CHAPTER V

MODEL SIMULATION

A mathematical model is developed to describe the behavior of DRI pellets submerged in liquid electric furnace slag. Nauman and Elliott^{58,57} have previously developed a model for heating an inert spherical object immersed in a liquid slag by translating Fourier's law of heat conduction and the dominant boundary conditions to finite difference equations and solving them by a step-by-step numerical method (cf. see II.B).

The evolution of gas from D-R pellets during their heating and melting period results in variation of the properties of materials and the conditions of the slag bath and influences the behavior of the DRImelting system. The experimental results described in Chapter IV show that the thickness of the solid shell of slag formed on the surface of a cold object decreases as a result of continued heating and because of the evolution of gas. Gas evolution changes the effective density of the frozen shell of slag as well as the liquid slag that surrounds the particle.

To construct a simple model that simulates the behavior of the DRIslag melting system, the contribution of four major items should be considered: (a) evolution of gas from DRI, (b) change of properties of materials, (c) solidification and melting of slag, and (d) condition of the bath of liquid slag. The roles of these items are described in the rest of this chapter. A copy of the computer program that was developed is also given in Appendix J.

A. Gas Evolution

An immersed D-R pellet (assumed spherical) is divided into spherical shells with a finite thickness Ar (Figure 5-1) to calculate the distribution of temperature and the evolution of gas from the pellet. The distribution of temperature in the pellet can be determined from solution of the heat conduction equation described in Section II.B. Knowing the temperature of an element, the volume of gas being evolved during heating of that element can be calculated. The total volume of the gas evolved from the pellet is then computed by summing the volumes of gases evolved from various elements of the pellet:

$$\mathbf{V} = (\mathbf{V}_1 \cdot \mathbf{W}_1 + \cdots \cdot \mathbf{V}_i \cdot \mathbf{W}_i + \cdots \cdot \mathbf{V}_n \cdot \mathbf{W}_n) / \mathbf{W}$$
(5.1)

where V is the total volume of gas evolved from unit weight of the pellet, V_i is the volume of gas formed per unit weight of element i, W_i is the weight of element i, and W is the total weight of the pellet. Assuming the density of the particle is constant along its radius and substituting for the weight terms in Eq. (5.1), the following equation is obtained:

$$\mathbf{V} = (\mathbf{V}_1 \cdot \mathbf{v}_1 + \dots + \mathbf{V}_i \cdot \mathbf{v}_i + \dots + \mathbf{V}_n \cdot \mathbf{v}_n) / \mathbf{v}$$
(5.2)

where v_i is the volume of element i and v is the total volume of the pellet. The volume of gas evolved from element i during the time interval $2\Delta t = t_{j+1} - t_{j-1}$ is evaluated from Eq. (5.3):

$$V_{i} = G_{i} (T_{i,j+1} - T_{i,j-1})$$
(5.3)



Fig. 5-1 Distribution of Temp. and Gas Volume for a D-R Pellet Immersed in Liquid Slag.

where T_i is the temperature of element i and G_i is "specific gas volume" for element i and is defined as the total volume of gas released per gram of DRI for a temperature increment of 1°K at temperature T_i .

The quantity, G_i , can be determined from the results of the bomb extractions. For simplicity, the temperature axis of the gas evolution curve (see Figure 5-2) is divided into 100°C intervals, then the mean derivative of gas volume is calculated for these intervals:

$$G_{i} = (V_{i+1/2} - V_{i-1/2})/(T_{i+1/2} - T_{i-1/2})$$
(5.4)

The results of the gas evolution experiments conducted at various heating rates show that the total volume of the gas evolved is not appreciably influenced by the rate of heating of DRI (see Section IV. A.2.a.3). The gas evolution patterns obtained for a rate of rise of temperature of 250°C/min are therefore used to calculate the specific gas volume G_i .

Since the volumes of the gases that evolve are almost proportional to the degree of metallization of DRI (Figure 4-10) when there is enough carbon in the sample to reduce the oxides completely, the volumes of the gases evolved can be expressed in terms of the degree of metallization or the oxygen content of DRI. The gas evolution data for a reference sample can thus be utilized to calculate the volume of gases evolved from a DRI sample as follows:

$$V_{\rm T} = V_{\rm T}^{\circ} \quad (\% {\rm Met}^{\circ} / \% {\rm Met}) \tag{5.5}$$

where ${\rm V}^{}_{\rm T}$ is the total volume of gas evolved from a DRI sample at

temperature T, V_T° is that of the reference, %Met° is the degree of metallization of the reference and %Met is that of the sample. Equation (5.5) can also be expressed in terms of the oxide content of DRI:

$$V_{\rm T} = V_{\rm T}^{\circ} ("FeO"/"FeO"^{\circ})$$
 (5.6)

This equation was inserted in the model to compute the gas evolution from a DRI sample. The results were tested against those obtained by utilizing the gas evolution patterns of different DRI samples as reference as well as those obtained by heating a pellet in slag (see Section VI.B.3).

The rate of evolution of gas is equal to the time derivative of the total volume of gas evolved from the pellet:

$$V_{j} = (V_{j+1} - V_{j-1})/2\Delta t$$
 (5.7)

where V is the total volume of gas evolved from the pellet from the time zero to the time j. Δt .

The influence of gas evolution on the transmission of heat from liquid slag to an immersed particle can be attributed to the following possible transport mechanisms: (a) partial shielding of the moving solid-liquid slag interface by departing gas bubbles, (b) replacement of cold solid and liquid layer in contact with the moving interface by "pumping" associated with bubbles departure,⁷⁸ and (c) circulation of the liquid slag due to the evolution of the rising gas bubbles.

The shielding of the particle by the evolved gas bubbles may result in a decrease or an increase in the rate of heating of the particle depending on temperature and thermal properties of the materials involved.



Fig. 5-2 Gas Evolution from DRI.



Fig. 5-3 Solidified Slag Shell Around an Active Gas Port on Ni Sphere.

The effect of this factor will be discussed in Section VI.B.2. The replacement of the layer of cold slag from the solid-liquid slag interface results in a decrease in the thickness of the solid slag shell. The effects of this factor and the circulation of the liquid slag due to the rising of gas bubbles will be described in Sections V.C and V.D.

B. Properties of Materials

A precise knowledge of the properties of the solid and liquid slag and of the metallic particles immersed in the slag is necessary to develop the mathematical model for melting of the pellets.

1. Properties of Slag

A detailed discussion of the thermo-physical properties is given in Appendix D. Thermo-physical properties of the slags utilized in heat transfer studies are summarized in Table 5-1. The Grashof and Rayleigh numbers of slags are calculated for bulk temperature of 1250°C and a constant particle radius of 1.8 cm including the thickness of the shell of slag. The chemical composition of the slags are given in Table 3-4.

2. Properties of Specimen

The physical properties of the specimens used in heat transfer studies are summarized in Table 5-2. The overall specific heat of DRI is calculated in Appendix F based on the contribution of the following items:

a. specific heat of the constituents as given in the thermodynamical tables,

b. enthalpy of the reduction reactions occurring during heating of DRI,

c. heat of the phase transformation of DRI materials:

Table 5-1 Properties of Slags. 58,59

	Slag A Slag B		Slag C			
Property	Sol.	Liq.	Sol.	Liq.	Sol.	Liq.
Melting range, °C	1140	1215	1125	1220	1230	1310
Heat of fusion, [*] cal/g.	80.7		102.0	-	130.0	·
Thermal expansivity, cm ³ /cm ³ . °C	-	0.00014	-	0.00014	-	0.00014
Conductivity, cal/cm. sec.°C	0.0059	0.0052	0.0043	0.0046	0.0028	0.0032
Density, g/cm ³	3.7	3.6	3.8	3.5	2.9	2.9
Specific Heat, cal/g. °C	0.25	0.28	0.25	0.28	0.24	0.28
Diffusivity, cm ² /sec.	0.0064	0.0052	0.0045	0.0047	0.0040	0.0040
Viscosity, poise	-	2	-	2	-	5
Kinematic viscosity, cm ² /sec.	-	0.56	_	0.57	-	1.72
Prandtl number	-	108	_	122	-	431
Grashof number	-	286	-	307	_	5
Rayleigh number	-	3.1x10 ⁴	_	3.7x10 ⁴	-	2.3x10 ³

*Based on heats of fusion of components (cf. Table 3-4).

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Specimen	Nickel Sphere		DRI Pellet E D	
Diameter, cm	1.84	3.00	1.60	1.62
Rad. of Thermocouple well, cm	0.22	0.38	0.15	0.15
Effective density, g/cm ³	8.29	8.00	2.60	2.33
Porosity, fraction	0.02	0.10	0.55	0.55
Radial distance of bead from center of particle, cm	0.35	0.72	0.08	0.08
Mass, g	25.5	106.4	5.8	5.2

Table 5-2 Physical Properties of Specimens Used forHeat Transfer Studies.

$$Fe_{3}C_{(s)} = 3Fe_{(\gamma)} + \underline{C}(\%) \quad \Delta H = -1.23 \text{ (cal. } g_{Fe_{3}C}^{-1}) \quad (5.8)$$

The effective thermal conductivity and heat of fusion of DRI and the constants used for calculation of the flow of heat transmitted to the thermocouple bead embedded inside the specimens are computed in Appendix E. A summary of the thermal properties of materials that are utilized in simulation of the computer model is given in Table 5-3.

C. Solid Shell of Slag

Because of transfer of heat from liquid slag to the cold immersed particle, a shell of slag freezes initially at the periphery of the particle and will remelt later. The thickness of the slag shell is a function of many variables such as time, temperature of the slag, initial temperature of the particle, properties of the slag and of the specimen, and motion of the slag relative to the specimen.

The thickness of the shell varies on the surface of the particle from place to place, becoming thicker as the distance from an active bubbling site increases, as represented in Figure 5-3.

Similar results are obtained for the shell of slag frozen on the surface of DRI pellets. For moderate rates of gas evolution $(1000 \text{ cm}^3/\text{min} \text{ for a 2-cm} \text{ diameter pellet})$ a number of active bubbling sites form on the surface of the solid shell which permit the evolution of gas from the pellet into the liquid slag. For higher rates of gas evolution $(3000 \text{ cm}^3/\text{min} \text{ for a 2-cm} \text{ diameter pellet})$, the shell of slag is highly porous and allows the evolution of gas from all over the surface. A comparison is made of the shells of slag solidified on the surface of a totally metallized pellet, a 95 percent, and an 87 percent metallized

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Property	Relationship	Temp., °K
Specific heat	0.13-8.01 E-6T - 2.27 E3T ⁻²	T`<903
cal/g. °K	$0.12 + 1.70 = 5T - 3.80 = 3T^{-2}$	T <u>></u> 903
Conductivity	0.25/0.22/0.19/0.17/0.16/0.16/0.16/0.1	7 T = 100 i
cal/sec. cm.°K	0.17/0.18/0.18/0.19/0.20/0.20/0.20	i = 2, 3,, 1
Heat of fusion of Ni ⁷⁷ , cal/g	71.70	M.P., 1726
Specific	C _M + 1.29 G(T)	T <t<sub>a</t<sub>
Heat of	C _M + 1.35 G(T)+CT	$T_{a} \leq T \leq T_{a} + 8$
DRI	C _M + 1.47 G(T)	T _a +8 <t<t<sub>b</t<t<sub>
Materials, [*] cal/g. °K	C _M + 1.35 G(T)	^T ≥ ^T b
Conductivity of	0.2/0.18/0.17/0.15/0.13/0.12/0.10/0.09	T = 100 i
11011-	0.07/0.07/0.07/0.07/0.07/0.08/0.08/0.1	0 i = 2,3,,1
"FeO"	0.0144	-
Fe ₃ C	0.0170	-
A1203	0.0190	-
SiO ₂	0.0069	-
Cal/sec. cm.°K		
Heat of fusion of DRI, ⁷⁷ cal/g	66 $W_{Fe} + 255 W_{Al_2O_3} + 34W_{SiO_2}$	1773

Table 5-3 Thermal Properties of Materials

*cf. Appendix F.

pellet in Figure 5-4. For the totally metallized pellet, the shell of slag is continuous and dense. For the 95% metallized pellet, there are several bubbling sites on the surface of the slag. For the 87% metallized pellet, the slag shell is very thin due to the vigorous disturbance introduced in the slag by gas bubbles.

The variation of the thickness of the shell of solid slag is computed in the model based on the difference of the heat which is transferred from the liquid into the surface of the solid particle and that which is conducted from the surface of particle to the cold core. Since the difference between the temperature of the bulk slag and the liquid-solid interface is constant, the flow of heat to the surface of solid particle is basically controlled by the condition of the bath which is quantified by the Nusselt number of the bath. The flow of heat transferred from the interface to the cold core is however determined from the temperature gradient in and the thermal conductivity of the solid shell which is influenced by the porosity and the pore diameter of the shell. The thermal conductivity of the shell is calculated from Equation (D.7) and the information given in Figure 4-28. Since the evolution of gas affects the porosity of the shell, it will indirectly influence the thermal conductivity and the rate of growth of the solid shell. These effects are inserted into the structure of the model and will be discussed further in Chapter VI.

D. Condition of Bath

The condition for transfer of heat from the liquid slag can be expressed in terms of an overall Nusselt number which is a dimensionless



Fig. 5-4 Shell of Slag Frozen on Surface of DRI Pellets: (a) Totally Metallized, (b) 95 Percent Metallized, (c) 87 Percent Metallized.

version of heat transfer coefficient. For a system in which the conditions of a moving solid-liquid interface prevail, the overall Nusselt number is defined as follows:

$$Nu \equiv 2h(R+\theta)/(\alpha\rho C_p)_{\ell}$$
(5.9)

where h is the heat transfer coefficient, R is the radius of the specimen, θ is the thickness of the shell of solid slag, and α, ρ and C_p are thermal diffusicity, density and specific heat of the liquid slag. The transmission of heat from hot liquid slag to the specimen is by conduction, free convection and forced convection as will be described in the subsequent sections.

Since the densities of slags do not change appreciably during solidification, the movements of the solid-liquid interface do not appear to affect the motion of the fluid around the particle significantly. The movements of the interface may, however, influence the coefficient of transfer of heat by changing the thickness of the thermal boundary layer of the slag. The Nusselt number in such a case will increase during the period that the shell grows and will decrease when the shell melts.

A simple calculation shows that the thickness of the thermal boundary layer is about 3 times greater than the thickness of the solid shell of slag when steady state transfer conditions prevail (Appendix G). The effects of the movements of the solid-liquid interface on the flow of heat to the particle were, for simplicity, neglected throughout the mathematical calculations.

1. Conduction

The Nusslt number for a stationary sphere submerged in a motionless body of liquid can be calculated from the solution of the conduction equation in spherical coordinates.⁸⁵ This solution is valid for short times when the velocities generated in the liquid because of development of nonuniform temperature profiles are small.

A simple manipulation of the conduction equation yields the following solution for the distribution of temperature outside a sphere of constant surface temperature, T_i (Appendix H):

$$\frac{T-T_{\infty}}{T_{i}-T_{\infty}} = \frac{R+\theta}{r} \operatorname{erfc} \frac{r-R-\theta}{\sqrt{\pi\alpha t}}$$
(5.10)

where T_{∞} is temperature of the bulk liquid, R is radius of the specimen, θ is thickness of the frozen shell, T is temperature at time t after immersion and at radial distance r>R from center of the sphere, α is thermal diffusivity of the liquid and erfc is the complementary error function defined in reference 85. The coefficient of transfer of heat determined from the above equation leads to the following correlation (see Appendix H):

$$Nu_t = 2 + 2(R+\theta)/\sqrt{\pi \alpha t}$$
 (5.11)

As is seen from Equation (5.11), the heat transfer coefficient is initially infinite. This is because of the sudden change of temperature at the surface of the sphere when immersed. But it decreases to a minimum of 2 after a long time has elapsed.

2. Natural Convection

If the temperature of the bath is substantially different from that of the surface of the particle, the effect of natural convection should also be included in computation of the Nusselt number. In contrast to the relatively rapid heating of the particle by conduction, the contribution of natural convection is not considerable during the initial transient period, when the Nusselt number for natural convection rises from zero to a maximum of about 4 (see Table 5-4).

Hellums and Churchill⁸⁶ have studied the transient natural convection of a fluid initially at rest on an isothermal vertical plate and inside a horizontal cylinder. Their results show that the time necessary for these systems to reach steady state is less than 3 seconds. This time is shorter than that of initial transient forced convection produced by sudden submersion of the particle (see V.D.3) and the time that must elapse until the contribution of conduction described by Equations (5.11) falls to that of natural convection. Since conduction and forced convection mechanisms are therefore initially dominant in the system (see also Section V.D.3) the effects of transient natural convection can be neglected.

The contributions of long term conduction and steady state free convection on transfer of heat to the particle are given in the following empirical expression:⁸⁷

$$Nu = 2 + 0.1 \text{ Gr}^{1/4} \cdot \text{Pr}^{1/3}$$
 (5.12)

when the quantity of the combination $Gr^{1/4}$. $Pr^{1/3}$ is no more than 200.

		Dom t i al a		Arro Sholl	c	Clar.	
_	No.	Type	Rad., cm	Thick., cm	Туре	Temp., °C	Nu
-	1	Ni	0.92	0.25	A	1250	3.43
	2	Ni	1.50	0.3	А	1250	3.97
	3	Ni	1.50	0.27	В	1250	4.07
	4	Ni	1.50	0.23	В	1275	4.13
	5	E	0.80	(0.10)	В	1250	3.18
	6	E	0.80	-	С	1600	3.30
	7	D	0.81	(0.10)	В	1250	3.19
	8	D	0.81	-	С	1600	3.31

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Table 5-4Average Nusselt Number for Natural Convection in
Liquid Slag Calculated from Eq. (5.12).

The average Nusselt numbers calculated from the above relationship for particles and slags of various types and conditions are given in Table 5-4. These quantities were utilized to compute the heating rate of neutral spheres and DRI pellets when submerged into a hot bath of slag.

3. Forced Convection

Transient forced convection may be generated when the particle is plunged into the liquid slag. Since the actual liquid velocities that may be produced by the plunged particle are not defined, the available correlations cannot be conveniently utilized to predict the contribution of forced convection to transfer of heat to the particle during the corresponding transient period. Because of the relatively large Prandtl number of the slags (and from the experimental results) this period does not appear to be long (cf. Section VI.B for the best fit of the data).

The evolution of gas from an immersed particle may also generate forced convection in the bath and increase the Nusslt number of the system. Mikic and Rohsenow⁷⁸ have studied the transfer of heat from a hot surface to the cold liquid of a nucleate pool boiling system. The physical model they have used consists of the removal of a part of the natural convection layer by each departing bubble when the areas of influence of the bubbles do not overlap.⁹¹ Using the transient solution of the heat conduction equation for calculation of the flow of heat to the layer of liquid in contact with the surface, they have been able to compute the rate of transfer of heat due to the evolution of gas bubbles from the surface into the pool.

Employing a similar physical model to that which Mikic et al.⁷⁸

have used and assuming the area of influence of gas bubbles is equal to their equatorial surface area, the local Nusselt number for transfer of heat to the immersed particles when gas evolution occurs into the slag bath may be computed as follows:

$$Nu_{b} = (\pi f \rho C_{p}/k)^{1/2} D_{b}^{2} n (R+\theta)$$
 (5.13)

where f is bubbling frequency, ρ , C_p and k are properties of the liquid slag, D_b is the diameter of gas bubbles when evolved from the particle, and n is the number of active bubbling sites per unit area of the particle. If N is the total number of active gas holes in the particle an average Nusselt number may be computed as follows:

$$\overline{Nu}_{b} = (f \rho C_{p} / \pi k)^{1/2} D_{b}^{2} N/4 (R+\theta)$$
(5.14)

A plot is made of $\overline{\mathrm{Nu}}_{\mathrm{b}}$ for particles with 2 active gas ports in Figure 5-5. It is to be noted that the areas of influence of gas bubbles do not overlap when the rate of evolution of gas from nickel spheres is less than 4000 cm³/min. port.

The evolution of gas may also result in generation of stirring in the liquid slag. The direction of motion is however opposite to that which is produced by natural convection. The produced stirring may therefore increase or decrease the rate of heating of the immersed sphere.

As is discussed in the next chapter, the Nusselt numbers determined by comparing the experimental results with the mathematical calculations are smaller than those which were calculated in this section. The overall Nusselt numbers for slags of various conditions which were utilized in



Fig. 5-5 Local Bubbling Nusselt Number for Particles and Slags Specified in Lines 1, 2 and 3 of Table 5-4.



Fig. 5-6 Natural and Forced Bubbling Convection in Liquid Slag.

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