Modelling the Reduction of an Iron Ore-Coal Composite Pellet with Conduction and Convection in an Axisymmetric Temperature Field

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Abstract—A mathematical model of the coal-based direct reduction process of iron ore in a pellet composed of coal and iron ore mixture is investigated using a finite-control volume method. Heat transfer by conduction in the solid, convection by gaseous media inside, and radiation from the surroundings of the pellet are included in the model. The pellet is assumed to be spherical initially and the temperature around the pellet is taken to be symmetric about an axis passing through the centre. The parameters of the process, such as thermal conductivity, specific heats, and heats of the reaction, are all temperature dependent. The shrinkage/swelling of the pellet is also considered. We find that the effect of convection on the temperature and on the overall average reduction is small. However, the effect on the local concentration of the reaction components is significant. We predict that a uniform surrounding temperature field around the pellet yields a better average reduction.

Keywords—Control volume, Iron ore direct reduction, Composite pellet, Axisymmetric heat transfer.

1. INTRODUCTION

Some coal-based iron ore direct reduction processes are based on formation of composite pellets which consist of a mixture of fines of iron-bearing oxide, carbonaceous material, for example, coal, coke, or char and a small amount of binder. Then, the pellets are placed on a rotary hearth and the iron ore is reduced to iron by chemical reactions. The nonuniformity of heating, heterogeneous...
reactions, the devolatilization of coal, and change in the pellet size make the reduction process very complicated.

There is considerable research on the mathematical modelling of direct iron ore reduction process (see, for example, [1-3]). Some papers describe models where the mixture of the fines of coal and iron ore are placed directly into a crucible and then heated at one end (see [1]). This results in one-dimensional mathematical models. Some papers assume that the rate of reduction in a pellet is governed by heat transfer by conduction only, and neglect the effect of convection due to gas flow in the pellet (see [2,3]). The equations describing these models are solved using finite-difference schemes.

In this paper, we develop a finite-control volume technique for solving the governing equations modelling the iron ore direct reduction process in a single pellet including both conduction and convection. The pellet is assumed to be spherical initially and the temperature surrounding it is taken to be axially symmetric about an axis, which we take to be vertical, passing through the centre. The properties of the mixture, such as the thermal conductivity, are all temperature dependent. The swelling and shrinkage of the pellet is also considered. A heat radiation condition is used on the surface of the pellet.

2. CHEMICAL REACTIONS

Assume that the iron ore contains haematite and magnetite and the coal contains carbon and volatile matter initially. The volatile matter evolves and releases carbon monoxide and carbon dioxide. The major chemical reactions in the pellet are now outlined. Part of the released carbon monoxide reacts with the haematite to produce magnetite and carbon dioxide,

\[ 3 \text{Fe}_2\text{O}_3 + \text{CO} \rightarrow 2\text{Fe}_3\text{O}_4 + \text{CO}_2. \]  

Part of the CO reacts with the magnetite to produce wustite and carbon dioxide,

\[ \text{Fe}_3\text{O}_4 + \text{CO} \rightarrow 3\text{FeO} + \text{CO}_2. \]

Part of the CO reacts with the newly produced wustite to produce metallic iron and carbon dioxide,

\[ \text{FeO} + \text{CO} \rightarrow \text{Fe} + \text{CO}_2. \]

Part of the carbon dioxide, released from both the volatile and the chemical reactions with the iron ore, reacts with carbon in the coal to produce more carbon monoxide via the Boudouard reaction,

\[ C + \text{CO}_2 \rightarrow 2\text{CO}. \]

The carbon monoxide so produced, in turn reacts with the iron oxides and produces more carbon dioxide. The gas, in excess to that required for the reactions, flows to the outside of the pellet. The volatile matter will be released completely after some time and then the reduction reactions depend on the supply of carbon monoxide from the Boudouard reaction (4). It is assumed that there is enough carbon to complete the reduction process.

3. MATHEMATICAL MODEL

We assume that the properties of the material within the pellet are initially uniform. The properties at each point depend on several parameters and the temperature is one of these. They become nonuniform after the reduction process starts since the temperature varies with time and becomes nonuniform. The pellet is assumed to be a sphere with radius \( r = r_0 \) initially. We also assume that the conditions on the surface are such that the internal fields are symmetric about a line passing through the centre of the sphere. Thus, this is an axially symmetric problem and
it is enough to consider the fields in half of the cross-section that passes through the symmetry line, as shown in Figure 1.

The pellet is porous with uniform initial porosity. As the reactions proceed, gases are released and flow through the pellet. Heat transfer inside the pellet is not only by conduction but also by convection. The porosity, $\omega$, varies from point to point during the reduction process since reactions are not uniform in the pellet. For simplicity, we do not distinguish the individual gas species but treat the gas phase as a mixture of all gas species. It is also assumed that the temperatures of the gas mixture and the solid phase are the same. With these assumptions, the governing equation for heat transfer in the spherical pellet with spherical coordinate system can be written as (see [4] for one-dimensional equation in rectangular coordinate system),

\[
\frac{(\rho C)_m}{\partial t} \frac{\partial T}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( k r^2 \frac{\partial T}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( k \sin \theta \frac{\partial T}{\partial \theta} \right) 
\]

\[
- \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \rho_f c_f V_r T \right) - \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( r \sin \theta \rho_f c_f V_\theta T \right) - \sum H_i,
\]

where $(\rho C)_m$ and $k$ are the sum of local heat capacities of the components of the mixture compound and thermal conductivity in the pellet, respectively. $T = T(t, r, \theta)$ is the temperature at the point $(r, \theta)$ and at the time $t$. $\rho_f$ and $c_f$ are the density and specific heat of the gas mixture, respectively. $V_r$ and $V_\theta$ are the radial and circumferential velocity components of the gas mixture averaged over the pellet volume element. $\sum H_i$ is the sum of rates of heat consumption per unit pellet volume associated with reactions in the reduction process of the iron ore in the pellet.

The gas conservation of mass equation is given by

\[
\frac{\partial}{\partial t} (\omega \rho_f) = - \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \rho_f V_r \right) - \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( r \sin \theta \rho_f V_\theta \right) + G.
\]

Here, $G$ is the production/consumption rate of gas mixture per unit volume of pellet in the reduction reactions. It is noted that there is no diffusion term in this equation since we treat the gas mixture as one type of fluid.
There are several approaches to describing the conservation of momentum of the gas mixture in porous media. The conservation of momentum comprises two component equations for the axisymmetric problem. For example, Zhang et al. [5] used the full Navier-Stoke equations to model the conservation of momentum of fluid in a spherically symmetric porous medium and Nguyen et al. [6] employed a set of approximate equations which involve both temporal and spatial variations of velocity, spatial variation of pressure as well as coupling with the temperature. These equations provide a more accurate description, but the computing times are also very much longer. In this paper, we use Ergun’s approximation for the momentum balance (see [7] for the equation in a rectangular coordinate system). These equations are written as

\[ B_1 V_r + B_2 V_r \sqrt{V_r^2 + V_\theta^2} = -\frac{\partial P}{\partial r}, \]

\[ B_1 V_\theta + B_2 V_\theta \sqrt{V_r^2 + V_\theta^2} = -\frac{1}{r} \frac{\partial P}{\partial \theta}, \]

with

\[ B_1 = 150 \frac{\mu \lambda^2 (1 - \omega^2)}{D_p^2 \omega^3}, \quad B_2 = 1.75 \frac{\rho_f \lambda (1 - \omega)}{D_p \omega^3}, \]

\( \mu \) being the viscosity of the gas mixture, \( \lambda \) being the shape factor taken to be 1.75, \( D_p \) being the mean diameter of the coal and iron ore particles assumed to be spherical. Here, \( P \) is the pressure of the gas mixture.

The temperature, pressure, and density of gas mixture are related by the perfect gas law,

\[ \frac{P}{V} = \frac{M_g P}{RT}, \]

with \( M_g \) being the molar mass of gas mixture and \( R \) being the absolute gas constant.

The rate of generation/loss of heat in the system is given by

\[ \frac{\partial H_i}{\partial t} = \hat{H}_H(T) + \hat{H}_M(T) + \hat{H}_W(T) + \hat{H}_C(T), \]

where \( \hat{H}_H(T), \hat{H}_M(T), \hat{H}_W(T), \) and \( \hat{H}_C(T) \) are the heats associated with reaction of one weight unit (kg) of the corresponding substance at the given temperature \( T \). The expressions of \( \hat{H}_i(T) \) for the reactions (1)–(4) are reported in papers by Donskoi and McElwain [3,8]. The quantities \( \hat{H}_H, \hat{H}_M, \hat{H}_W, \) and \( \hat{H}_C \) are the rates of the transformation from haematite to magnetite, magnetite to wustite, wustite to iron, and carbon to carbon monoxide at temperature \( T \), respectively. Donskoi and McElwain [9] report the expressions for these rates (also see equations later).

At early stage of the process, the generation of gases comes from two sources: devolatilization of coal volatile matter and the reactions. It can be seen that the reduction reactions (1)–(3) do not change the overall concentration of gas mixture since each reaction consumes one mole of carbon monoxide and produces one mole of carbon dioxide. The Boudouard reaction produces one extra mole of gas (carbon monoxide) while consuming one mole of carbon. Later, when the volatile matter has completely evolved, the Boudouard reaction is the only source for gas (carbon monoxide). The rate of production/consumption of gas mixture (mass per unit time per unit volume) can therefore be written as

\[ G = \frac{dV_v}{dt} + M_g \hat{H}_C, \]

where \( V_v \) measures the mass of volatile matter per unit current volume already released from the coal char up to time \( t \) and \( M_g \) is molar mass of the gas mixture which is taken to be the mean value of those of carbon monoxide and carbon dioxide (= 0.036 kg/mole). The rate of devolatilization is modelled as an \( n \)-th-order reaction, (see [3]),

\[ \frac{dV_v}{dt} = k_v \exp \left( -\frac{E_{\text{act}}}{RT} \right) \left[ V_v^* - V_v \right]^n, \]
where $V_v^*$ is the value of $V_v$ as $t \to \infty$; $k_v$ and $E_{av}$ are the apparent frequency factor and the apparent activation energy of the devolatilization process, and $n$ is the order of the reaction. The parameters $n$, $k_v$, and $E_{av}$ depend on the rate of heating ($\frac{dT}{dt}$) as adopted in [3].

The rates of change of concentration of haematite (H), magnetite (M), wustite (W), and iron (F) are given by

$$\frac{dH}{dt} = -\dot{R}_H,$$

$$\frac{dM}{dt} = x\dot{R}_H - \dot{R}_M,$$

$$\frac{dW}{dt} = y\dot{R}_M - \dot{R}_W,$$

$$\frac{dF}{dt} = z\dot{R}_W,$$

where

$$\dot{R}_H = Hk_H \exp\left(-\frac{E_H}{RT}\right),$$

$$\dot{R}_M = Mk_M \exp\left(-\frac{E_M}{RT}\right),$$

$$\dot{R}_W = Wk_W \exp\left(-\frac{E_W}{RT}\right),$$

are the rates of transformation from haematite to magnetite, magnetite to wustite, wustite to iron in consecutive reactions (1), (2), (3), respectively. H, M, W, and F are the concentrations of haematite, magnetite, wustite, and iron. The weight coefficients ($x$, $y$, and $z$), the apparent frequency factors ($k_H$, $k_M$, and $k_W$), and the apparent activation energies ($E_H$, $E_M$, and $E_W$) are all constant. The rate of the carbon consumption is given by

$$\frac{dC}{dt} = -\dot{R}_C = -Q_H\dot{R}_H - Q_M\dot{R}_M - Q_W\dot{R}_W,$$

where $Q_H$, $Q_M$, and $Q_W$ are coefficients depending on weight relationships and equilibrium conditions for the corresponding reaction.

The local change of volume consists of two competing processes, swelling and shrinkage. The rate of change of volume is expressed as (see [3,8]),

$$\frac{dV}{dt} = V(S_w - S_h).$$

The shrinkage term $S_h$ is modelled as

$$S_h = 0.012\omega^2 \exp\left(-\frac{4372}{T}\right),$$

where, as discussed above, $\omega$ is the porosity of the pellet. The swelling term $S_w$ is modelled as

$$S_w = 2.9 \times 10^{-7}\frac{WF}{\sigma} \exp\left(-\frac{(T - T_0)^2}{2\sigma^2}\right),$$

where $W$ and $F$ are concentrations of wustite and iron. The swelling term has Gaussian dependence on temperature with a mean temperature, $T_0$ of 1193° K and a standard deviation, $\sigma$, of 60° K. The local change of volume results in the overall change of the pellet size.

The properties of the pellet vary with time and it is necessary to update the properties at each time step of the calculation. We adopt the routines used in [8,9] to calculate the properties.

The surface of the pellet is irradiated from the surroundings. This condition can be written as

$$k \frac{\partial T}{\partial r} = \sigma_s \varepsilon (T_{\text{surf}}^4 - T^4),$$

where
where $T_{surr}$ is the temperature of the surrounding medium and a particular form is adopted in this work, namely, $T_{surr} = 0.5(T_{max} + T_{min}) + 0.5(T_{max} - T_{min}) \cos \theta$, with $T_{max}$ and $T_{min}$ ($T_{max} > T_{min}$) being temperatures at $\theta = 0$ and $\theta = \pi$ respectively, $a_s = 5.67 \times 10^{-8}$W/m$^2$K$^4$ is the Stefan-Boltzmann constant, and $\epsilon$ is the emissivity/absorptivity of the pellet surface taken to be 0.8.

We assume that the pressure on the surface of the pellet is uniform, independent of time and equal to the atmospheric pressure,

$$P = P_{atm}. \quad (22)$$

For the numerical calculation, in addition to those parameters that have been specified, we use the following. The viscosity and specific heat of gas mixture depend on the temperature according to

$$\mu = \left( -12.2187 + 1.6544 \sqrt{T} \right) \times 10^{-6} \text{N/m s},$$

$$c_f = 23.400 + 36.351 \times 10^{-3} T - 20.123 \times 10^{-6} T^2 + 4.175 \times 10^{-9} T^3 \text{J/mol K}.$$ 

These correspond to the mean values of carbon monoxide and carbon dioxide. The expression for the viscosity is obtained from data given in [10] and the specific heats are reported in [8].

4. CONTROL VOLUME SCHEME DISCRETISATION

We employ a control volume method to discretise the problem and follow the technique used in Patankar [11]. The method was used and compared with finite-difference schemes in [12,13] for the analysis of direct reduction of iron ore by heat conduction only. Assume that half of the circular section is meshed by $N$ circumferential circular curves, $r = r_i$ ($0 = r_1 < r_2, \ldots, r_{j-1} < r_j < r_{j+1}, \ldots, r_N = r_N$) and $M$ radially straight lines, $\theta = \theta_j$ ($0 = \theta_1 < \theta_2, \ldots, \theta_{j-1} < \theta_j < \theta_{j+1}, \ldots, \theta_M = \pi$). The distances between the circumferential curves and the angles between the radial straight lines need not necessarily be the same for the method, but we use equidistant and equiangular meshes in this paper. The values of the dependent variables, except for the velocity components, are calculated at the nodes which are the intersection points of the circumferential curves and the radial straight lines. The velocity components are calculated at the midpoints between the nodes.

Let the $i^{th}$ circumferential circular curve and the $j^{th}$ radial straight line intersect at node $P$. For an interior node, $P$, it has neighbouring nodes denoted by $E$, $W$, $N$, and $S$. The control volume (area) associated with the node $P$ is the shaded area in Figure 1 and it has four faces: east face (e), west face (w), south face (s), and north face (n). The meshing circular curves and straight lines intersect the faces at the points e, w, s, and n, respectively, as shown in Figure 1. Although the positions and orientation of the faces are arbitrary, in this paper, we let the faces bisect the distances between the node $P$ and its neighbouring nodes (see Figure 1).

Following Patankar [11], we linearize the heat production/consumption term $-\sum H_i$ in the heat equation (5) in the form of $S_C + S_P T$. Here, $S_C$ and $S_P$ may depend on the temperature $T$. If so, they are approximated by being evaluated using the temperature at the previous (not present) time step, or at the previous iteration if an iterative scheme is used.

The governing equations (5) and (6) are singular at the origin and on the symmetry lines $\theta = 0$ and $\theta = \pi$. In order to eliminate the singularities, we multiply the equations by $r^2 \sin \theta$. Now, we integrate the resulting equations with respect to $r$ and $\theta$ over the control volume around node $P$, from the west face (w) to the east face (e) in radial direction and from the south face (s) to the north face (n) in the circumferential direction, and approximate the time derivatives on the left-hand side of the equations by a forward finite difference. For the heat transfer equation, (5), with Patankar’s [11] notation, we get the following equation,

$$a_r T_P = a_e T_E + a_w T_W + a_N T_N + a_s T_S + b. \quad (23)$$
Integration of the balance equation of mass of gas mixture over the control volume (shown in Figure 1) can be converted into a discretized equation for pressure. To this end, following the same procedure as for the equations of heat transfer, we multiply by $r^2 \sin \theta$ and integrate the conservation equations of the momentum of the gas mixture, (7) and (8), over the control volume.
volumes shown in Figure 2a and 2b, respectively, and obtain

\[
(V_r)_e = -\Phi_e (P_E - P_P), \quad (V_\theta)_n = -\Phi_n (P_N - P_P), \tag{24}
\]

with

\[
\Phi_e = \frac{3}{2} \frac{r_E^2 + r_P^2}{r_E^2 - r_P^2} \frac{1}{B_1 e + B_2 e \sqrt{r_E^2 + r_P^2}},
\]
\[
\Phi_n = \frac{3}{4} \frac{r_E^2 - r_P^2}{r_E^2 - r_P^2} \sin \theta_N \sin \theta_P \frac{1}{\cos \theta_P - \cos \theta_N B_1 n + B_2 n \sqrt{r_N^2 + r_P^2}}.
\]

It is noted that the velocity components are not calculated at the nodes where the temperature and pressure are calculated. Substituting the perfect gas law (9), the expressions for velocity (24) and the similar expressions for \((V_r)_w\) and \((V_\theta)_s\) from the neighbouring control volumes into the resulting integration equation of the mass balance of the gas mixture, and manipulating the resulting equation, we derive an equation for pressure \(P_P\), namely,

\[
\bar{a}_P P_P = \bar{a}_E P_E + \bar{a}_W P_W + \bar{a}_N P_N + \bar{a}_S P_S + b. \tag{25}
\]

The equations (23)-(25) are applicable at the interior nodes. For the nodes on the surface, we use the control volumes shown in Figures 1 and 2 with the pellet surface as the east face and node \(P\) as the point \(e\), i.e., \(r_e = r_P\). The pressure at the surface nodes are specified as the atmosphere pressure, so we have condition for pressure,

\[
P_P = P_{\text{atm}} = 1.01325 \times 10^5 \text{N/m}^2.
\]

The radial velocity component on the surface is determined by extrapolation from the values near the surface. Since the pressure on the surface is uniform, the tangential velocity component is zero on the surface. For the temperature on the surface, integrating the governing equation (5) over the control volume as shown in Figure 1 on surface and applying condition (21) to the term involving \(\partial T / \partial r\), similar equation to (23) is obtained with \(a_x = 0\) and \(b\) having extra term,

\[
2 \frac{r_E}{r_E + r_W} C_\theta \Delta t a_x e (T_{\text{surr}}^4 - T_P^4). \tag{26}
\]

On the symmetry line \(\theta = \pi\), we use the control volumes shown in Figures 1 and 2 with the symmetry line as the “north” face and node \(P\) as the point \(n\), i.e., \(\theta_n = \theta_P\) and \(r_n = r_P\). Integrating the governing equation (5) for the temperature over the control volume and applying the symmetry conditions \(\partial T / \partial \theta = 0\) and \(V_\theta = 0\) on the north face, we find that the equation for temperature can be represented by (23), too, by putting \(a_n = 0\). Similarly, equation (25) with \(\bar{a}_N = 0\) gives an approximation to the pressure on this symmetry line.

On the symmetry line \(\theta = 0\), we use a similar procedure. The equations for temperature and pressure are the same as (23) and (25) with \(a_x = 0\) and \(\bar{a}_S = 0\), respectively.

For node \(P\) at the centre of the pellet, we employ a control volume with cross-section a semi-circular disc initially, as shown in Figure 1. Due to the nonuniform swelling/shrinkage, it will not remain circular after the process starts. Integrating the governing equations over the cross section by adding up the contribution from the integrations over regions which are originally fan sections formed by the radial straight lines for the interior control volumes and the circular curve \(r = \Delta r/2 = (r_2 - r_1)/2\), we obtain the following forms for each term. For the temperature, the left-hand side term is

\[
\frac{1}{24} \rho C_m \frac{T_P - T_P^{(0)}}{\Delta t} \Psi,
\]
with $T_p^{(0)}$ being the temperature at node $P$ at the previous time step, and

$$
\Psi = \sum_{j=1}^{M} \Delta r_j^3 \Delta \theta_j C_{\theta j}.
$$

Here, $\Delta r_j$ is the distance between the centre and the $j$th neighbouring node on the curve originally being the circle $r = r_2$, $\Delta \theta_j = \theta_{n_j} - \theta_{s_j}$ with $\theta_{s_j}$ and $\theta_{n_j}$ representing the angles of the two faces of the $j$th fan region and $C_{\theta j}$ as value of $C_{\theta}$ at the $j$th region. Similarly, the source term is

$$
\frac{1}{24} (S_c + S_p T_p) \Psi.
$$

The term from the heat flux in the radial direction results in

$$
\frac{1}{4} \left( \sum_{j=1}^{M} (D_{E_j} - F_{E_j}) T_{2,j} - \sum_{j=1}^{M} (D_{E_j} + F_{E_j}) T_p \right),
$$

with

$$
D_{E_j} = k_{\Delta r/2,j} \Delta r_j C_{\theta_j} \Delta \theta_j, \quad F_{E_j} = \frac{1}{2} (\rho_f c_f V_r) \Delta r_{2,j} \Delta r_j^2 C_{\theta_j} \Delta \theta_j,
$$

(27)

$k_{\Delta r/2,j}$ being the thermal conductivity at the intersecting point of the $j$th radial straight mesh line and curve originally from the circle $r = \Delta r/2$, $T_{2,j}$ being the temperature at the $j$th neighbouring node on the curve originally being the circle $r = r_2$. The term from the heat flux in the circumferential direction vanishes due to the cancellation of the flux from two neighbouring regions. Collecting all the terms and rearranging, we obtain the equation for temperature at the centre, $T_p$, from

$$
\left[ \left( \frac{\rho c}{\Delta t} - S_p \right) \Psi + 6 \sum_{j=1}^{M} (D_{E_j} + F_{E_j}) \right] T_p = \left( \frac{\rho c}{\Delta t} T_p^{(0)} + S_c \right) \Psi
$$

$$
+ 6 \sum_{j=1}^{M} (D_{E_j} - F_{E_j}) T_{2,j},
$$

(28)

For the pressure at the centre, integrating the equation of mass balance over the control volume and making use of relation (24), we obtain

$$
6 \Omega P_p = 6 \sum_{j=1}^{M} \Omega_j P_{2,j} + \left[ G - \omega \frac{\left( \rho_f - \rho_f^{(0)} \right) \rho}{\Delta t} \right] \Psi,
$$

(29)

with $\rho_f^{(0)}$ being the gas density at the previous time step,

$$
\Omega = \sum_{j=1}^{M} \Omega_j, \quad \Omega_j = (\rho_f)_{\Delta r/2,j} \Phi_{ej} \Delta r_j^2 \Delta \theta_j C_{\theta j}.
$$

Here, $\Phi_{ej}$ is the value of $\Phi_e$ evaluated for the $j$th fan region.

The equations describing the stepwise reductions, volatilization and carbon consumption have time derivatives only and are evaluated at each time step at each node. After the temperature and pressure are determined, the densities of gas mixture and the pellet and the other parameters can be evaluated.
5. COMPUTING PROCEDURE

We have obtained two systems of discrete algebraic equations for the temperature and pressure at the mesh nodes using a control volume method. They are coupled and nonlinear, and the nonlinearity derives from,

1. dependency of the material properties on temperature,
2. the surface condition,
3. the form of the heat and gas production/consumption terms.

Therefore, an iterative scheme is needed. For each time step, the iterative scheme is as follows. The nonlinear terms (the material properties, surface condition, and source terms) at each node are evaluated using the values from the previous iteration. The temperature and pressure at the centre are calculated from the temperature and pressure at the surrounding nodes from the previous iteration. For the nodes on a radial mesh line, we use the temperatures on the neighbouring radial mesh lines from the previous iteration to obtain a system of tridiagonal linear equations for the temperatures at the present iteration. The system of linear equations are solved using the Thomas algorithm (see [11]) for the temperatures at nodes on a radial mesh line. After the temperatures for all nodes are calculated line-by-line for this iteration, they are used in the equations for the pressure. Then, the pressure is calculated line-by-line in the same way. With the new values of temperature and pressure for the iteration, the velocity, and density of the gas mixture are computed and next iteration is performed if a specified accuracy criterion is not satisfied. The accuracy criterion used here demands that the maximum of relative differences between the temperatures and pressures of two successive iterations at all the nodes is less than a specified value. After the temperature and pressure approximations are obtained, then the other quantities can be calculated for that time step. To reduce the computing time, we do not update the computation domain, i.e., the volume of the pellet, and the quantities of haematite, magnetite, wustite, and iron every time step, rather we do so every ten time steps. This does not affect the solution significantly.

6. NUMERICAL RESULTS

The initial value of porosity is taken to be 0.3 and the mean diameter of the particles composing the pellet $D_p$ to be 50μm. To examine the effect of convection, we first use a large value, 0.02 m, for the radius of the pellet and large proportion of volatile in the coal, with a radially symmetric surrounding temperature field $T_{\text{max}} = T_{\text{min}} = 1373.15 \, \text{K}$. Of the initial material of the pellet, 82% is iron ore (haematite) and 18% is coal by weight, of which 40% is volatile matter. The mesh consists of 21 points on the radial lines and 33 points on the circumferential curves. The time step is 0.01 s.

With these parameters, it is found that the effects of convection on the temperature and average reduction, which is overall effect over the whole pellet, are very small in the spherical pellet. For example, the maximum relative difference of temperatures with and without, convection is 0.24%, occurring at temperature of about 1055 K. The maximum difference in the average reduction fraction with and without, convection is 0.0019, 0.49% of the average reduction value of 0.3903. For a smaller pellet and/or a smaller volatile matter proportion, the effect is even smaller. Overall, the convection lowers the temperature. Sun and Lu [1] also found that the effect of gas convection on temperature in a one dimensional situation is small. However, the effects of the convection on the concentrations of the reaction components, which are local characteristics in the pellet, are significant. The maximum absolute differences of concentrations with and without convection and the maximum values of the concentration are shown in the Table 1. The average reduction is closely related to the change of concentration of the reactants, but the above findings are not inconsistent. This is because the average reduction is an integral characteristic over the pellet while the concentrations of the reaction components are calculated locally. With the parameters
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Table 1. Maximum values of the components, maximum absolute differences of concentrations with and without convection and the percentage.

<table>
<thead>
<tr>
<th>Component</th>
<th>Haematite</th>
<th>Magnetite</th>
<th>Wustite</th>
<th>Iron</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum Value</td>
<td>1582.</td>
<td>1645.</td>
<td>1534.</td>
<td>922.</td>
</tr>
<tr>
<td>Maximum Diff.</td>
<td>32.7</td>
<td>31.1</td>
<td>14.5</td>
<td>3.9</td>
</tr>
<tr>
<td>%</td>
<td>2.1</td>
<td>1.9</td>
<td>0.9</td>
<td>0.4</td>
</tr>
</tbody>
</table>

used here, we also found that the nonlinear velocity terms in the Ergun’s equations can be neglected.

Then, we investigated the effect of the surrounding temperature field on the reduction process. For this investigation, the radius of the pellet was taken to be 0.007 m, a typical value for industrial process and the volatile matter contained in the coal was 6.48%. Figure 3 shows the variations of the average reduction over the whole pellet with time for three different surrounding temperature fields. The three fields are

1. radially symmetric case, $T_{\text{max}} = T_{\text{min}} = 1373.15 \text{ K}$,
2. $T_{\text{max}} = 1473.15 \text{ K}$ and $T_{\text{min}} = 1273.15 \text{ K}$, and
3. $T_{\text{max}} = 1573.15 \text{ K}$ and $T_{\text{min}} = 1173.15 \text{ K}$.

Notice that the average of the surrounding temperature fields is the same for all three cases. These fields might not represent the real situation in a multi-pellet-layer process where the temperatures from the surrounding pellets are not controlled. These have been chosen to compare the effects of different nonradially symmetrical temperature fields. It can be seen that overall uniform surrounding temperature distribution is better for reduction. However, early in the process, the reduction from the nonuniform temperature field is higher than that from a uniform temperature field. This is also the case when the number of mesh points on the radial lines are doubled, i.e., it is not an artifact of the numerical scheme. The same effect has also been shown by Donskoi et al. [2] using finite-difference method for pellet with conduction as the only heat transfer mechanism.

Figure 4 shows the variations of temperatures with time at four points: the centre and three points on surface where $\theta = 0, \pi/2, \pi$ for a surrounding temperature field with $T_{\text{max}} = 1473.15 \text{ K}$ and $T_{\text{min}} = 1273.15 \text{ K}$. It is noted that at later stage, the temperature at point $\theta = \pi$ on the surface is higher than the surrounding temperature at the point. This is due to the heat transfer from the high temperature part to law temperature part through the pellet. The effect of the surrounding temperature fields on the temperature at the centre is illustrated in Figure 5, which shows the time variation of differences of the central temperatures between the two nonradially symmetric cases and the radially symmetric case. The maximum difference between the central temperatures of the nonradially symmetric case with $T_{\text{max}} = 1573.15 \text{ K}$ and $T_{\text{min}} = 1173.15 \text{ K}$ and the radially symmetric case is about 52 K, i.e., about 4% of the average temperature.

The variations of the pressure at the centre with time for the three surrounding temperature fields are shown in Figure 6. The main change in the pressure occurs in the first 100 s and it first increases and then decreases. The maximum pressure at the centre occur at the time of about 40 s. Due to the steepness of the curves around the time, the difference between the curves is not very noticeable. In order to display the differences, the time variation of the differences of the central pressures between the two nonradially symmetric fields and the radially symmetric field is shown in Figure 7. It is noticed that at 30 s, the central pressure in the radially symmetric case is higher than those in the nonradially symmetric cases and the difference is about 506 N/m², about 0.49% relative difference. At 50 s, the pressure in the nonradially symmetric cases are higher than that in the radially symmetric case and the maximum difference is about 451 N/m², about 0.44% relative difference. To see if this is phenomenon related to the mesh size, the number of mesh points on the radial lines was doubled and the same pattern is found.

Figure 8 shows the pressure distributions along the line $\theta = \pi/2$ at four times for the surrounding temperature field with $T_{\text{max}} = 1473.15 \text{ K}$ and $T_{\text{min}} = 1273.15 \text{ K}$. At the four times,
the pressure at 50 s is highest and this can also be seen from Figure 6. The pressure becomes almost uniform on the line at 600 s. It is noted that the pressure distributions at 100 s, 200 s, and 600 s from the other two surrounding temperature fields (not shown) are very close to the corresponding curves shown in Figure 8. However, at 50 s, the pressure distributions from the three temperature fields are distinct, as shown in Figure 9.

The time variations of the velocity of the gas mixture at four points for the three different surrounding temperature fields are shown in Figure 10. For the nonradially symmetric temperature fields, there are two times at which the velocities at the points on the surface exhibit high peaks, (see Figure 10a and 10b). These peaks correspond to the maximum rate of devolatilization and the maximum rate of the carbon reaction. The gas mixture flows outwards faster at the points where the surrounding temperature is higher than at the points where the surrounding temperature is lower at early stage, and at later stage the flow is slower at the points where the surrounding temperature is higher than at the points where the surrounding temperature is lower. In the nonradially symmetric cases, the gas velocity at the centre is nonzero. The positive direction of velocity at the centre is assumed to be in the outward radial direction of the line \( \theta = 0 \). It can be seen that the velocity at the centre changes direction several times during the early stages. As expected, in the radially symmetric case, the velocity at the centre is zero and at the surface points, the velocities are the same, see Figure 10c.

Figure 11 shows the velocity fields on eight lines in the pellet at 50 s and 100 s in the case where the surrounding temperature field has \( T_{\text{max}} = 1573.15 \text{ K} \) and \( T_{\text{min}} = 1173.15 \text{ K} \). It can be seen that at 50 s, the velocity around the centre of the pellet has considerable circumferential component, while at 100 s, the velocity is almost in radial direction.

For the radially symmetric case, the pellet first swells and the radius of the outer surface reaches 0.00733 m, compared with the initial value of 0.007 m. Then, it shrinks and the radius reaches 0.00726 m at 600 s. For the nonradially symmetric cases, the pellet changes its shape since the
Figure 5. Time variation of central temperature differences between the nonradially symmetric cases and the radial symmetric case.

Figure 6. Variation of pressure at the centre with time for three surrounding temperature fields.

Figure 7. Time variation of central pressure differences between the nonradially symmetric cases and the radial symmetric case.

Figure 8. Pressure distribution on line $\theta = \pi/2$ at four times with the surrounding temperature field: $T_{\text{max}} = 1473.15\,\text{K}$ and $T_{\text{min}} = 1273.15\,\text{K}$.
Figure 9. Pressure distributions on line $\theta = \pi/2$ at 50s for the three surrounding temperature fields.

Figure 10. Variations of radial velocity with time at four positions: the centre and three on the surface, for the three surrounding temperature fields.

(a). $T_{\text{max}} = 1573.15\text{K}$ and $T_{\text{min}} = 1173.15\text{K}$.

(b). $T_{\text{max}} = 1473.15\text{K}$ and $T_{\text{min}} = 1273.15\text{K}$.

(c). Radially symmetric case $T_{\text{max}} = T_{\text{min}} = 1373.15\text{K}$—the three on the surface coincide.
shrinkage/swelling is not uniform. For the case where $T_{\text{max}} = 1473.15 \text{ K}$ and $T_{\text{min}} = 1273.15 \text{ K}$, the pellet first swells in all directions and then shrinks at the point where the surrounding temperature is 1473.15 K. It continues swelling at the point where the surrounding temperature is 1273.15 K until the end of 600 s. For the case where $T_{\text{max}} = 1573.15 \text{ K}$ and $T_{\text{min}} = 1173.15 \text{ K}$, the point on the surface where the surrounding temperature is 1573.15 K first moves outwards (swelling) slightly and then moves inwards (shrinkage). At the end of 600 s, the distance between the point and the original centre becomes 0.00685 m. The point where the surrounding temperature is 1173.15 K first moves inwards (shrinkage) slightly and then moves outwards (swelling). The distance between the point and the original centre becomes 0.00761 m at the end of modelling time.

7. CONCLUSION

The coal-based direct iron ore reduction process in pellet is investigated using a finite-control volume method. Besides the conduction in the mixture, convection due to the movement of the gas medium in the pellet is taken into account. For simplicity, the gas species are not distinguished when conservations of their mass and momentum are considered. The temperatures of solid and gas are taken to be the same. The formulation is outlined for axially symmetric temperature, pressure and other fields.

It is found that the effects of convection in the gas medium on the temperature and the overall average reduction are very small. The effects of the convection on the concentrations of the reaction components at some local position are not insignificant. Overall, a uniform surrounding temperature field around the pellet produces a better average reduction.

REFERENCES