top of the scrap. This layer then remelts and if conditions are suitable the scrap will not begin to melt immediately after the layer is gone. In this case the scrap is heating up and the solidus and liquidus temperatures are solved using the iron-carbon phase diagram. Once the liquidus and solidus temperatures are equal the scrap begins to melt. The modeling concepts used in this case are explained in detail. The current paper is based on a previous conference article [10]. This article has now been completely rewritten and is presented with new results and data.

2 Basic model for scrap melting

Melting process of scrap is influenced by heat and mass transfer. Thus differential equations for enthalpy and carbon concentration are necessary. The geometry consists of a 1-D model which describes the average scrap piece thickness. The model predicts a melting curve for the scrap. The enthalpy equation for moving grid is

$$\frac{\partial}{\partial t} \int_V \rho h dV - \int_S \rho h (\mathbf{U}_{grid} \cdot \mathbf{n}) dS = \int_S k \nabla T \cdot \mathbf{n} dS, \quad (1)$$

and for carbon concentration the equation is

$$\frac{\partial}{\partial t} \int_V \rho Y dV - \int_S \rho Y (\mathbf{U}_{grid} \cdot \mathbf{n}) dS = \int_S \rho D \nabla Y \cdot \mathbf{n} dS, \quad (2)$$

where, h is specific enthalpy, ρ is density, $\mathbf{U}_{grid}$ is grid velocity, V is volume, S is surface, k is thermal conductivity, D is diffusion coefficient and Y is carbon mass fraction. The enthalpy method [11] is used to solve equation (1). The details involving the discretization and solution of these equations are explained in reference [9].

3 Conservation equations for hot metal

The hot metal region is modeled with a 0-D approach. A single spacial point will approximate the average melt properties. Ideal mixing is assumed for the hot metal. Enthalpy equation for the melt is

$$\begin{aligned} \frac{\partial}{\partial t} \int_V \rho h dV &= \frac{(h\rho V)^{n+1} - (h\rho V)^n}{\Delta t} = \Psi^h \\ &= \Psi_{scrap}^h + \Psi_{phase}^h + \Psi_{reactions}^h, \end{aligned} \quad (3)$$

where, volume integral over the whole balance area with changing volume has been discretized and where, Ψ^h represents the source terms for the hot metal region. Time index $n+1$ represents new unknown values and n indicates known values from current time level. Next iteration index

v is utilized and specific enthalpy is linearized with respect to temperature as follows:

$$h^{v+1} = h^v + \frac{dh}{dT} (T^{v+1} - T^v). \quad (4)$$

Iteration index $v+1$ indicates unknown values at new iteration step and v last known values from current iteration step. At the end of the iteration loop $n+1$, $v+1$ and v values are all equal. Equations (3) and (4) are combined to form

$$\frac{[h^v + \frac{dh}{dT} (T^{v+1} - T^v)](\rho V)^v - (h\rho V)^n}{\Delta t} = \Psi^h, \quad (5)$$

which is solved for new temperature value:

$$T^{v+1} = T^v + \left(\frac{\Delta t \Psi^h + (hm)^n}{m^v} - h^v \right) \bigg/ \frac{dh}{dT}, \quad (6)$$

where, m is the total hot metal mass. With enthalpy-temperature curves and equation (4) new enthalpy values are calculated. The new iteration value for melt mass m is calculated as

$$m^{v+1} = m^n - \dot{m}_{phase} \Delta t, \quad (7)$$

where, $\dot{m}_{phase}$ is phase change mass flux. If $\dot{m}_{phase}$ is positive, the melt will solidify and if $\dot{m}_{phase}$ is negative, the scrap will liquefy. Equation for hot metal carbon concentration is

$$\begin{aligned} \frac{\partial}{\partial t} \int_V \rho Y dV &= \frac{(Y\rho V)^{n+1} - (Y\rho V)^n}{\Delta t} = \Psi^Y \\ &= \Psi_{scrap}^Y + \Psi_{phase}^Y + \Psi_{reactions}^Y, \end{aligned} \quad (8)$$

where, Ψ^h represents the source terms for the hot metal region. The equation can be solved as follows:

$$Y^{v+1} = \frac{\Delta t \Psi^Y + (Ym)^n}{m^v}. \quad (9)$$

The source terms for heat and carbon mass transfer into the solid scrap are

$$\begin{aligned} (a) \Psi_{scrap}^h &= -N\beta_T S_{s-m} (T_{melt} - T_L), \\ (b) \Psi_{scrap}^Y &= -N\rho\beta_Y S_{s-m} (Y_{melt} - Y_L), \end{aligned} \quad (10)$$

where, β_T and β_Y are convective heat and mass transfer coefficients. S_{s-m} is the area between solid and melt for a reference scrap piece. N is the ratio of the initial total scrap mass and initial reference scrap piece. The 1-D scrap melting model calculates the profiles for the reference scrap piece. N multiplied with S_{s-m} represents the overall area between the solid and liquid phases. When phase changes occur, total enthalpy and carbon balance in the hot metal must change accordingly. The phase change source terms are

$$\begin{aligned} (a) \Psi_{scrap}^h &= -\max(0, m_{phase}) (h_{melt} - h_L) - m_{phase} h_L, \\ (b) \Psi_{scrap}^Y &= -\max(0, m_{phase}) (Y_{melt} - Y_L) - m_{phase} Y_L, \end{aligned} \quad (11)$$

where, the max () operator chooses the maximum value inside the parentheses. Therefore, the enthalpy and carbon mass changes are not symmetric for melting and solidification. This is done to preserve the combined total energy and carbon mass for hot metal and scrap. The source terms for taking into account chemical reactions are

$$\Psi_{reaction}^h = -\dot{m}_{O_2}\Delta h_{reaction} - \dot{m}_{CO}(h_{CO}^{out} - h_{CO}^{in}), \quad (12a)$$

$$\Psi_{reaction}^Y = -\dot{m}_c, \quad (12b)$$

where, the equation (12a) takes into account carbon oxidation into CO and the heat loss due to CO leaving the converter. Equation (12b) is a drain term for carbon due to formation of CO. The mass flux parameters $\dot{m}_{O_2}$, $\dot{m}_{CO}$ and $\dot{m}_c$ have constant values. When the interface velocity is known, the phase change mass flux is solved from:

$$\dot{m}_{phase} = U_{IF}\rho_S S_{S-m} N. \quad (13)$$

4 Further model development including interfacial solid/liquid phenomena

Boundary conditions have to be determined for the scrap melting model. These will be used to solve the solid/liquid interface velocity and temperature. Since the scrap is cold, it is expected that initially the hot metal will solidify on top of the scrap increasing the thickness. After this, the layer remelts.

4.1 Hot metal solidification and melting

The phase change rate for the layer is only dependent on heat transfer, because the composition of the layer and the melt is the same. Therefore, boundary conditions are set up differently when the scrap thickness L is larger than the initial thickness L_i compared to $L < L_i$. So when $L > L_i$ and interface velocity $U_{IF} > 0$ indicating solidification of the hot metal, the heat balance for the interface is

$$\begin{aligned} U_{IF}\rho(h_{melt} - h_I) &= k_{S,1}\left(\frac{\partial T}{\partial x}\right)_1 - \beta_T(T_{melt} - T_{L,1}) \\ U_{IF}\rho(h_{melt} - h_I) &= k_{S,1}\left(\frac{T_{S,1} - T_I}{0.5\Delta x}\right) - \beta_T(T_{melt} - T_{L,1}), \end{aligned} \quad (14)$$

where, h_I is the enthalpy on the control volume next to the interface in the scrap melting model. The index 1 indicates corresponding points on the iron-carbon phase diagram for solidification of the hot metal. The phase change paths of hot metal and scrap are presented in Figure 1.

In the hot metal phase change path $Y_L = Y_S = Y_{melt}$. When $U_{IF,1} < 0$ indicating melting of the pig iron layer, the heat balance is as follows:

$$U_{IF}\rho(h_{L,1} - h_I) = k_{S,1}\left(\frac{\partial T}{\partial x}\right)_1 - \beta_T(T_{melt} - T_{L,1}). \quad (15)$$

Fig. 1. Phase change paths in iron-carbon phase diagram.

To conserve overall heat balance with melt balance equation (3) the liquidus enthalpy $h_{L,1}$ is used in equation (15).

4.2 Scrap melting

After the layer has disappeared, the scrap begins to melt. Then, the melting is affected both by heat transfer and mass transfer of carbon. So when $L < L_i$ and $U_{IF} < 0$, equation for enthalpy balance is

$$U_{IF}\rho(h_{L,2} - h_I) = k_{S,2}\left(\frac{\partial T}{\partial x}\right)_2 - \beta_T(T_{melt} - T_{L,2}), \quad (16)$$

and equation for carbon balance is

$$U_{IF}(Y_{L,2} - Y_I) = D_{S,2}\left(\frac{\partial Y}{\partial x}\right)_2 - \beta_Y(Y_{melt} - Y_{L,2}), \quad (17)$$

at the interface according to Figure 1. In equations (16) and (17) the temperatures T_S and T_L have the same values, which is visualized in Figure 1. Iron-carbon phase diagram is used to determine the interface temperature as well as corresponding carbon concentrations for solidus and liquidus. These two equations are valid only for $U_{IF} < 0$, because scrap melting and melt solidification are not reversible.

4.3 Special situation after the layer has disappeared

It is possible that after the disappearance of the pig iron layer, the solution of the equations (16) and (17) give a positive velocity for the interface. This means that the scrap is not melting. These equations are defined for $U_{IF} < 0$ so equation (14) should be used in this instance. But in this case the equation (14) gives negative velocity for the interface velocity indicating melting. Logically this is not possible since there is no layer left. So the model is now giving contradicting predictions for phase change. In other words, the iron-carbon phase diagram and balance equations for interface fail to give logical predictions for scrap melting with the assumption that $T_S = T_L$. This problem can be solved by setting the interface velocity

Fig. 2. The scrap solidus and liquidus temperature evolution during a time period without phase changes.

$U_{IF} = 0$. Now equations (16) and (17) change into

$$\lambda_S \frac{\partial T}{\partial x} - \beta_T (T_{melt} - T_L) = 0, \quad (18)$$

and into

$$D_S \frac{\partial Y}{\partial x} - \beta_Y (Y_{melt} - Y_L) = 0, \quad (19)$$

respectively. Equations (18) and (19) can be used to solve T_S and T_L . In this special case liquidus and solidus temperatures are not equal. As long as $U_{IF} > 0$ solved from equations (16) and (17) with the assumption $T_S = T_L$, the actual interface velocity is set to zero. For this special situation there are no phase changes and the scrap is heating up. During this heating stage the scrap and solidus temperatures rise. When T_S and T_L have equal values, equations (16) and (17) can now be used to solve the interface velocity for scrap melting with the assumption that $T_S = T_L$, and nonzero interface velocity. This situation is presented in Figure 2.

4.4 The complete algorithm

The equations for 1-D scrap melting, interface velocity and temperature with melt properties are iterated together inside a time-step. The calculation of local material properties such as thermal conductivity and diffusion coefficient in the scrap are explained in reference [9].

In Figure 3, flowcharts for the scrap melting and interface programs are presented. The scrap melting algorithm begins by initializing the necessary variables. Then, implicit Euler time integration is started. Inside the time integration loop there is an iteration loop, which contains the solution for the temperature and carbon concentration 1-D profile solutions for scrap, solution for U_{IF} , T_S , T_L , Y_S , Y_L at the interface and the solution of conservation equations for the hot metal phase, respectively. The interface quantities are solved in the interface algorithm, which contains an iteration loop as well. In the beginning the iteration loop is divided into two paths.

One is for the melting and solidification of the layer. The other path is for the scrap melting. The layer path is chosen if the current scrap thickness L is equal or higher than the initial thickness L_i . The scrap melting path is chosen if $L < L_i$. In the layer path, the solidus and liquidus compositions are equal to the melt concentration. If the last known value for the interface velocity U_{IF} is smaller than zero indicating melting, the new value for it is solved from equation (15). If $U_{IF} \geq 0$ indicating solidification of hot metal, the new value for it is solved from equation (14). This concludes the layer path. In the scrap melting path U_{IF} and $T_{S,L}$ are solved from equations (16) and (17). If $U_{IF} < 0$ indicating scrap melting, the scrap melting path is finished. On the other hand, if $U_{IF} > 0$, equation (14) is used to compute a second value for $U_{IF,2}$. If this value is less than zero, then no phase changes are taking place. In this case $U_{IF} = 0$ and the solidus temperature T_S and liquidus temperature T_L are solved from equations (18) and (19). This concludes the scrap melting path. If $U_{IF,2} > 0$, this would indicate that another layer would be forming after the first layer has disappeared. This never happened in test calculations. If another layer begins to form, the ratio of scrap and hot metal masses are most likely too high and the process is not able to produce enough heat to melt the scrap. Once the difference between new and last known values for U_{IF} is small enough, the iteration loop is discontinued and the algorithm ends.

In many steel plants, ore additions are performed during the blowing for temperature adjustment and slag conditioning. If bigger amounts of ore are added into the furnace, the melt temperature can decrease so much that a new layer solidifies on the scrap surface. The effect of ore additions during the blow was examined and modeled by Gaye et al. [7,8]. In the current model this situation can be taken into account by changing the “Interface Algorithm”. If in the scrap melting path $U_{IF,2} > 0$, the L_i variable can be set equal to the current scrap thickness L . This enables the possibility of a new layer formation when the algorithm returns to the beginning of the iteration loop. The ore can be added all in a single batch or in many small additions. In general, a single large ore addition causes the melt temperature to decrease very close to the liquidus in the iron-carbon phase diagram, which can cause problems in the converter operation. Adding the ore in many increments makes the changes in the melt temperature much smoother. The behavior of the melt temperature evolution affects naturally the scrap melting rate.

Furthermore, it is a common practice to mix heavy and light scrap in steel converter operation. As a consequence, the scrap melting evolution is changing. Gaye et al. [7,8] observed that mixing light and heavy scrap can considerably decrease the melting rate of the heavy scrap when compared to a case without light scrap.

The current model can be modified to take this phenomenon into account by creating 1-D melting models for all scrap types. These 1-D models then exchange heat and mass with the melt conservation equations.

Fig. 3. Flowcharts for scrap melting and interface algorithms.

5 Numerical results

Numerical results are calculated for steel converter containing 100 tons of hot metal with 4.5 w-% of carbon. Other initial values are presented in Table 1.

The calculations are done for different scrap thicknesses $L = 1.0, 2.0, 4.0, 8.0$ cm. The shape of the scrap is plate and since the total initial mass is not varied, the surface area between the melt and the scrap changes with thickness. The estimation of the convective heat and mass transfer coefficients goes as follows. Gaye et al. [7] estimated the convective heat transfer coefficients for Lance-Bubbling-Equilibrium (LBE) and for Lance-Equilibrium-Tuyeres (LET) steel converters at values 17000 and 25000 $\frac{W}{m^2K}$, respectively. The values were estimated by fitting the modeling results with plant data. The convective heat transfer coefficient for this work is chosen to be $\beta_T = 20000 \frac{W}{m^2K}$, which is in the range of Gaye's estimations. In a previous work [9] the ratio between the heat and mass transfer coefficients was found to be approximately $\frac{\beta_T}{\beta_Y} = 1e8$. Therefore, the value for mass transfer coefficient in this work is $\beta_Y = 0.0002 \frac{m}{s}$. The coefficients are kept constant for each case.

Oxygen mass flow rate is set to value $\dot{m}_{O_2} = 6.0 \frac{kg}{s}$ which means that all of the carbon will be oxidized in 16 minutes. Enthalpy flux of reactions is estimated to be $\dot{H}_{reactions} = \dot{m}_{O_2} \Delta h_{reactions} = -7.7e7 J/s$. The drain term for carbon concentration is $\dot{m}_C = -\frac{3}{4} \dot{m}_{O_2}$ according to the oxidation reaction and with the assumption of constant oxidation rate. The CO heating enthalpy is estimated as $\dot{m}_{co} (h_{co}^{out} - h_{co}^{in}) = 1.947e7 J/s$. The numerical results are

Table 1. Initial conditions for calculations.

	Hot metal	Scrap	
Carbon	4.5	0.25	w-%
Temperature	1322	25	°C
Mass	100	20	ton

presented in Figures 4–9 for all initial scrap thicknesses. In Figure 4 the evolutions of half of the scrap thicknesses are presented.

First, a solidified layer with melt composition accumulates on top of the scrap in all cases. After a short time the layer remelts and disappears. Then, there is a short period in all cases where the scrap is heating up and not melting. Next the scrap begins to melt. The melting rates are different for the layer and the scrap. This is due to the higher temperature difference between the bulk melt and liquidus in the case of the layer material, which can be seen in Figure 1. Also, the scrap melting rate is highly dependent on carbon mass transfer from the hot metal to the scrap. The thicker the scrap the more time is needed for complete melting. The absolute thickness increase is quite similar for all cases. Since the surface area between the melt and the scrap increases as initial thickness decreases, the melt mass curves experience more solidification for thinner scrap which is shown in Figure 5.

The melt temperatures in Figure 6 are much lower for thin scrap at the time of shell solidification and melting. This happens again because of the higher surface area. In

Fig. 4. Melting curves for different scrap thicknesses.

Fig. 7. Hot metal carbon concentrations for all cases.

Fig. 5. Hot metal mass profiles as a function of time.

Fig. 8. The evolution of liquidus and solidus temperatures for scrap thickness $L = 4.0$ cm.

Fig. 6. Hot metal temperatures for different scrap thicknesses.

Figure 7 the carbon concentrations in hot metal are presented. Here, the drain term dominates the behavior of the concentration decrease. The dilution effect of the scrap is strongest in the thinnest case due to faster melting.

Fig. 9. Melt temperature and carbon concentration evolution compared with liquidus and solidus from iron-carbon phase diagram.

In Figure 8 the evolution of the solidus and liquidus temperatures for scrap thickness $L = 4.0$ cm are presented. While the solidified layer is present the solidus temperature

is constant for the duration of 65 s since the solidus is at the eutectic isotherm. The continuous decrease in carbon concentration in the melt is causing the increase in the liquidus temperature. Between 65 and 73 s, a process similar to Figure 2 is taking place. Here, the solidus temperature begins to rise and at the 73 s mark the liquidus and solidus temperatures are equal. At this point the scrap begins to melt, while the interface temperature is in continuous rise. The melt temperature and carbon concentration evolution in an iron-carbon phase diagram are presented in Figure 9. Time stamps have been marked for every 100 s for the scrap thickness $L = 8.0$ cm. As expected in the thinnest scrap case the melt temperature is the closest to the liquidus and vice versa for the thickest scrap.

The validation of the model against measurements from industrial scale converter is important. However, the authors are not aware of any data from literature, which contains a sufficient measurement campaign for validation purposes. In the future it would be helpful if the following information could be available for validation:

- initial and final composition as well as temperature of the iron melt and slag phase;
- initial and final masses of the iron melt and slag phase;
- temperature measurements as a function of time from the iron phase;
- initial scrap mass, temperature, thickness and composition;
- estimation of total scrap mass as a function of time during the process.

6 Conclusions

A 1-D scrap melting model for steel converter was further developed to include the hot metal temperature and carbon composition change during converter operation. The melt model includes a simple chemical reaction source term assuming constant reaction rate for oxidation. The scrap melting and melt models were linked with a solid/liquid interface model. Interface properties are determined with enthalpy and carbon balance equations and iron-carbon phase diagram. The interface model contains a possibility for situation, where no phase changes are present and the scrap is heating up. This has not been taken into account in the models from literature. The interface balance equations are used to solve solidification and melting rate with heat and mass transfer rates between the solid and liquid phases. The new converter scrap melting model was tested for varying scrap thickness.

Nomenclature

ρ	Density (kg/m ³)
β_T	Convective heat transfer coefficient (W/(m ² K))
β_Y	Convective mass transfer coefficient of carbon (m/s)

Ψ	Source term
h	Specific enthalpy (J/kg)
H	Enthalpy (J)
V	Volume (m ³)
S	Surface area (m ²)
T	Temperature (K)
U	Velocity vector (m/s)
m	Mass (kg)
n	Surface unit normal vector
k	Thermal conductivity (W/(mK))
L	Scrap half-thickness (m)
t	Time (s)
Y	Carbon mass fraction
D	Diffusion coefficient of carbon (m ² /s)

Subscripts

L	Liquidus
S	Solidus
s	Solid
m	Melt
IF	Interface

Superscripts

n	Time level index
v	Iteration index
h	Enthalpy
Y	Carbon mass fraction

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