Weld Metal Microstructure Calculations from Fundamentals of Transport Phenomena in the Arc Welding of Low-Alloy Steels

Agreement between computation and experiment indicates promise for predicting weld metal microstructure on the basis of transport phenomena fundamentals

BY K. MUNDRA, T. DebROY, S. S. BABU AND S. A. DAVID

ABSTRACT. In recent years, significant progress has been made toward understanding the development of the weld pool shape and size from the numerical calculations of heat transfer and fluid flow in the weld pool. Although such calculations have provided detailed information about the welding processes, no efforts have been made to understand the development of fusion zone microstructures from the fundamentals of transport phenomena. The aim of this work is to address this.

Heat transfer and fluid flow during manual metal arc welding of low-alloy steels containing different concentrations of vanadium and manganese were investigated by solving the equations of conservation of mass, momentum and energy in three-dimensional transient form. The model incorporates fluid flow in the weld pool resulting from surface tension, electromagnetic and buoyancy forces. The cooling rates are calculated at various locations in the weldment. The weld metal compositions are used to calculate the time-temperature-transformation (TTT) diagrams on the basis of an available phase transformation model. The calculated cooling rates and the TTT diagrams are then coupled to determine the continuous cooling transformation (CCT) behavior and volume percentages of acicular, allotriomorphic and Widmanstätten ferrites in various low-alloy steel weldments. The computed microstructures are found to be in good agreement with the experimentally observed microstructures. The agreement indicates significant promise for predicting weld metal microstructure from the fundamentals of transport phenomena.

Introduction

The integrity and the performance of a welded joint depend on the weldment microstructure and properties (Refs. 1, 2). During welding, the interaction of the heat source and the material leads to rapid heating, melting and vigorous circulation of the molten material in the weld pool. As the heat source moves away from the molten region, solidification of the material takes place. The resulting thermal cycle plays an important role in determining weldment structure and properties.

An accurate prediction of the thermal cycle in the weld metal is a prerequisite for a reliable prediction of weld metal microstructure. Direct accurate measurements of temperature profiles in a weld pool are difficult. Furthermore, noncontact techniques for the measurement of temperature profiles in the weld pool are still evolving (Ref. 3). Earlier models to calculate temperature-time history in the weld were based on the solution of conservation of energy equations (Refs. 4-7) and neglected the effect of fluid flow in the weld pool. Fluid flow in the weld pool can significantly affect the time-temperature history experienced by a weld metal.

In the past decade, significant progress has been made in the solution of equations of conservation of mass, momentum and energy in the weld pool (Refs. 8-13). The role of Marangoni, electromagnetic and buoyancy forces on the weld pool geometry has been investigated (Refs. 8, 9). The effect of surface active elements on the transient development of weld pool geometry has also been examined in detail (Ref. 14). Furthermore, simple features of solidification structure, such as secondary dendrite arm spacings, have been predicted from the cooling rate data calculated from the fundamentals of transport phenomena (Ref. 10). These developments have provided significant insight into the welding process. However, accurate transient temperature calculations from comprehensive fluid flow and heat transfer models have not been used to predict fusion zone microstructures.

The work reported here was aimed at predicting the weld metal microstructure from the fundamentals of transport phenomena in the weld pool and the phase transformations in the fusion zone during cooling. The heat transfer and fluid flow in the top bead of multipass welds of low-alloy steels fabricated by using the manual metal arc welding process were investigated by numerically solving the equations of conservation of mass, momentum and energy in the weld pool. The fluid flow and heat transfer models take into account the circulation of the molten metal in the weld pool owing to surface tension, electromagnetic and buoyancy forces. The cooling rates at various locations in the weld metal were computed as a function of time. The cooling rates and the CCT diagram generated from the phase transformation model (Ref. 15) are then used to determine the volume fractions of acicular, Widmanstätten and allotriomorphic ferrites in the top bead of the multipass welds containing different levels of vanadium and manganese in iron-carbon-silicon low-alloy steel weldments. The
Model Framework

Assumptions in the Model Formulation

During manual metal arc welding, the energy is transferred to the workpiece both from the arc and from the metal droplets generated from the consumable electrode. The energy distribution from the arc does not change significantly with time, and the distribution is Gaussian in nature in most cases. However, the energy transfer from the droplets depends on various parameters such as the drop frequency, the drop transfer mode, and the drop shape, size, and temperature. Because of the transient nature of these parameters and the resulting complexity in integrating these phenomena in the numerical scheme, a time average energy transfer rate was considered in the model for simplicity. It is thought that, irrespective of the mode of droplet transfer, the rapid mixing of the metal in the weld pool will minimize temporal variation of cooling rates in the solidified weld pool. Because all the droplets do not impinge exactly on the same location on the weld pool surface, the time-average energy density distribution was assumed to be Gaussian in its spatial distribution. The energy distributions from the arc and metal droplets from the electrode were coupled and expressed in the form of an overall energy transfer efficiency. In principle, the shape of the energy density distribution vs. distance profiles for the arc and for the metal drops may be different. Our assessment of this effect, considering different energy distributions, resulted in somewhat different peak temperatures and a minor change in the weld pool geometry. However, no significant difference in temperature-time history was observed in the range 1100–700 K (827–427°C). The temperature-time history in this temperature range governs the microstructural development in low-alloy steel weldments (Ref. 15). Therefore, the time-average values of the energy transport, assumed in the formulation of the model, are justified for the purpose of this research. For simplicity, the weld pool surface was considered to be flat. The fluctuations in the mass of the weld pool due to droplet addition were approximated by a time-average constant mass of the metal in the weld pool. Furthermore, because the weld metal did not contain significant quantities of volatile alloying elements, the possible composition change of the weld metal owing to alloying element

computed microstructures in different regions of the weldment are then compared with the experimentally observed microstructures (Ref. 16).
vaporization was ignored. The transport of momentum from the droplets to the weld pool was ignored. The resulting inaccuracy in the cooling rate in the fusion zone in the 1100–700 K range depends on the magnitude of the Peclet number for heat transfer and its change due to additional momentum from the metal drops. At low values of Pe (<0.5), the impact of momentum from the droplets is negligible. However, at high values of Pe (=60), a 17% change in Pe resulting from the momentum transfer from the droplets leads to roughly a 1.5% change in the average cooling rate in the 1100–700 K range.

The spatial variation of the inclusion characteristics and the effects of this variation on the microstructure development are ignored. It should be noted that the detailed theoretical models to describe the development of inclusions are still evolving (Refs. 17, 18). Furthermore, the elemental segregation (Ref. 19) was not considered in the microstructure model. The preceding discussion indicates both the complexity of the welding process and the need for simplification to keep the computational task within practical limits.

### Fluid Flow and Heat Transfer in the Weld Pool

The following equations describe the velocity and temperature fields in a stationary workpiece welded by using a moving heat source.

**Equation of Continuity**

\[ \nabla \cdot V = 0 \]  

(1)

where \( V \) is the velocity vector and \( U, V, W \) are the x, y and z components of the velocity vector, respectively. The coordinate system is shown in Fig. 1. The density of the material is assumed to be a constant.

**Momentum Equations**

\[
\begin{align*}
\rho \frac{\partial V}{\partial t} + \rho V \cdot \nabla V &= -\nabla P + \\
\mu \nabla^2 V &= -\nabla P + S_v
\end{align*}
\]  

(2)

where \( \rho \) is the density, \( \mu \) is the viscosity, \( P \) is an effective pressure, \( t \) is the time and \( S_v \) is the source term that takes into account the combined effects of buoyancy, Marangoni and electromagnetic forces.

**Energy Equation**

The technique used here to account for the phase change has evolved from the works of Voller and Prakash (Ref. 20) and Brent, et al. (Ref. 21). The total enthalpy of the material, \( H \), is represented as a sum of the sensible heat, \( h = f C, T \), and the latent heat content, \( \Delta H, i.e. \).

![Fig. 3 -- Typical fusion zone microstructure in a low-alloy steel weld. The allotriomorphic ferrite delineating the prior austenite grain boundary is marked as “AL” and acicular ferrite is marked as “AF.” Weld metal composition: 0.066% C, 0.82% Si, 1.66% Mn, 0.026% Ti and 0.084% O. The joint was prepared by using submerged arc welding with 29 V and 390 A at a welding speed of 9.1 mm/s.](image)

![Fig. 4 -- Schematic diagram of the various steps involved in the calculation of fusion zone microstructure (Ref. 15) and the heat transfer and fluid flow model developed in the present work.](image)
The energy equation is written in terms of the sensible heat, $h$, as follows:

$$\frac{\partial h}{\partial t} + \rho \nabla \cdot (\rho \mathbf{V} \cdot \mathbf{V} h) = -\rho \nabla \cdot (\rho \mathbf{V} \cdot \mathbf{V} h) + \nabla \cdot (k \nabla h) + S_h + S_I$$  \hspace{1cm} (4)

In Equation 4, $C_p$ is the specific heat, $k$ is the thermal conductivity, $S_h$ is the source term that accounts for the latent heat of melting and convective transport of latent heat in the two-phase region (mushy zone). Thus, the equation for the sensible enthalpy is the same as that for the case with no phase change, except for the source terms, $S_h$, which is given by (Ref. 20)

$$S_h = -\left( \rho \frac{\partial (\Delta H)}{\partial t} + \rho \nabla \cdot (\rho \mathbf{V} \Delta H) \right)$$  \hspace{1cm} (5)

where $\Delta H = F(T)$ is the latent heat content, is defined as a function of temperature, $T$, and is given by

$$F(T) = \begin{cases} L & T > T_l \\ \frac{T - T_s}{T_l - T_s} L & T_s \leq T \leq T_l \\ 0 & T < T_s \end{cases}$$  \hspace{1cm} (6)

where $L$ is the latent heat, $T_l$ is the liquidus temperature and $T_s$ is the solidus temperature.

The numerical solution of Equations 1-6, with appropriate boundary conditions, requires a large number of fine grids for accurate representation of heat input from the source, which is marching in time, and a small time step to ensure conservation of mass, momentum and energy during each time step. This makes the computation time very large. In addition, a large volume of data is generated and meaningful analysis of the data becomes time consuming and, sometimes, depending on the grid size, impractical. Therefore, the transient problem has been reduced to a steady-state problem by solving in a coordinate system that moves with the heat source as shown in Fig. 1. In this coordinate system, the velocity and the enthalpy fields will be independent of time. As a consequence, the time required for computation and data analysis is reduced significantly.

**Transformed Momentum and Energy Equations**

Let $\mathbf{V}$ be the velocity at any point with respect to the moving frame. Then $\mathbf{V}$ can be expressed as

$$\mathbf{V} = \overline{\mathbf{V}} + \mathbf{V}_s$$  \hspace{1cm} (7)

where $\overline{\mathbf{V}}$ is the convective component of the velocity and $\mathbf{V}_s$ is the scanning velocity. Because $\mathbf{V}_s$ is known, we can treat $\overline{\mathbf{V}}$ as the primary unknown in the solution of momentum equations. The transformation of Equations 2-5, using Equation 7, results in the following equations:

$$\rho \nabla \cdot (\rho \overline{\mathbf{V}}) = -\rho \nabla \cdot (\rho \mathbf{V}_s) + \nabla \cdot (k \nabla h) + S_h + S_I$$  \hspace{1cm} (8)

$$\rho \nabla \cdot (\overline{\mathbf{V}} h) = \nabla \cdot (k \nabla h) + S_h + S_I$$  \hspace{1cm} (9)

$$S_I = \rho \nabla \cdot (\mathbf{V} \Delta H) + \rho \nabla \cdot (\mathbf{V} \Delta H)$$  \hspace{1cm} (10)

The last terms in Equations 8-10 result from the transformation of the coordinate system. Alternatively, because in this work the $y$ and $z$ components of the scanning velocity, $\mathbf{V}_s$, are zero and the $x$ component is the experimental scanning velocity, $U_s$, Equations 8-10 are obtained by using the transformation $x = x + U_s t$.

**Boundary Conditions and Source Terms**

The source term in Equation 6, $S_h$, incorporates the buoyancy force, the Marangoni stress, and the electromagnetic force. Assuming the Boussinesq treatment to be valid, the density is assumed constant in all terms. The natural convection effect, i.e., the buoyancy force, is taken into account by defining the buoyancy source term, $S_b$, to be

$$S_b = \rho g \beta (T - T_{ref})$$  \hspace{1cm} (11)

where $\beta$ is the thermal expansion coefficient and $T_{ref}$ is any arbitrarily selected reference temperature.

Because the temperature varies on the surface of the weld pool, a shear stress
(Marangoni stress) is produced on the free surface. The effective tangential stress, $\tau$, due to this effect on the free surface, was calculated as follows:

$$\tau = \frac{\mathrm{d}y}{\mathrm{d}T} \frac{\gamma}{\kappa T}$$

where $\frac{\mathrm{d}y}{\mathrm{d}T}$ is the temperature coefficient of the surface tension and $\kappa$ is the fraction of liquid. The value of $\kappa$ (liquid fraction) was computed from the linear relationship between $\kappa$ and temperature between the solidus and liquidus temperatures. The limiting values of $\kappa$ are zero at or below the solidus temperature and one at or above the liquidus temperature. The multiplication of the shear stress with $\kappa$ takes into account the decrease in the shear stress in the mushy region.

The condition that the velocity is zero in the solid region is enforced by incorporating a source in the momentum equation as follows:

$$S_i = -\frac{\mathrm{A}(\kappa)}{\kappa} \mathbf{V}_i$$

where the constant $A$ is determined according to the Carman-Koseny equation (Refs. 20, 21) for flow through porous media as follows:

$$A = -C \left( \frac{1 - \kappa}{\kappa + B} \right)$$

where $B$ is a very small positive number introduced to avoid division by zero, and by choosing a large value of $C$, the velocity of the solid region ($\kappa = 0$) is forced to be zero. The electromagnetic force, $F_e$, is given by:

$$F_e = J \times B$$

where $J$ is the current density vector and $B$ is the magnetic flux vector. Because the heat source is axisymmetric, the electromagnetic force term, $F_e$, was calculated by use of the formulation given by Kou, et al. (Ref. 11).

The calculations were performed only for half of the workpiece, because there is symmetry about the $y = 0$ plane — Fig. 1. Along the plane of symmetry, the following boundary conditions were defined for the velocity components:

$$\frac{\mathrm{d}U}{\mathrm{d}y} = 0$$
$$\mathbf{V} = 0$$
$$\frac{\mathrm{d}W}{\mathrm{d}y} = 0$$

Because the weld pool surface was assumed to be flat, the $z$ component of the velocity, $W$, was defined as zero at the top surface.

The source term for enthalpy equation, $S_h$, included the prescription of the heat exchange between the surface of the sample and the heat source and the radiative and convective heat loss to the surroundings.

$$S_h = \frac{Q \eta}{\pi r_i^2} \left[ \frac{3(\xi^2 + y^2)}{r_i^2} \right] -$$
$$\frac{\sigma (T_i^4 - T_g^4)}{h}$$

where $Q$ is the power input, $\eta$ is the process efficiency, $r_i$ is the arc/beam radius, $T_i$ is the local weld pool surface temperature, $T_g$ is the ambient temperature, $\sigma$ is the Stefan-Boltzmann constant, and $h$ is the heat transfer coefficient. At the plane of symmetry, the gradient of enthalpy was zero.

$$\frac{\mathrm{d}h}{\mathrm{d}y} = 0$$

At the other surfaces of the sample, the temperature was prescribed as the preheat temperature.

Solution Procedure

The governing equations were repre
sent in a finite difference form and solved iteratively on a line-by-line basis utilizing a tridiagonal matrix algorithm (TDMA). The semiimplicit method for pressure-linked equations (SIMPLE) algorithm was employed for the discretization of the equations. The details of the procedure are described elsewhere (Ref. 22). The model used a 65 x 39 x 17 grid system for the calculation of the enthalpies and velocities. Spatially nonuniform grids were used for maximum resolution of variables.

Calculation of Temperature-Time Data

From the steady-state temperature field, obtained by solving the transformed momentum and enthalpy equations, temperature as a function of time at different locations (x,y,z) can be calculated by using the following relation:

\[ T(x,y,z,t_2) = \frac{T(\xi_2,y,z) - T(\xi_1,y,z)}{\xi_2 - \xi_1} \left[ U_x(t_2 - t_1) + \sum \right] T(x,y,z,t_1) \]

where \(T(\xi_2,y,z)\) and \(T(\xi_1,y,z)\) are the steady-state temperatures at coordinates \((\xi_2,y,z)\) and \((\xi_1,y,z)\), respectively; \(\xi_2 - x_1\) is the distance traveled by the arc/bear in time \((t_2 - t_1)\), \(T(x,y,z,t_1)\) and \(T(x,y,z,t_2)\) are the temperatures at location \((x,y,z)\) at times \(t_1\) and \(t_2\), respectively.

Phase Transformation Model

A simplified sequence of microstructure development in a low-alloy steel weld metal is shown in Fig. 2. As the steel weld pool cools, various phase transformations that occur as a function of temperature are inclusion formation, solidification of liquid to delta ferrite, transformation of delta ferrite to austenite, and finally subsequent transformation of austenite to various ferrite morphologies. The final low-alloy steel weld microstructure consists of allotriomorphic ferrite, Widmanstätten ferrite and acicular ferrite. On cooling, the allotriomorphic ferrite is the first phase to transform from austenite and it nucleates along austenite grain boundaries and grows by a reconstructive diffusion mechanism (Ref. 15). As the weld cools further, Widmanstätten ferrite nucleates from the allotriomorphic ferrite as thin wedge-shaped plates and grows into the austenite grain. On further cooling, the acicular ferrite in the form of thin lenticular plates nucleates on inclusions within the austenite grain and produces typical interlocking microstructure as shown in Fig. 3. The small amount of residual austenite that remains after the above ferrite transformation transforms into complex martensite-austenite-carbide aggregates called microphases. The variables that influence the volume percentage of the various ferrite morphologies are listed below (Refs. 23–25).

1) Inclusion characteristics.
2) Solidification features such as the segregation patterns and austenite grain size.
3) Transformation kinetics of austenite to various ferrite morphologies, which is controlled by the weld metal composition.
4) Weld metal cooling rates in the temperature range 1100–700 K, which are controlled by the welding process conditions.

A comprehensive model developed by Bhadeshia, et al. (Refs. 15, 17, 26), can predict the volume percentage of ferrite morphologies as a function of weld metal composition and process conditions by considering most of the above mentioned variables. In this model, weld metal cooling rates are calculated for a given welding process conditions, using a semiequilibrium approach developed by Svensson, et al. (Ref. 26). This method of calculation is based on experimental measurements of cooling rates in steel welds with various welding conditions and processes and is explained below briefly.

To describe the cooling rates in the 1100–700 K temperature range, Svensson, et al. (Ref. 26), measured the cooling rates experimentally by harpooning platinum and platinum-rhodium thermocouples into the weld pool region of a standard ISO 2560 weld, for various welding conditions and processes. They then fitted the experimentally measured cooling rates to the following equation:

\[ \frac{dT}{dt} = \frac{C_1(T - T_i)^{C_2}}{q_\eta} \]

where \(C_1\) and \(C_2\) are adjustable constants, \(T\) is the temperature of interest, \(T_i\) is the preheat temperature, \(q\) is the net energy input to the weld per unit length and \(\eta\) is the heat transfer efficiency of the welding processes. They assumed that the constants \(C_1\) and \(C_2\) were indepen-
The coupled fluid flow, heat transfer and phase transformation model described above was used to predict microstructures for the experimental conditions published by Evans (Ref. 16). He has measured the volume percentages of ferrite morphologies in the top bead of multipass welds with different levels of vanadium and manganese in iron-carbon-silicon low-alloy steel welds. These weld beads were deposited by use of manual metal arc welding processes. The welding conditions are given in Table 1, and the weld metal compositions are given in Table 2. The weld joint geometry was that of an ISO 2560 joint (Ref. 16). For the above conditions, thermal histories at different locations in the weldment were predicted using the fluid flow and heat transfer model. The calculated cooling rates and the experimental austenite grain size data (Ref. 16) were then used to calculate the microstructure within the fusion zone for all the weld metal compositions given in Table 2. In each case, the predicted volume percentages of ferrite morphologies in the top bead are compared with the corresponding experimental results.

Experimental Validation

The coupled fluid flow, heat transfer and phase transformation model described above was used to predict microstructures for the experimental conditions published by Evans (Ref. 16). He has measured the volume percentages of ferrite morphologies in the top bead of multipass welds with different levels of vanadium and manganese in iron-carbon-silicon low-alloy steel welds. These weld beads were deposited by use of manual metal arc welding processes. The welding conditions are given in Table 1, and the weld metal compositions are given in Table 2. The weld joint geometry was that of an ISO 2560 joint (Ref. 16). For the above conditions, thermal histories at different locations in the weldment were predicted using the fluid flow and heat transfer model. The calculated cooling rates and the experimental austenite grain size data (Ref. 16) were then used to calculate the microstructure within the fusion zone for all the weld metal compositions given in Table 2. In each case, the predicted volume percentages of ferrite morphologies in the top bead are compared with the corresponding experimental results.

Results and Discussion

Heat Transfer and Fluid Flow

The three-dimensional steady-state temperature field obtained by solving the transformed equations of conservation of mass, momentum and energy for the shielded metal arc welding of low-alloy steels (Ref. 16) is shown in Fig. 5. The thermophysical properties used in the calculations are presented in Table 3. The peak temperature attained by the weld pool surface just below the arc was found to be 2490 K (2217°C). The general features of the temperature field are consistent with the results reported in the literature (Ref. 11) for a moving heat source. In front of the heat source, the temperature gradient is greater than that behind the heat source. The higher temperature gradient results in slightly greater liquid metal velocities in front of the heat source than behind it. This can be observed from the velocity fields on the
weld pool surface and along the plane of symmetry (y = 0), plotted in Fig. 6A and B, respectively. The weld pool surface flow also shows that the liquid metal moves from the center (point of maximum temperature) to the periphery of the weld pool. This is expected for a metal with a very low concentration of surface active elements that results in a negative temperature coefficient of surface tension, dy/dT, over much of the weld pool surface. In the calculation, a constant negative dy/dT was assumed. The temperature field shows a typical elongated weld pool. Moreover, the weld pool size was found to be similar to the experimental results of Evans (Ref. 16).

The effect of convection on heat transfer on the weld pool geometry, for the welding conditions investigated, can be characterized by the calculation of Peclet number, Pe. The Pe is a measure of the relative magnitudes of convective and conductive heat transfer and is given by

\[ Pe = \frac{V_{\text{max}} L}{\kappa} \]  

(23)

where \( V_{\text{max}} \) is the maximum velocity, \( \kappa \) is the thermal diffusivity of the liquid metal given by \( k/(\rho C_p) \) and \( L \) is the characteristic length that can be taken as the length of the weld pool. Using the data presented in Table 3, the weld geometry and the maximum velocity presented in Fig. 6A and B, the Peclet number is found to be 60. The high value of Pe (>1) shows that convection plays an important role in heat transfer under the conditions investigated for manual metal arc welding of low-alloy steels.

The calculations show that the length of the mushy zone at the trailing edge of the weld pool was longer than all the other regions. The area of the mushy zone controls the extent of solute segregation and also the solidification features. The phase transformation model by Bhadeshia, et al. (Ref. 15), considers the solute segregation and takes this into account while calculating the TTT diagram, as shown in Fig. 4. The solidification features may affect the prior austenite grain size within the weld pool.

However, in the present work, experimentally measured austenite grain size was used and the variations in austenite grain size within the weld pool were assumed to be negligible.

### Thermal Cycles and Cooling Rates

From the computed temperature field, the temperature-time data at different locations were computed by making use of Equation 21. Figure 7A shows the temperature contour profiles calculated by using the model, and the profiles describe the weld pool shape and size. The temperature contour corresponding to the solidus temperature of 1745 K (1472°C) represents the weld interface. The region between the weld interface and the temperature contour corresponding to solidus temperature 1785 K (1512°C) represents the solid-liquid region. The temperature-time data at four different locations A, B, C and D are shown in Fig. 7B. The positions of these four points on a cross section of the weldment normal to the welding direction are marked in Fig. 7A. The temperature-time data at any other cross section, normal to the welding direction, will be the same except for the time lag between the responses at the two cross sections. The results in Fig. 7B show that thermal cycles vary from location to location. It is interesting to note from Fig. 7B that the peak temperatures are not reached at the same time at all locations. The time it takes for any point to attain its peak temperature depends on that point's distance from the heat source.

In the present work, the cooling rates are computed at all locations of the weldment. Figure 8 shows the cooling rates predicted by the present work as a function of temperature at various locations. The calculations show that the differences on cooling rates at different locations are not significant in the temperature range 1100–700 K. Because there are no significant differences in the cooling rates as a function of position within the fusion zone, the spatial difference in microstructure is also expected to be negligible, which will be discussed later. Figure 8 also shows the comparison of cooling rates predicted by the present work and by the semiempirical approach of Svensson, et al. (Ref. 26), i.e., Equation 22. The cooling rates predicted by the present work are significantly higher than those predicted by Equation 22. This difference in cooling rate will influence the microstructural prediction.

### Microstructure Calculation

The cooling rates predicted by the present work are used in calculating the volume percentages of ferrite morphologies in the fusion zone for various iron-carbon-silicon-manganese-steel weld compositions given in Table 2 (Ref. 16). The calculated microstructural constituents at location B (marked in Fig. 7A) are compared with the experimentally observed values in Table 4. The table also contains the microstructural predictions by the original model proposed by Bhadeshia, et al. (Ref. 15), where the cooling rates are calculated from Equation 22. Because the cooling rates predicted by the present work are higher than those predicted by using Equation 22, the allotriomorphic ferrite volume percentage predicted by the present work is slightly lower than that predicted by the original Bhadeshia, et al., model. The volume percentage of Widmanstätten ferrite predicted by the present work is approximately the same as that of the original Bhadeshia, et al., model. Due to a reduction in the predicted allotriomorphic ferrite volume percentage, the volume percentage of acicular ferrite calculated in this work is higher than that predicted by the original Bhadeshia, et al. (Ref. 15), model. On the whole, the calculations showed negligible spatial variations in the volume percentages of various ferrite morphologies in different locations. This is indeed expected, because the calculations showed roughly identical cooling rates calculated at locations A, B and C — Fig. 7. The present results support the assumption of Svensson, et al. (Ref. 26), and Watt, et al. (Ref. 27), that the variation in the cooling rates within the fusion zone may not be significant enough to induce a drastic microstructural difference.

The comparison of overall predicted microstructural constituents (Fig. 9) with the experimental data showed slightly better correlation than the calculations using the original Bhadeshia, et al. (Ref. 15), model. It is important to note that the present work is the first attempt at coupling a comprehensive transport phenomenon with a fundamental phase transformation model. The correlations between predicted and experimental data are expected to improve with refinement in the models used. Because the semiempirical approach used by Bhadeshia, et al. (Reqs. 15, 26), yields approximately similar results to those of the present work, one may choose not to use a comprehensive, detailed, and computationally intensive fluid flow and heat transfer model to describe thermal histories experienced by the fusion zone. However, it is noteworthy that the semiempirical approach used by Bhadeshia, et al. (Reqs. 15, 26), cannot be used directly for different weld joint geometries and new welding processes, i.e., for
every new set of welding conditions, the constants $C_1$ and $C_2$ have to be determined experimentally. Moreover, this approach is incapable of calculating the spatial variation of weld metal cooling rates within the fusion zone.

Spatial Variation of Microstructure

It is important to note that the microstructure in the fusion zone may not be spatially uniform in all cases. For example, in some highly alloyed steels such as iron-carbon-chromium-molybdenum welds, a small change in the cooling rate may lead to a significant difference in the microstructural development in two locations of the fusion zone as shown below.

The cooling rate calculations at various locations, presented in Fig. 8, were applied to a weld composition of Fe-0.07C-0.45Si-1.0Mn-0.5Ni-1.0Mo-2.25Cr (wt-%) weld and the computed results are presented in Table 5. The formation of allotriomorphic ferrite and Widmanstätten ferrite is predicted only in location C, whereas in locations A and B 100% acicular ferrite is predicted. This is because the cooling rates at locations A and B are slightly higher than the critical cooling rate for nucleation and growth of allotriomorphic ferrite at the austenite grain boundary. As a consequence, at these locations, allotriomorphic ferrite formation is completely suppressed. At location C, the cooling rates are lower than the critical cooling rates leading to the formation of the allotriomorphic ferrite. Because there are no available experimental data on the spatial variation of the volume percentages of various ferrite morphologies within the fusion zone, the above predictions cannot be validated. However, such calculations can be used in the theoretical design of weldment and welding procedures. For example, it has been reported that in cases where allotriomorphic ferrite formation is completely suppressed (e.g., at locations A and B), the acicular ferrite microstructure may be replaced by a bainitic microstructure (Ref. 28). The bainitic microstructure is deleterious to the weld metal properties. As a consequence, the weld properties for the iron-chromium-molybdenum carbon weld considered above may be inferior at locations A and B compared to those of location C. However, by changing the weld composition or weld metal cooling conditions appropriately, bainitic microstructure development can be suppressed and the acicular ferrite microstructure may be promoted by allowing a small amount of allotriomorphic ferrite all along the austenite grain boundaries (Ref. 28).

Summary and Conclusions

1) A model to calculate transient heat transfer and fluid flow in the weld pool in three dimensions resulting from surface tension, electromagnetic and buoyancy forces has been applied to manual metal arc welding of low-alloy steels. Numerical calculations indicate that the weld pool shape and size are determined by convective heat transfer for the welding conditions investigated in this work.

2) The cooling rate calculated from the fluid flow and heat transfer was coupled with an existing phase transformation model to predict the volume percentages of acicular, Widmanstätten and allotriomorphic ferrites in the top bead of multipass welds containing different concentrations of vanadium and manganese in iron-carbon-silicon low-alloy steel welds. Numerical calculations with ten weldment compositions predicted volume percentages of different ferrite morphologies that are in agreement with experimental data.

3) For the ten compositions of the low-alloy steels presented in Table 2, small variations in the cooling rates at different locations in the fusion zone did not result in significant spatial variations of the microstructure in the fusion zone.

4) Theoretical calculations indicate that for a small difference in the cooling rate at different locations, for certain weld compositions (e.g., Fe-0.07C-0.45Si-1.0Mn-0.5Ni-1.0Mo-2.25Cr (wt-%)), significant microstructural variation may result in the weldment. This can lead to spatial variation of the properties in the weld metal.

5) The above calculation features and the agreement between experimental and predicted measurements indicate significant promise for predicting weld metal microstructure evolution and properties in fusion welds, for any given low-alloy steel composition and welding process, from the fundamentals of transport phenomena.

Acknowledgments

The authors are grateful to Dr. H. K. D. H. Bhadeshia, Department of Materials Science and Metallurgy, University of Cambridge, Cambridge, U.K., for allowing the authors to use his computer program to predict microstructure in steel welds. This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science, under grant numbers DE-FG02-84ER45158 with Pennsylvania State University and DE-AC05-84OR22140 with Martin Marietta Energy Systems, Inc.

References