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COUPLED HEAT AND MASS TRANSFER APPROACH TO SIMULATE THE SCRAP DISSOLUTION IN STEELMAKING PROCESS

Ajay Kumar Shukla[1] ,Prof Brahma Deo[1]

[1]Department of Materials and Metallurgical Engineering,
Indian Institute of Technology Kanpur, 208016, India
Email: {shukla@,bdeo@}iitk.ac.in

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ABSTRACT

Scrap is used as one of the basic iron bearing charge materials in steelmaking processes, in addition to hot metal. The kinetics of dissolution of scarp can be a limiting factor in the control of the temperature trajectory of a steelmaking process. It is also known to affect the slag formation, slag foaming and the post combustion ratio in the initial stages of the blow. The mechanism of scrap dissolution comprises of simultaneous heat transfer and mass transfer (of carbon) in the bulk metal and in the scrap. A proper understanding and accurate prediction of the scrap dissolution rate is a key factor to design a suitable dynamic control strategy for a steelmaking process. In the present work, both analytical and numerical models have been developed to predict the dissolution behavior of scrap in an oxygen steelmaking converter. The effect of various shapes (only cylindrical) and sizes of scrap, the carbon composition of metal, temperature and the carbon composition trajectory in the bulk under forced convection conditions of heat and mass transfer are incorporated into the model. For the first time, a comparison is made between the analytical and numerical solutions for the case of a complex moving boundary problem. The results of the calculation obtained from both the models have been critically analyzed and the important parameters are evaluated. The models can be directly used to predict the limiting size and also the optimal ratio of liquid metal to scrap in a steelmaking process.

INTRODUCTION

Scrap is added as raw material which compensates for the excess heat generated due to various chemical reactions in steelmaking process . The process is coming under the special category of solidification and melting problems called as moving boundary problems with phase change (Stefan problems). Depending upon the heat efficiency of the process it is possible to consume scrap by 30% in oxygen steelmaking process.

Several studies have been carried out to investigate the process of scrap dissolution in steelmaking converters . Most of the models have been developed for heat transfer in a single direction where heat and mass transfer coefficients between solid and liquid melt were estimated by semi-empirical correlations under the conditions of natural and forced convection . Since there is lot of turbulence in the bath due to rigorous chemical reactions such as decarburization and bottom stirring so effort has been made to correlate the heat transfer coefficient as a function of total energy input to the system . There exists relationship between heat and mass transfer coefficients under forced convection condition known as Chilton-Colburn analogy . Since during dissolution of scrap boundary layer at solid liquid interface is also moving so the actual values of heat and mass transfer coefficients are different from the bulk values . Heat and mass transfer equations obtained in this way are coupled together to estimate the dissolution behavior of cylindrical shape scrap for various sizes under different conditions like trajectory of Temperature and Carbon composition in the bulk , parent scrap composition , operation parameters of the process (blowing regime and decarburization profile) etc . The estimated values of dissolution behavior and total time for dissolution is coming in close agreement with the observations .

THEORETICAL CONSIDERATIONS

Solidification and melting process is goverened by heat and mass transfer between liquid and solid phases . The heat and mass transfer equations are coupled together to arrive at the desired solution . Let us consider the interface between liquid and solid steel during dissolution process .

Figure 1 – Schematic diagram of temperature and composition profile in scrap and metal

Figure 1 shows the temperature and carbon composition profile for melting of solid scrap in liquid melt . The bulk has a temperature of Tb and carbon composition of Cb. The solid scrap has the uniform temperature and carbon composition of Ts and Cscrap respectively . The temperature and composition of solid-liquid interface are Ti and Ci respectively . There exists thermodynamic equilibrium between solid and liquid carbon composition at the interface from which the composition of scrap in solid at the interface is estimated as Cs .The following mathematical equations have been used to describe the dissolution behavior of scrap in the liquid melt (calculations done for heat and mass transfer in one dimension) :

$$\rho Hv + h(Tb - Ti) = \lambda \left.\frac{dT}{dX}\right|_{x=0} \qquad \text{[E1]}$$

$$\alpha \frac{\partial^2 T_{sc}(x,t)}{\partial x^2} = \frac{\partial T_{sc}(x,t)}{\partial t} \qquad \text{[E2]}$$

$$v(Ci-Cs)=k(Ci-Cb) \qquad \text{[E3]}$$

ρ =mass density of the scrap
α =thermal diffusivity of solid scrap
h=heat transfer coefficient between liquid and solid
k=mass transfer coefficient between liquid and solid
v=the moving velocity of the interface (solidification/melting rate)
H=the latent heat of melting
$\lambda =$ thermal conductivity in the solid steel .

Equation [E1] represents heat balance at the interface, and equation [E2] represents the heat conduction in the solid scrap and equation [E3] describes mass balance of carbon at the interface .The estimated velocity of interface may be positive(solidification) or negative(melting) depending upon the dominance of the heat transfer by conduction inside the scrap .Therefore overall dissolution process is defined as simultaneous heat and mass transfer (of carbon) in the melt and inside the scrap . Initial melt is getting solidified on cold parent scrap followed by remelting of the solidified shell and melting of the parent scrap .

DESCRIPTION OF THE MATHEMATICAL MODEL

Equation [E1] and [E2] has been solved by analytical method along with suitable initial and boundary conditions obtaining solution as a Fourier series in our previous work[1] .In order to study the scrap dissolution process in a complete way , heat and mass transfer equations have been coupled together where heat transfer coefficient in bulk has been estimated as a function of total input energy to the oxygen steelmaking process and mass transfer coefficient by chilton-colburn analogy for the forced convection situation . Further mathematical treatment is given to estimate the heat and mass transfer coefficients for the moving boundary situation . The velocities estimated by heat and mass transfer equations are compared for different values of interface carbon till they are converged to give the correct solution . Following set of assumptions are made for formulating the model :

1. Thermal conductivity ,density are same for scrap as well as liquid melt.
2. Actual values of heat and mass transfer coefficients are calculated from moving boundary layer concept.
3. The solid scrap at the interface is carburized and is in equilibrium with the liquid at the interface . This is subject to the condition that the estimated equilibrium composition in the solid scrap at the interface cannot be lesser than the parent composition . It is defined in the following way :
   If Cs estimated in the following way is greater than Cscrap then

$$Cs = \left(\frac{\alpha Cb}{\alpha + (1-\alpha)\exp\left(\frac{-v}{k}\right)} \right) \qquad \text{Otherwise} \quad Cs = Cscrap \qquad (1)$$

4. The composition of the solidified shell in early stage of solidification is calculated from the equation :

$$Velocity = \beta \times \ln((Ci - Cs)/(C\infty - Cs)) \quad (2)$$

Where Ci and Cs are in thermodynamic equilibrium with each other .

5. Liquidus Line of Fe-C system is defined for the interface Temperature and Carbon composition as following :

$$Ti = 1836 - 93 \times Ci \quad (3)$$

6. Velocity of the moving interface is constant for small time step .
7. The latent heat of solidification does not include the additional term to account for the energy required to raise the temperature of melting mass from interface temperature to the bulk temperature .This effect is taken care in equation (5) ,while defining the actual heat transfer coefficient .

8. The scrap is assumed to be uniformly exposed to all the surfaces .

Mathematical Formulation :

1.Heat Transfer Coefficient :

For moving boundary layer ,thickness of the thermal boundary is given as :

$$\delta t = k / h \quad (4)$$

Actual value of heat transfer coefficient is given as :

$$h' = \rho m \times Cpm \times Velocity /(1 - Exp(-\rho m \times Cpm \times Velocity / h)) \quad (5)$$

2. Mass Transfer Coefficient :

The thickness of the concentration boundary layer is given as :

$$\delta m = Dc / \beta \quad (6)$$

Actual value of mass transfer coefficient is given as :

$$\beta' = Velocity /(1 - Exp(-Velocity / \beta) \quad (7)$$

3.Heat flux balance at the solid-liquid interface :

$$h'(2\pi Rl)(T\infty - Ti) = \rho(2\pi Rl)(-\Delta Hfe') \times Velocity + k \times (2\pi Rl) \times (dT / dr)\big|r = R \quad (8a1)$$

where :

$$\frac{dT}{dr}\Big|r = R \;=\; -\sum_{i=1}^{i=20}\frac{2(Tsci - T'(R,t')}{R}Exp\left[-\alpha\left(\frac{\beta oi}{R}\right)^2 t\right] \qquad (8a2)$$

$\Delta Hfe' = \Delta Hfe$; During solidification (8b)

$\Delta Hfe' = \Delta Hfe + Cp(T' - Tav)$; During fast and normal melting (8c)

where average Temperature of the melting shell is given as

$$Tav = \frac{\int_{R}^{R-velocity\times t} Tsc(r',t)r'dr'}{R(R - Velocity\times t)} \qquad (8d1)$$

4. Mass flux at interface :

$$-Velocity(Cs - Ci) = \beta'(Ci - C\infty) \qquad (9)$$

5. Change in the heat content of the melt :

Solidification :

$$CpWm(dT\infty / dt) = -h(2\pi Rl)(T\infty - T') \qquad (10)$$

Fast and Normal melting :

$$CpWm(dT\infty / dt) = -h(2\pi Rl)(T\infty - T') + Cpm(T\infty - Tav)(dWsc / dt) \qquad (11)$$

where :

$$(dWsc / dt) = (2\pi Rl)\rho \times Velocity$$

6 . Change in Carbon content of the melt :

Solidification :

$$Wm(dC\infty / dt) = (C\infty - rCi)(2\pi Rl)\rho \times Velocity \qquad (12)$$

Fast and Normal Melting

$$Wm(dC\infty / dt) = (C\infty - Cs)(2\pi Rl)\rho \times Velocity \qquad (13)$$

7 . Assumed Carbon and Temperature trajectory for the case when scrap is not charged :

$$C\infty = Cinitial - 0.172 \times t^{1.4} \quad \text{if} \quad 0 \le t < 3$$
$$= Cinitial - 0.238 \times t \quad \text{if} \quad 3 \le t \le 15$$
$$= 0.50 \times Exp(-0.479 \times t) \quad \text{if} \quad C\infty < 0.50 \qquad (14)$$

$$T\infty = Tinitial + 0.116524 \times t^3 - 4.81238 \times t^2 + 75.2857 \times t \qquad (15)$$

where t is the time in minutes.

8. Temperature profile estimation inside the scrap :

$$Tsc(r,t) = T'(R,t') + \sum_{i=1}^{i=20} \frac{2(Tsci - T'(R,t'))}{\beta oi. \times J_1(\beta oi)} J_o(\frac{\beta oi}{R} r) Exp\left[-\alpha \left(\frac{\beta oi}{R} \right)^2 t \right] \qquad (16a)$$

9. Relationship between heat and mass transfer coefficient :

Heat and mass transfer coefficients for fixed boundary situation may be related by Chilton-Colburn similarity as following :

$$\beta = \left(\frac{Dc}{\alpha} \right)^{0.6667} \left(\frac{h}{\rho m \times Cpm} \right) \qquad (17)$$

Calculation Procedure :

1. Process is divided into a number of time steps .
2 .Temperature profile is calculated inside the scrap at every time step
3. Heat and Carbon mass transfer equations are coupled together in the following way depending upon the the ratio between the conductive and convective heat flux at the interface :

If $\left(\frac{Conductive\_Heat\_Flux\_at\_Interface}{Convective\_Heat\_Flux\_at\_Interface} \right) > 0.001$

Velocity of the moving interface is calculated as following :

$$Velocity = \frac{1}{\rho(-\Delta Hfe')} \left[h'(T\infty - T') - k \times \frac{dT}{dr} \Big| r = R \right] \qquad (18)$$

$$Velocity = -\beta \times \ln\left(\frac{(Cs - C\infty)}{(Cs - Ci)} \right) \qquad (19)$$

Where (19) is coming after plugging in value of β' in equation (9).
Equation (18),(19)along with (3) are solved simultaneously by iteration method for three unknowns namely Velocity,Ti and Ci.

If $\left(\frac{Conductive\_Heat\_Flux\_at\_Interface}{Convective\_Heat\_Flux\_at\_Interface}\right) < 0.001$

Then $(dT/dr)\big|_{r=R}$ may be neglected and by combining equation (18) and (5) we have follwing equation :

$$\text{Velocity} = -\left(\frac{\alpha}{\rho m \times Cpm}\right) \ln\left[1+\frac{Cpm \times \rho m \times (T\infty - T')}{\rho m \times \Delta Hfe'}\right] \quad (20)$$

After coupling this equation with equation (19) and by Chilton-Colburn analogy for relationship between heat and mass transfer coefficient ,we have :

$$\ln\frac{(Cs - C\infty)}{(Cs - Ci)} = \left(\frac{\alpha}{Dc}\right)^{0.6667} \ln\left[1+\frac{Cpm \times \rho m \times (T\infty - T')}{\rho m \times \Delta Hfe'}\right] \quad (21)$$

Equation (21) along with (3) may be solved for two unknowns Ti and Ci and from them Velocity may be calculated using equation (20) .

5. $C\infty$ and $T\infty$ are updated at each time step as explained from equation (10) to (15) .
6. Wm and Wscr are updated at each time step as following :

$$Wm(t) = Wm(t') - \rho(2\pi Rl) \times Velocity \times \Delta t$$
$$Wscr(t) = Wscr(t') + \rho(2\pi Rl) \times Velocity \times \Delta t \quad (22)$$

Process Conditions for which simulation has been done :

Wt of liquid melt	= 130000 Kg
Scrap Ratio	= 0.10
Initial Temperature	= 1573 K
Melt Carbon Composition	= 4.5 %
Scrap Carbon Composition	= 0.25 %
h_frac	= 0.50
Lance Angle	= 14 degrees
Number of openings in lance	= 6
Throat Diameter	= 2.46 cm
Bath Depth	= 1.30 m
Lance Oxygen Flow Rate	= 400 NM3/Min
Bottom Stirring Flow Rate	= 2 Nm3/min

Blowing Regime is defined as following :

If 0< t < 135 ; Lance height = 2.20 m
If 135< t <225 ; Lance height = 2.00 m
If 225 < t < 300 ; Lance Height = 1.80 m
If t > 300 ; Lance Height = 160 cm

RESULTS AND DISCUSSIONS

Mass transfer vs heat transfer control

Based upon the calculated results , following different zones of control of process with respect to heat and mass transfer have been outlined :

If $(T_b > T_l)$ and $(C_b > C_s)$, The Process is controlled by heat and mass transfer both for smaller differences of T_b and T_l . For larger differences heat transfer is the only controlling mechanism .

If $(T_b > T_l)$ and $(C_b < C_s)$,The Process is controlled only by the heat transfer.

If $(T_b < T_l)$ and $(C_b > C_s)$, The Process is controlled only by the mass transfer.

If $(T_b < T_l)$ and $(C_b < C_s)$, Dissolution does not take place ,

As it is verified from figure 2 that rate of dissolution is slow and mass transfer controlled as long as the temperature of the melt is below the liquidus temperature of the scrap . When temperature of the melt is greater than the liquidus temperature of the scrap , rate of dissolution increases very fast as it is heat transfer controlled .

Above findings give an impression that the blowing strategy must be developed in such a manner that decarburization rate in early moment should not be fast enough to reduce the carbon level of the melt significantly .

; Dimension and Bulk Temperature (at reduced scale) of cylindrical shape scrap (Heat Transfer Coefficient calculated as a function of

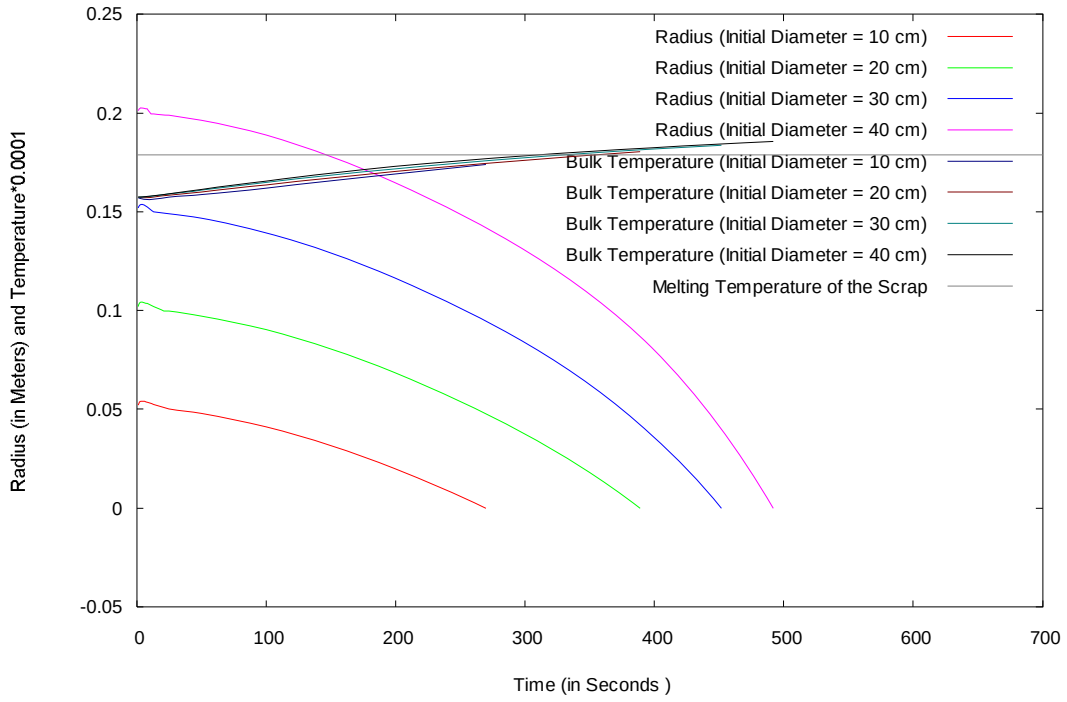

Figure -2 : Dissolution behavior of cylinder wrt bulk temperature

Heat transfer coefficient vs dissolution behaviour

In figure 3-4 dissolution behavior is plotted for the heat transfer coefficient value given in literature (47500 W/M^{2}K) and for the value calculated as a function of blowing conditions for cylindrical geometries . The total time for dissolution is coming is coming in between 5 to

10 minutes which is in close agreement with the industrial observations . The results are almost same for both the cases which proves that average heat transfer coefficient as given in literature is in close agreement with what has been calculated by the consideration of average energy input to the system .Total time for dissolution is decreasing on increasing the heat transfer coefficient and also not proportional to the initial size of the scrap which is contrary to the previous findings[8].

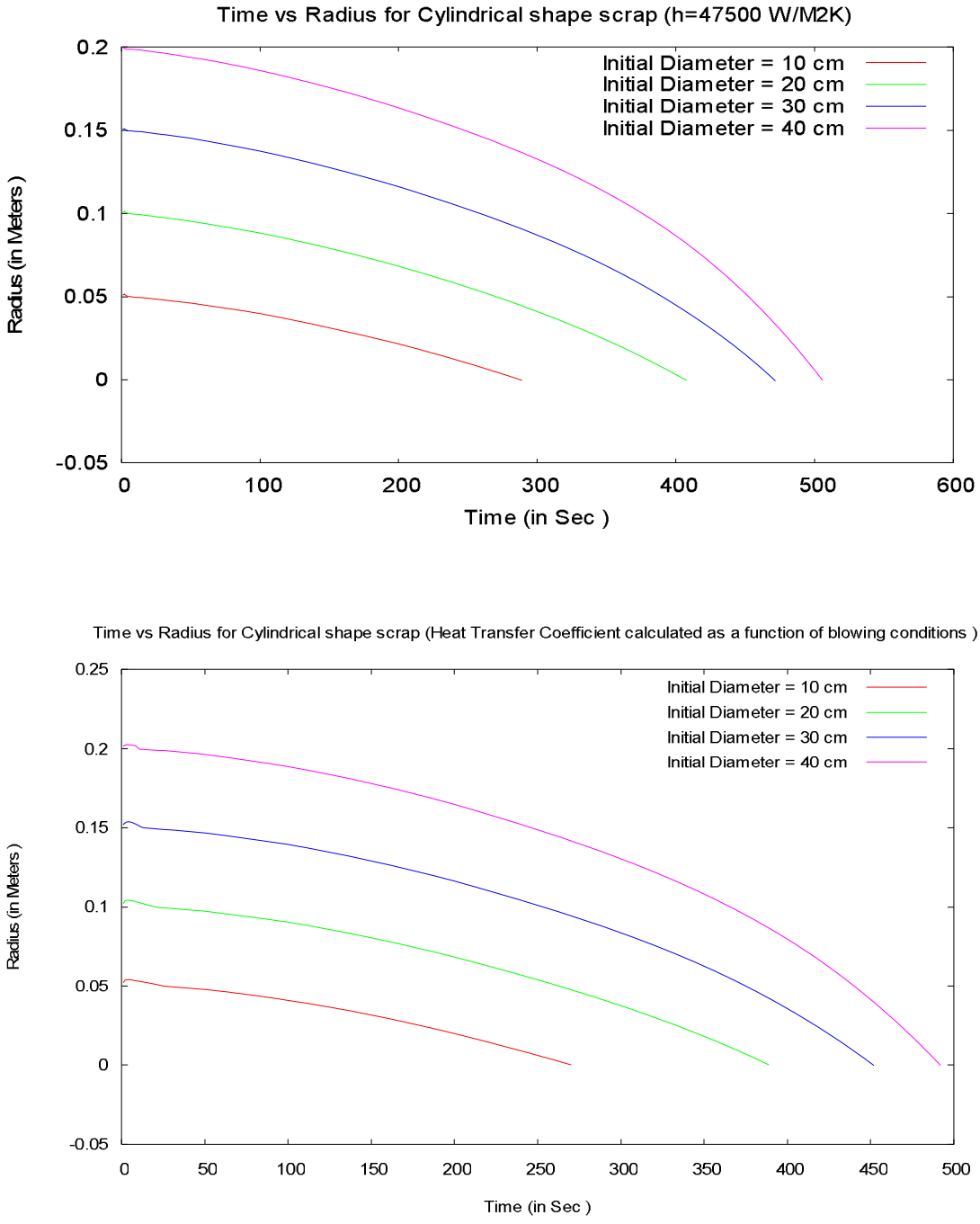

Figure-3 : Dissolution behavior of cylindrical shape scrap

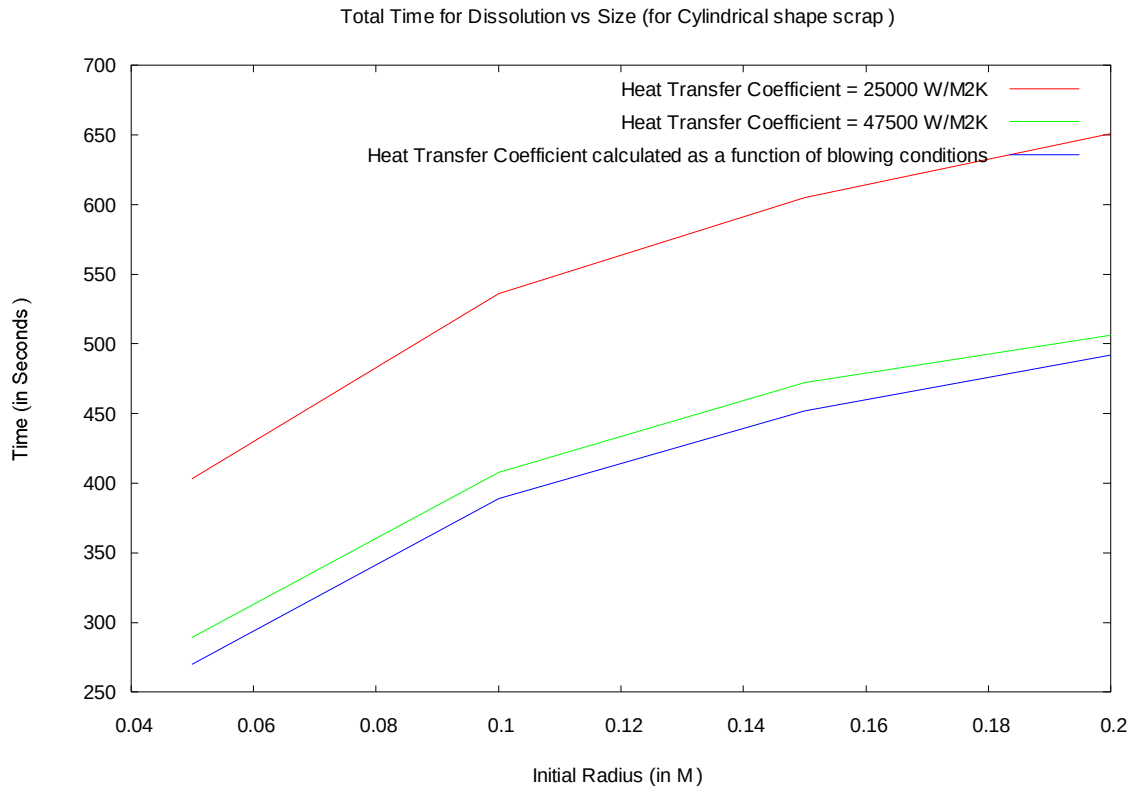

Figure 4 : Total time for complete dissolution vs dimension

CONCLUSION

Mathematical model for dissolution of scrap in high carbon melt is developed by coupled heat and mass transfer approach where temperature profile in the scrap is described as power series based solution[1].and the heat transfer coefficient is estimated as a function of energy input to the system . The results prove that it is a good approximation to assume the value of heat transfer coefficient as 47500 $W/M^2/K$ which is in agreement with the calculations of D Hertog and Snoeijer[2]. Further work is going on to estimate the complete analytical solution by Green's function approach for the same . It is also a matter of investigation to find out the level of contact between solidified shell and the parent scrap by performing experiments however requisite modification in heat transfer coefficient may be introduced to take care of it[17]. The results of numerical method using FDM were compared with analytical results in my previous work where role of mushy zone in calculations is well described[1] . Work is under progress to develop a model by numerical method for pure metal considering only the heat transfer control .

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NOMENCLATURE :

Notation	Description	Units
Cp	Specific Heat of Scrap	J/Kg K
Wm	Wt of the melt	Kg
Wscr	Wt of scrap	Kg
Velocity/v	Velocity of moving interface	m/s
t‘	Time till Previous time step	seconds
t	Current process time	seconds
Cpm	Specific heat of the melt	J/Kg K
ρm	Density of the melt	Kg/m3
α	Thermal diffusivity of the melt	m2/s
Dc	Diffusion Coefficient of Carbon in the melt	m2/s
k	Thermal conductivity of the melt	W/m K
$C\infty$	Melt bulk Carbon composition	%
Ci	Interface carbon composition	%
Cs	Scrap composition at the interface	%
Tsci	Initial Scrap Temperature	%
Tsc Eig	Temperature inside the scrap at different locations Eigen Value	K
$T\infty$	Melt Bulk Temperature	K
T’	Interface Temperature	K
ΔHfe	Latent heat of solidification/melting	J/Kg
h	Heat transfer Coefficient for fixed boundary	W/m2 K
h’	Actual heat transfer Coefficient	W/m2 K
β	Mass transfer Coefficient for fixed boundary	m/s
β'	Actual mass Transfer Coefficient	m/s
J_o	Bessel’s function of Zero order	
J_1	Bessels function of first order	
βoi	i th root of bessels function	
Cinitial	Carbon composition of melt at t = 0	
Tinitial	Temperature of the melt at t = 0	
r	Equilibrium ratio of carbon composition between solid and liquid phase	
Cscrap	Composition of the Parent Scrap	%

APPENDIX I

Estimation of heat and mass transfer coefficients for moving boundary

The mass transfer equation in the liquid melt adjacent to the the scrap interface is given as :

$$D\frac{d^2C}{dX^2}+v\frac{dC}{dX}=0 \qquad \text{[A1]}$$

With the following boundary conditions :

C = Ci at x =0
C = Cb at x= δ c

Solution of the above equation comes as following :

$$k=\frac{v}{1-\exp(-v/k_0)} \qquad \text{[A2]}$$

$$\delta c = \frac{D}{k}$$

The heat transfer equation in the liquid melt adjacent to the the scrap interface is given as :

$$\alpha\frac{d^2C}{dX^2}+v\frac{dC}{dX}=0 \qquad \text{[A3]}$$

Where

$$\alpha=\frac{\lambda}{\rho C_p}$$

With the following boundary conditions :

T = Ti at x =0
T = Tb at x= δ t

Solution of the above equation is as following :

$$h=\frac{\rho C_p v}{1-\exp(-\rho C_p v/h_0)} \qquad \text{[A4]}$$

$$\delta t=\frac{\lambda}{ho}$$

APPENDIX B

Estimation of absolute value of heat transfer coefficient as a function of input energy to the steelmaking system

Following set of mathematical expressions are used to estimate the heat transfer coefficient where total energy input to the steel bath is considered under combined influence of top lance and bottom stirring system :

$$E_t^0 = 6.32 \times 10^{-7}.\cos\varphi.\frac{Q_t^3.M}{W.n^2.d_t^3.X}$$

$$Q_{decarb} = \frac{d[C]}{dt}.W.\frac{10^6 \times 22.4 \times 60}{12}$$

$$E_{decarb}^0 = 6.18 \times \frac{Q_{decarb}\,T_l}{W}(\ln[1+\frac{\rho.g.H.h\_frac}{p_{atm}}]+[1-\frac{T_0}{T_l}])$$

$$E_b^0 = 6.18 \times \frac{Q_{bottom}.T_l}{W}.(\ln[1+\frac{\rho.g.H}{p_{atm}}]+[1-\frac{T_o}{T_l}])$$

$$E_{total}^o = E_{top}^o \times 0.10 + E_b^o + E_{decarb}^0$$

$$h = 5000.E_{total}^{o\ 0.33}$$

where φ is the angle of the lance tip from vertical , Q_t is Oxygen flowrate ,W is weight of steel , n is the number of openings of the lance , X is the lance height above metal bath during blowing , H is the average height of the formation of CO bubbles , h_frac is the average depth fraction at which CO bubble formation takes place , d_t is the throat diameter , T_o is the Temperature of the bottom stirring gas at input , T_l is the average Temperature of the liquid Steel , p_{atm} is the atmospheric pressure and h is the heat transfer coefficient