Supersonic O_2 -jet Impingement on Liquid Iron with Surface Chemistry

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This paper describes numerical analysis of a supersonic O_2 -jet impingement on carbon-contained liquid iron under vacuum circumstances. The gas phase is assumed to be composed of O_2 , CO, CO_2 , O and C. Since gas temperature is elevated over 1 000 K in the vicinity of the surface of liquid iron, high-temperature gas effects, namely vibrational energy excitation and dissociation, are included in the analysis. Therefore, the flow field is expressed by Navier–Stokes equations consisting of mass conservation, momentum, overall energy, vibrational energy and species mass conservation equations. Furthermore, surface reactions for O_2 –C and O–C encounters are included in surface boundary conditions. Cavity geometry is determined from the balance of pressure, shear stress, surface tension and liquid buoyancy. Based on the numerical results, sensitivity of mass fraction for each species to the probability of surface reaction is discussed. In addition, the effect of the surface reactions on the cavity geometry is clarified.

KEY WORDS: jet impingement; supersonic jet; surface reaction; thermochemical nonequilibrium.

1. Introduction

A supersonic oxygen jet is widely employed for vacuum oxygen decarburization (VOD). The jet impinges on liquid metal to produce a cavity for certain conditions. The experimental visualization of such cavity formation is actually very difficult, so that the structure of the jet impingement on high-temperature liquid metal is not completely understood yet. In the past, investigations of a jet impingement on liquid have been extensively conducted to reveal the structure of the cavity and lip geometry.^{1–5)} Banks and Chandrasekhara¹⁾ conducted experiments of an air jet impingement on water, and measured the cavity depth, diameter and lip height. The role of surface tension in affecting the cavity depth was discussed. They also developed analytical models of a penetrating jet. Olmstead and Raynor²⁾ and Fagela-Alabastro and Hellums³⁾ carried out numerical calculations of the geometry of liquid surface in a two-dimensional jet impingement. Turkdogan,⁴⁾ through experiments of incompressible fluid, found correlations between jet flow rate and cavity depth and between surface tension and critical impact pressure to cause splash. The influence of surface reactions on cavity geometry was clarified by Cheslak *et al.*⁵⁾ After these works, an interest moved to the solution of splash mechanism. References 1)–5) were concerned with the experiments at atmospheric pressure and there are no papers treating the jet impingement on liquid in vacuum circumstance.

The present paper is concerned with the numerical analy-

sis of a supersonic O_2 -jet impingement on carbon-contained liquid iron (see Fig. 1). Not only surface reactions but also gas phase chemistry are considered and so the analysis uses a thermochemical nonequilibrium model. The thermal nonequilibrium is expressed by separating temperature into translational-rotational temperature and vibrational temperature. Namely, a two-temperature model is used here. The cavity geometry is dependent on properties of a jet. When impact pressure is small, a steady-state cavity is just formed. On the other hand, a lip can appear at larger impact pressures. Further large pressure causes splash and ripples on the liquid surface. The present analysis is limited to a steady jet impingement in vacuum circumstance and does not treat splash and ripples.

Fig. 1. Flow field of a supersonic-jet impingement on liquid iron.

2. Flow Model

The flow field considered here is described below. As shown in Fig. 1, a supersonic O_2 -jet, which is issued from a sonic nozzle, impinges on the surface of carbon-contained liquid iron. A part of O_2 molecules reacts with carbon on the surface, and then produced CO diffuses into the gas phase. Oxygen gas impinging on the surface is heated due to heat conduction from the high-temperature liquid iron ($T_w = 1840$ K). On the other hand, radiative heat flux can be neglected because the gas-temperature increase by the radiation is below 1 K. High-temperature gas will excite molecular vibration, so that the contribution of vibration on specific heat must be included into the analysis, while electronic excitations are not needed to be put in the analysis. Therefore, a two-temperature model composed of translational-rotational temperature (T_{tr}) and vibrational temperature (T_{vib}) was selected. Chemical species contained in the gas phase are O_2 , CO, CO_2 , O and C. Nozzle-flow conditions are given in Table 1.

The liquid iron works as heat bath, so that the liquid surface is taken to be isothermal. A flow inside the liquid iron induced by surface shear-stress of gas phase is not considered to simplify the analysis.

3. Chemistry in Gas Phase

Six chemical reactions for O_2 , CO, CO_2 , O and C contained in the gas phase have been taken from Evans *et al.*'s work.⁶⁾ They are shown in Table 2. Rate constants for forward and backward reactions are given by

$$k_{f,r} = A_{f,r} T_f^{B_{f,r}} \exp(-C_{f,r}/T_f) \dots\dots\dots (1a)$$

$$k_{b,r} = A_{b,r} T_b^{B_{b,r}} \exp(-C_{b,r}/T_b) \dots\dots\dots (1b)$$

In Eqs. (1a) and (1b), $A_{f,r}$, $B_{f,r}$, $C_{f,r}$, $A_{b,r}$, $B_{b,r}$ and $C_{b,r}$ are the constants, where the subscripts f and b denote the for-

ward and backward reactions, respectively. For $r=1, 2$ and 3, T_f is modeled as $\sqrt{T_{tr} T_{vib}}$. For the other forward and backward reactions, $T_f = T_{tr}$ and $T_b = T_{tr}$. In this paper, in order to simplify the model, such chemistry at the liquid surface as shown in Table 3 was employed, where backward reactions are not included in the present analysis.

4. Cavity Geometry

A cavity will be formed due to the interaction of the jet with the surface. The cavity geometry was determined from the balance of impact pressure, shear stress, surface tension and buoyancy of the liquid iron. Figure 2 illustrates the balance of the forces on the cavity surface. The top view of the cavity is shown in Fig. 3. Let α be the angle of the cavity surface, and then we have the following expression for the force acting on the small area of a ring with a width of ds :

$$\text{Impact pressure: } (p_w - p_f) \cos \alpha \times 2\pi y ds \dots\dots\dots (2)$$

where p_w and p_f are the pressure at the surface of liquid iron and the ambient pressure, respectively.

Similarly, the force due to shear stress (τ), buoyancy and force due to surface tension are written as follows:

$$\text{Force due to shear stress: } \tau \sin \alpha \times 2\pi y ds \dots\dots\dots (3)$$

$$\text{Buoyancy: } (\rho_l - \rho_w) g h \times 2\pi y ds \cos \alpha \dots\dots\dots (4)$$

$$\begin{aligned} \text{Surface tension: } & (\sigma \sin \alpha)_{y+dy} \times 2\pi(y+dy) \\ & - (\sigma \sin \alpha)_y \times 2\pi y \dots\dots\dots (5) \end{aligned}$$

Table 3. Chemistry at liquid surface.

r	Reaction
1	$C + O_2 \rightarrow CO + O$
2	$C + O \rightarrow CO$

Fig. 2. Balancing of force on surface of cavity.

Fig. 3. Top view of cavity.

Table 1. Nozzle-flow conditions.

Reservoir pressure	1.0×10^4 Pa
Reservoir temperature	300 K
Ambient pressure	5.0×10^2 Pa
Ambient temperature	300 K
Mach number at nozzle exit	1.0
Nozzle exit diameter (D)	1.0 cm
Initial distance between nozzle exit and liquid surface	3.0 cm

Table 2. Chemistry in gas phase.

r	Reaction
1	$CO + M \rightleftharpoons C + O + M$
2	$CO_2 + M \rightleftharpoons CO + O + M$
3	$O_2 + M \rightleftharpoons O + O + M$
4	$CO + CO \rightleftharpoons CO_2 + C$
5	$CO + O \rightleftharpoons O_2 + C$
6	$CO_2 + O \rightleftharpoons O_2 + CO$
$M = O_2, CO, CO_2, O, C$	

where ρ_l is the density of liquid iron, ρ_w is the density of the gas phase at the surface, g is the gravity and h is the depth of the cavity.

The balance of the above forces in the perpendicular direction, therefore, can be written as

$$(p_w - p_f) - \tau \tan \alpha = (\rho_l - \rho_w)gh + \frac{1}{y} \frac{d}{dy} (y\sigma \sin \alpha) \dots (6)$$

The cavity geometry was determined by solving Eq. (6).

5. Numerical Analysis

5.1. Governing Equations

The flow field of the supersonic jet impingement in a steady state is numerically calculated by integrating in time the unsteady equations and obtaining its large-time limit. The problem is described by Navier–Stokes equations consisting of equations of mass conservation, momentum, overall energy, vibrational energy and mass conservation for each species in unsteady form.¹⁰⁾ Using cylindrical coordinates given in Fig. 1, the governing equations are written as follows:

• Mass conservation equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\rho v}{y} = 0 \dots (7)$$

• x-momentum conservation equation

$$\begin{aligned} \frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2 + \rho)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} + \frac{\rho uv}{y} \\ = \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\tau_{xy}}{y} \dots (8) \end{aligned}$$

• y-momentum conservation equation

$$\begin{aligned} \frac{\partial(\rho uv)}{\partial t} + \frac{\partial(\rho uv)}{\partial x} + \frac{\partial(\rho v^2 + p)}{\partial y} + \frac{\rho v^2}{y} \\ = \frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{2\mu}{y} \left(\frac{\partial v}{\partial y} - \frac{v}{y} \right) \dots (9) \end{aligned}$$

• Energy conservation equation

$$\begin{aligned} \frac{\partial e}{\partial t} + \frac{\partial[(e+p)u]}{\partial x} + \frac{\partial[(e+p)v]}{\partial y} + \frac{(e+p)v}{y} \\ = \frac{\partial \beta_x}{\partial x} + \frac{\partial \beta_y}{\partial y} + \frac{\beta_y}{y} \dots (10) \end{aligned}$$

• Mass conservation equation of species s

$$\begin{aligned} \frac{\partial \rho_s}{\partial t} + \frac{\partial(\rho_s u)}{\partial x} + \frac{\partial(\rho_s v)}{\partial y} + \frac{\rho_s v}{y} \\ = -\frac{\partial J_{x,s}}{\partial x} - \frac{\partial J_{y,s}}{\partial y} - \frac{J_{y,s}}{y} + \dot{w}_s \dots (11) \end{aligned}$$

• Vibrational energy equation

$$\begin{aligned} \frac{\partial e_{\text{vib}}}{\partial t} + \frac{\partial(e_{\text{vib}} u)}{\partial x} + \frac{\partial(e_{\text{vib}} v)}{\partial y} + \frac{e_{\text{vib}} v}{y} \\ = -\frac{\partial q_{\text{vib},x}}{\partial x} - \frac{\partial q_{\text{vib},y}}{\partial y} - \frac{q_{\text{vib},y}}{y} + Q_{T-V} + \dot{q}_{\text{vib}} \dots (12) \end{aligned}$$

In Eqs. (7)–(12), u and v are the gas velocity in x - and y -directions, respectively, p is the pressure of the gas phase, ρ is the density of the gas phase, ρ_s is the density of the species s , and $\dot{w}_s$ is the mass production rate of the species s .

In Eqs. (8) and (9), τ_{ij} is the viscous stress tensor written as¹¹⁾

$$\tau_{xx} = \mu \left[\frac{\partial u}{\partial x} + \frac{\partial u}{\partial x} - \frac{2}{3} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{v}{y} \right) \right] \dots (13)$$

$$\tau_{yy} = \mu \left[\frac{\partial v}{\partial y} + \frac{\partial v}{\partial y} - \frac{2}{3} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{v}{y} \right) \right] \dots (14)$$

$$\tau_{xy} = \tau_{yx} = \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \dots (15)$$

In Eq. (10), e is the total energy per unit volume, which is expressed by¹²⁾

$$e = e_{\text{tr-rot}} + e_{\text{vib}} + \frac{1}{2} \rho(u^2 + v^2) \dots (16)$$

where $e_{\text{tr-rot}}$ is the internal energy for translation–rotation and e_{vib} is the internal energy for vibration and β_x and β_y denote, respectively,

$$\beta_x = \tau_{xx} u + \tau_{xy} v - q_x \dots (17)$$

$$\beta_y = \tau_{yx} u + \tau_{yy} v - q_y \dots (18)$$

where q_x and q_y are the heat fluxes in the x - and y -direction, respectively, which are expressed by¹³⁾

$$q_x = -\lambda_{\text{tr}} \frac{\partial T_{\text{tr}}}{\partial x} - \lambda_{\text{rot}} \frac{\partial T_{\text{tr}}}{\partial x} - \lambda_{\text{vib}} \frac{\partial T_{\text{vib}}}{\partial x} + \sum_s^{ns} J_{x,s} H_s \dots (19)$$

$$q_y = -\lambda_{\text{tr}} \frac{\partial T_{\text{tr}}}{\partial y} - \lambda_{\text{rot}} \frac{\partial T_{\text{tr}}}{\partial y} - \lambda_{\text{vib}} \frac{\partial T_{\text{vib}}}{\partial y} + \sum_s^{ns} J_{y,s} H_s \dots (20)$$

In the above equations, H_s is the enthalpy of the species s , and λ_{tr} , λ_{rot} and λ_{vib} are, respectively, thermal conductivities for translation, rotation and vibration. $J_{x,s}$ and $J_{y,s}$ are the diffusive mass-fluxes of the species s .

$$J_{x,s} = -\rho D_{sm} \frac{\partial Y_s}{\partial x} \dots (21)$$

$$J_{y,s} = -\rho D_{sm} \frac{\partial Y_s}{\partial y} \dots (22)$$

where D_{sm} is the effective diffusion coefficient of the species s , Y_s is the mass fraction of the species s .

In Eq. (12), $q_{\text{vib},x}$ and $q_{\text{vib},y}$ are the vibrational heat fluxes expressed by

$$q_{\text{vib},x} = -\lambda_{\text{vib}} \frac{\partial T_{\text{vib}}}{\partial x} + \sum_{s=M} J_{x,s} E_{\text{vib},s} \dots\dots\dots(23)$$

$$q_{\text{vib},y} = -\lambda_{\text{vib}} \frac{\partial T_{\text{vib}}}{\partial y} + \sum_{s=M} J_{y,s} E_{\text{vib},s} \dots\dots\dots(24)$$

where $E_{\text{vib},s}$ is the vibrational energy of the species s , and $\sum_{s=M}$ means the summation over molecular species. $Q_{\text{T-V}}$ is the energy transfer rate between translational and vibrational energy modes and $\dot{q}_{\text{vib}}$ denotes the production of vibrational energy due to chemical reactions. The expressions for $Q_{\text{T-V}}$ and $\dot{q}_{\text{vib}}$ are given later.

5.2. Boundary Conditions

Chemical reactions at the surface are assumed to be steady. Let k_s be the rate constant of surface reaction, and then we have

$$k_s Y_{s,w} = -\mathfrak{D}_{sm,w} \left(\frac{\partial Y_s}{\partial x} \right)_w \dots\dots\dots(25)$$

The rate constant of surface reaction k_s is given by

$$k_s = \alpha_s \sqrt{\frac{R_s T_w}{2\pi}} \dots\dots\dots(26)$$

where R_s is the gas constant of the species s and T_w is the surface temperature. α_s is the probability for surface reaction, which must satisfy the following condition:

$$0 \leq \alpha_s \leq 1 \quad \text{or} \quad \sum_r \alpha_{s,r} + \alpha_{\text{elastic}} = 1 \dots\dots\dots(27)$$

In the above equation, $\alpha_{s,r}$ is the probability for the reaction r of the species s , and α_{elastic} is the probability for elastic collision of the gas. However, $\alpha_{s,r}$ is still unknown, so that numerical calculations used Park *et al.*'s ablation model.⁽⁸⁾ In addition, the calculations for α_{elastic} were also conducted.

Park *et al.*'s ablation model gave the following relations⁽⁹⁾:

$$\alpha_{\text{O}_2} = \frac{1.43 \times 10^{-3} + 0.01 \exp(-1450/T_w)}{1 + 2 \times 10^{-4} \exp(13000/T_w)} \dots\dots\dots(28)$$

$$\alpha_{\text{O}} = 0.63 \exp(-1160/T_w)$$

Boundary conditions for pressure and velocities at surface are given by

$$\left(\frac{\partial p}{\partial x} \right)_w = -u_w \left(\frac{\partial \rho u}{\partial x} \right)_w \dots\dots\dots(29)$$

$$u_w = \left(1 - \frac{M_{\text{O}} + M_{\text{CO}}}{M_{\text{O}_2}} \right) k_{\text{O}_2} Y_{\text{O}_2} + \left(1 - \frac{M_{\text{CO}}}{M_{\text{O}}} \right) k_{\text{O}} Y_{\text{O}} \dots\dots\dots(30)$$

$$v_w = 0$$

where M_s is the molecular weight of the species s .

5.3. Energy Exchange

The energy transfer considered here is translation–vibration. The translation–vibration energy transfer rate is written in the following well-known form⁽¹⁴⁾:

$$Q_{\text{T-V}} = \sum_{s=M} \rho_s \frac{E_{\text{vib},s}^{\text{eq}}(T_{\text{tr}}) - E_{\text{vib},s}(T_{\text{vib}})}{\tau_{\text{v},s}} \dots\dots\dots(31)$$

where $E_{\text{vib},s}^{\text{eq}}(T_{\text{tr}})$ is the vibrational energy per unit mass at equilibrium, and $E_{\text{vib},s}(T_{\text{vib}})$ is the vibrational energy per unit mass, given by

$$E_{\text{vib},s}^{\text{eq}}(T_{\text{tr}}) = \frac{R_s \Theta_{\text{vib},s}}{\exp(\Theta_{\text{vib},s}/T_{\text{tr}}) - 1} \dots\dots\dots(32)$$

$$E_{\text{vib},s}(T_{\text{vib}}) = \frac{R_s \Theta_{\text{vib},s}}{\exp(\Theta_{\text{vib},s}/T_{\text{vib}}) - 1} \dots\dots\dots(33)$$

where $\Theta_{\text{vib},s}$ is the characteristic temperature of the species s for vibration. $\tau_{\text{v},s}$ is the vibrational relaxation time⁽¹⁵⁾ expressed by

$$\tau_{\text{v},s} = \frac{\sum_r^{ns} Z_r}{\sum_r^{ns} Z_r / \tau_{\text{v},s-r}} \dots\dots\dots(34)$$

Z_r is the molar weight of the species r , and $\tau_{\text{v},s-r}$ is the vibrational relaxation time of Millikan and White⁽¹⁶⁾ for the $s-r$ encounter given by

$$\ln(p \tau_{\text{v},s-r}) = c \mu_{sr}^{1/2} \Theta_{\text{vib},s}^{4/3} (T_{\text{tr}}^{-1/3} - 0.015 \mu_{sr}^{1/4}) - 18.42 \dots\dots\dots(35)$$

where

$$\begin{cases} c = 1.01 \times 10^{-3} & (\text{for } s = \text{O}_2) \\ c = 1.05 \times 10^{-3} & (\text{for } s = \text{CO}) \end{cases}$$

The relaxation time for CO_2 was taken from Camac⁽¹⁷⁾ and modified to a multi-component system in this work as follows:

$$p \tau_{\text{v},\text{CO}_2-r} = \exp[36.5(T_{\text{tr}}^{-1/3} - 0.015 \mu_{\text{CO}_2,r}^{1/4}) - 2.714] \times 10^{-6} \dots\dots\dots(36)$$

μ_{sr} appearing in Eq. (35) is the reduced mass given by

$$\mu_{sr} = \frac{10^3 M_s M_r}{M_s + M_r} \dots\dots\dots(37)$$

The vibrational energy loss owing to dissociation and recombination $\dot{q}_{\text{vib}}$ was calculated by

$$\dot{q}_{\text{vib}} = \sum \dot{w}_s E_{\text{vib},s} \dots\dots\dots(38)$$

5.4. Method of Numerical Analysis

A set of governing equations are numerically solved using the second order upwind TVD scheme of the Harten–Yee type^(18,19) for the convection terms and the second order central difference for viscous, heat-conductive and diffusive terms. Calculations were done for the right half region of the jet ($x/D=3$; initial condition and $y/D=8$), composed of upper boundary (orifice and ambient), right boundary (outflow boundary), left boundary (jet axis) and lower boundary (liquid surface boundary) (see Fig. 1). The grid locations in x -direction are remapped depending upon the cavity geometry. At the nozzle exit, sonic conditions are

imposed and a parallel flow is assumed, so that $v=0$. The sonic conditions were calculated from the specified reservoir conditions given in Table 1. Ambient conditions are given by $u=v=0$, $T_{tr}=T_{vib}=300$ K and $p=5.0 \times 10^2$ Pa (see Table 1). Ambient species conditions are shown in Table 1. On the axis, axisymmetric conditions are employed.

Fig. 4. Flow patterns of O_2 -jet.

Fig. 5. Contours of O_2 and CO mass fractions for Park *et al.*'s ablation model.

6. Results and Discussion

6.1. Flow Pattern of a Supersonic Jet

In Fig. 4 are shown contours of Mach number, axial velocity u and radial velocity v . The jet structure is characterized by Mach disc, jet boundary and barrel shock. After exhausting from the nozzle exit, the O_2 gas expands to the ambient pressure. Axial velocity u decreases abruptly behind the Mach disc, and impinges onto the liquid iron. After impinging on the liquid iron, the gas flows to the radial direction. As shown in Fig. 4, at the lip of the cavity, the gas jumps toward the upper direction.

6.2. Species Mass Fractions for Park *et al.*'s Ablation Model

Figure 5 illustrates mass fraction contours of O_2 and CO which were obtained by using Park *et al.*'s ablation model.^{8,9)} The radial profiles of species mass fractions on the surface are shown in Fig. 6. The mass fraction of C is not illustrated in this figure because of very small mass fraction (10^{-20}). It can be seen that dominant species in the vicinity of the center is O_2 . However, in the region of

Fig. 6. Radial profiles of species mass fractions on liquid surface for Park *et al.*'s ablation model.

Fig. 7. Contours of O_2 and CO mass fractions for $\alpha_s = 1$.

$y > 0.03$ m, the mass fraction of O_2 decreases, while the mass fraction of CO increases. At $y > 0.07$ m, the mass fraction of CO becomes larger than that of O_2 . The lip of the cavity is located around $y = 0.03$ m, so that it may be mentioned that surface reactions are significant outside the cavity in the present conditions. According to Park *et al.*'s ablation model, the reaction probabilities at the surface temperature of 1840 K are approximately 0.5% for O_2 and 34% for O. Such low probability for O_2 is considered to make surface reactions inactive. It is seen from the figure that the mass fraction of CO_2 is in the orders of 10^{-5} – 10^{-4} . Hence, CO_2 can be neglected.

6.3. Species Mass Fractions for $\alpha_s = 1$

In the second stage, calculations for the reaction probability of unity were performed to examine the effect of the reaction probability on species mass fractions in the gas phase. Figure 7 shows mass fraction contours obtained by taking the probability for surface reaction to be unity, namely $\alpha_s = 1$. In contrast to the result shown in Fig. 5, CO mass fraction is higher just on the cavity surface and O_2 mass fraction almost vanishes at the peripheral zone of the cavity on the liquid surface.

In Fig. 8, on-axis mass fractions are shown for both cases of thermal non-equilibrium ($T_{tr} \neq T_{vib}$) and thermal equilibrium ($T_{tr} = T_{vib}$). In the figure, "Non-Eq" and "Eq" mean, respectively, thermal non-equilibrium and thermal equilibrium. The result for C is also not shown in the figure because of very small mass fraction. The comparison of the results for thermal non-equilibrium and equilibrium shows no significant difference in relation to the on-axis mass fractions. Computed on-axis translational and vibrational temperatures show that these two temperatures are almost equal downstream of the Mach disc ($x \approx 0.023$ m), so that the rate constants of the reactions 1 to 3 in Table 2, which is governed by $\sqrt{T_{tr} T_{vib}}$, give almost equal value for both of thermal equilibrium and non-equilibrium. In the range from the nozzle exit ($x = 0$) to $x = 0.035$ m, the mass fraction of O_2 does not alter, which leads to no reactions there. However, the mass fraction of O_2 very rapidly decreases near the surface, while those of CO and O increase there. This is caused by very active surface reactions. Generated CO and O diffuse away from the surface.

Fig. 8. On-axis species mass fractions for $\alpha_s = 1$.

Figure 9 shows the mass fractions on the surface for both cases of thermal non-equilibrium and equilibrium. The most dominant species is CO, having the mass fraction close to unity. There is no difference between the results for both cases except for CO_2 .

In the vicinity of the center, the mass fraction of CO_2 shows almost the same value for thermal non-equilibrium and equilibrium but CO_2 mass fraction for thermal non-equilibrium is a little less than that for thermal equilibrium at $y > 0.02$ m. This can be explained as follows: CO is generated by the surface reactions in Table 3. Thus generated CO produces CO_2 according to the reaction of $r = 2$ shown in Table 2, so that CO and CO_2 mass fractions are determined by the forward and backward reactions. Its reaction temperature for thermal non-equilibrium is slightly lower than that for equilibrium. This temperature difference seems to cause the difference of CO_2 mass fraction along the surface downstream of $y = 0.02$ m.

6.4. Mass Transfer due to Surface Reactions

Mass flux of carbon from the surface of the liquid iron is shown in Fig. 10. As shown in this figure, decarbonization of the liquid iron mainly occurred inside the cavity where O_2 jet impinges. The mass flux of C simulated by use of

Fig. 9. Radial profiles of species mass fractions on liquid surface for $\alpha_s = 1$.

Fig. 10. Mass flux of carbon from liquid iron surface.

 Fig. 11. Radial profiles of u on cavity surface.

 Fig. 12. Radial profiles of stresses on surface for $\alpha_s = 1$.

Park *et al.*'s ablation model is smaller than that simulated by use of $\alpha_s = 1$.

Radial profiles of u on the surface are depicted in Fig. 11, where the curve for $u=0$ is shown as "without reactions" for reference. As regards the results for $\alpha_s = 1$, thermal nonequilibrium and equilibrium provide similar results. The sign of u is negative, which means a net mass release from the surface. O_2 , which reaches the surface, reacts with C and then $2CO$ is released from the surface. Therefore, it follows that the net mass leaves the surface. This is the reason why the sign of u is negative. When Park *et al.*'s ablation model is used, u is very small, because the reaction probability is so small as afore-mentioned.

6.5. Stresses Acting on Liquid Surface

Radial profiles of pressure, shear stress and surface tension on the surface are shown in Fig. 12. It can be understood that the surface tension acts against pressure. The shear stress is active only at $y \approx 0.03$ m where the cavity lip is located. The sum of stresses balances with the buoyancy of liquid iron, which leads to forming a cavity. Surface stresses obtained for no surface reactions are shown in Fig.

Fig. 13. Radial profiles of stresses on surface without surface reaction.

Fig. 14. Cavity geometries.

13 for comparison with Fig. 12. It can be seen from the comparison of these two figures that pressure at $y \approx 0.025$ is less in the case with surface reactions than in the case without them. Correspondingly, the surface tension there is also increased in the case with surface reactions. However, a significant difference of the sum of stresses cannot be found between the results with and without surface reactions.

6.6. Cavity Geometry

A comparison of cavity geometries with surface reactions for thermal non-equilibrium and equilibrium is shown in Fig. 14. A difference between both results cannot be identified. The cavity geometry without surface reactions is also illustrated in Fig. 14, from which it can be seen that the effect of the surface reactions on the cavity geometry is very small.

Cavity geometries had been already investigated for the converter in order to clarify the reaction site of O_2 jet. In the atmospheric pressure, the non-dimensional equation for the calculation of cavity depth (h) are proposed as follows,^{20,21)}

$$h/D^* = C \cdot \{MV/(\rho_1 \cdot g \cdot D^3)\}^m \cdot \{L/D\}^n \dots \dots \dots (39)$$

where, L is the distance between the liquid level and the nozzle tip, h is the cavity depth, MV is the momentum of a jet and D is the diameter of the nozzle throat. In the equation, C , m and n are the constants determined from experimental data as $C=0.81$, $m=0.56$, $n=-0.18$ for $L/D<28$ and $C=2.71$, $m=0.56$, $n=-0.54$ for $L/D>28$, respectively. According to Eq. (39), $h/D=8$ has been obtained for the present condition, $L/D=3$. However, this value is larger than the present result of $h/D=0.8$. The reason for this discrepancy is that the present ambient pressure is very low compared with the previous experimental conditions.²⁰⁾ There are no experimental works under such low pressure conditions (10–100 torr) as used in the present computations. Therefore, measurements of the cavity depth at low pressures are needed to confirm the simulated results.

7. Concluding Remarks

The system of governing equations applicable to a supersonic O_2 -jet impingement on high-temperature liquid metal with surface chemistry was developed. In order to numerically reproduce the exact flowfield of the jet impingement, a high-temperature gas effects, namely vibrational energy excitation and gas phase chemistry, were included in the analysis. Moreover, a two-temperature model composed of translational-rotational and vibrational temperatures was used to express thermal nonequilibrium. Nevertheless, the effect of thermal nonequilibrium on species mass fraction could not found except for CO_2 . The effect of thermal nonequilibrium on cavity geometry could not be identified, either.

Two models for the probability of the surface reaction were employed, *i.e.*, Park *et al.*'s ablation model and the probability of unity. The former model provided very slight surface reactions, but when the latter model was used, the most dominant species on the surface was CO. However, it was seen that the surface reactions are active outside the cavity in both models. The sensitivity of the cavity geometry to surface reactions was appreciable in the present calculation model.

Nonmeclature

$A_{b,r}$, $B_{b,r}$, $C_{b,r}$:	Constants for backward reaction r
$A_{f,r}$, $B_{f,r}$, $C_{f,r}$:	Constants for forward reaction r
D :	Throat diameter
D_{sm} :	Effective diffusion coefficient of species s
e :	Total energy per unit volume
e_{tr-rot} :	Internal energy for translation–rotation per unit volume
e_{vib} :	Internal energy for vibration per unit volume
$E_{vib,s}$:	Vibrational energy of species s per unit mass
$E_{vib,s}^{eq}$:	Vibrational energy of species s per unit mass at equilibrium
g :	Gravitational acceleration
$J_{x,s}$, $J_{y,s}$:	Diffusive mass-fluxes of species s
h :	Depth of cavity
H_s :	Enthalpy of species s
$k_{f,r}$:	Rate constant for forward reaction r
$k_{b,r}$:	Rate constant for backward reaction r

k_s :	Rate constant of surface reaction
L :	Distance between liquid level and nozzle tip
M_s :	Molecular weight of species s
MV :	Momentum of jet
p :	Pressure of gas phase
p_f :	Ambient pressure
p_w :	Pressure at surface of liquid iron
q_x , q_y :	Heat fluxes in x - and y -direction
$q_{vib,x}$, $q_{vib,y}$:	Vibrational heat fluxes in x - and y -direction
Q_{T-v} :	Energy transfer rate between translational and vibrational energy modes
$\dot{q}_{vib}$:	Production rate of vibrational energy due to chemical reaction
R_s :	Gas constant of species s
T_f :	Temperature for forward reaction
T_b :	Temperature for backward reaction
T_{tr} :	Translational–rotational temperature
T_{vib} :	Vibrational temperature
T_w :	Temperature of liquid iron
u , v :	Gas velocity in x - and y -direction
$\dot{w}_s$:	Mass production rate of species s
x , X :	Coordinates of axial direction
y , Y :	Coordinates of radial direction
Y_s :	Mass fraction of species s
Z_r :	Molar weight of species r
α :	Angle of cavity surface
$\alpha_{elastic}$:	Probability for elastic collision of gas
α_s :	Probability for surface reaction
$\alpha_{s,r}$:	Probability for reaction r of species s
$\Theta_{vib,s}$:	Characteristic temperature of species s for vibration
λ_{tr} , λ_{rot} , λ_{vib} :	Thermal conductivities for translation, rotation and vibration
μ :	Viscosity
μ_{sr} :	Reduced mass of species s and r
ρ :	Density of gas phase
ρ_l :	Density of liquid iron
ρ_s :	Density of species s
ρ_w :	Density of gas at surface of liquid iron
τ :	Shear stress
τ_{ij} :	Viscous stress tensor
$\tau_{v,s}$:	Vibrational relaxation time of species s
$\tau_{v,s-r}$:	Vibrational relaxation time of Millikan and White for species s – r encounter

Subscripts

f, b:	Forward and backward reactions
r :	Reaction r
w:	Surface of liquid iron

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