Role of Thermophysical Properties in Weld Pool Modeling

The effects of variations in thermophysical properties in models on heat transfer and fluid flow is examined

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ABSTRACT. The results of numerical simulation of heat transfer and fluid flow in the weld pool strongly depend on the physical processes considered and the input data used in the model. The aim of this paper is to examine the impact of the thermophysical properties on the results of such calculations. The effects of various thermophysical properties such as the viscosity, thermal diffusivities of both the solid and liquid, the temperature coefficient of surface tension and the energy absorption coefficient on the depth and the diameter of the weld pool, and the weld pool surface velocities and temperature distributions are analyzed. The relative importance of the various thermophysical properties are identified from the computed results.

Introduction

The structure and properties of the welds are strongly affected by heat transfer and metal flow in the weld pool and alloying element loss from the weld surface. Although the diagnostic techniques for measuring pool temperatures are currently being evaluated and developed, direct reliable measurements of velocities, temperatures and species concentrations in the weld pool are extremely difficult since the weld pool is small in size and often covered by an intense plasma (Refs. 1–3). A recourse is to simulate the temperature and velocity fields by mathematical modeling of the essential physical features of a welding process. For the prediction of the weld pool geometry, the temperature fields and the cooling rates, the traditional heat conduction models (Refs. 4–6) are being increasingly replaced by more accurate calculation procedures (Refs. 7–22), which take into account the weld pool convection due to the combined effects of the buoyancy, electromagnetic and the surface tension forces. Indeed, the modeling of heat transfer, fluid flow and mass transfer has already been successful in revealing detailed insight about various aspects of the welding process which could not have been obtained otherwise.

Despite the success of the modeling approach in welding, insufficient help is available to most beginner researchers to enable them to meaningfully apply this powerful tool to achieve trustworthy results in a realistic time frame. Currently, there are at least two main difficulties in using mathematical modeling to solve welding problems. First, since the welding processes are more complicated than most other high-temperature thermochemical processes, practical simulation of heat and mass transfer and fluid flow in the weld pool mandates considerable simplification in the modeling efforts. A fully comprehensive modeling of weld pool heat transfer and fluid flow is computationally intensive. As a consequence, one is confronted with the precarious task of having to make some sort of judgment about what level of simplification is adequate for a particular application. In practice, this involves making a decision to choose, often without any objective basis, which physical processes are to be considered important and emphasized in the construction of the model and which others must be considered as less important details and, consequently, greatly simplified or even completely ignored in the mathematical framework. Recent welding simulation literature is a testimony of the large numbers of such choices. Three-dimensional vs. two-dimensional simulations, transient vs. steady state, flat weld pool surface vs. free deformable surface, laminar structure of flow in the weld pool vs. turbulent flow simulated using various turbulence models of different degrees of sophistication are all examples of the choices that must be consciously made prior to undertaking the numerical simulation. While it is expedient to weigh heavily in favor of a particular set of simplifications because of the availability of an existing software or other computational conveniences, the consequences of such choices vary depending upon the goals of the simulation effort.

KEY WORDS

Weld Pool Modeling
Thermophysical Prop.
Numerical Simulation
Heat Transfer
Fluid Flow
Viscosity
Thermal Diffusivity
Surface Tension
Power Absorption
Weld Pool Simulation

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A more fundamental limitation is imposed by the lack of necessary thermophysical data required for the calculations. Our existing database of high-temperature materials processing was developed, to a large extent, to understand the manufacture and the subsequent processing or use of metals and alloys. Unlike welding, these operations are seldom carried out at a temperature much above the melting point of metals. Furthermore, in most thermochemical processing, the processing environment does not contain plasma. In contrast, in many welding operations, the peak temperature in the weld pool can reach very close to the boiling point of the metal and the weld metal is surrounded by plasma. Thermophysical data for such high-temperature systems are scarce, if not unavailable. Thus, apart from the difficulty in adapting rigorous simulation of the highly complex welding process, an in-depth understanding of the behavior of the welding process is often impeded by the lack of appropriate thermophysical data.

The authors have recently investigated the difference in the computed results obtained by using temperature-dependent and constant thermophysical properties (Refs. 21, 22). The analysis showed that if the temperature dependency of physical properties is not considered, significant inaccuracies in the predictions can occur. Since material properties are temperature dependent, the actual temperature experienced by the weld can influence weld pool development by altering physical properties. This was also clearly demonstrated in the previous study of surface tension effects (Refs. 18, 19) where the development of the weld pool was found to be very sensitive to changes in surface tension brought about by changes in the peak temperatures experienced in the molten weld pool. Therefore, it is of vital importance that computational modeling studies of the welding processes consider accurate representation of the material properties.

In the present study, the relative importance of the various material properties are considered. The impact of the variation in thermophysical properties on the calculation of heat transfer and fluid flow in welding is examined. It is to be emphasized here that the calculations were done for various combinations of constant thermophysical properties since the objective was to find out the sensitivity of the results to these properties. Laser beam welding in the conduction mode is utilized as an example, since both the buoyancy and the electromagnetic forces can be neglected for simulation. The roles of liquid metal viscosity, temperature coefficient of surface tension, laser beam absorption coefficient, and the thermal diffusivities of solid and liquid metal on the pool geometry and the velocity and temperature distributions are discussed in this paper.

Theoretical Considerations

In laser beam welding, the absorption of the laser beam energy produces a molten pool rapidly and a steady-state is reached in a very short time (Ref. 18). The steady state heat transfer and fluid flow phenomena in the axisymmetric laser melted pool are represented by the following equations of conservation of mass, momentum and enthalpy.

Conservation of Mass:

$$\frac{1}{r}\frac{\partial}{\partial r}(\rho r u_r)+\frac{\partial}{\partial z}(\rho u_z)=0 \tag{1}$$

Conservation of Momentum:

Radial Direction:

$$\rho u_r\frac{\partial u_r}{\partial r}+\rho u_z\frac{\partial u_r}{\partial z}= -\frac{\partial p}{\partial r}-\mu\left\{\frac{\partial^2 u_r}{\partial r^2}+\frac{\partial^2 u_r}{\partial z^2}+\left(\frac{1}{r}\frac{\partial u_r}{\partial r}-\frac{u_r}{r^2}\right)\right\} \tag{2}$$

Axial Direction:

$$\rho u_r\frac{\partial u_z}{\partial r}+\rho u_z\frac{\partial u_z}{\partial z}= -\frac{\partial p}{\partial z}-\mu\left(\frac{\partial^2 u_z}{\partial r^2}+\frac{\partial^2 u_z}{\partial z^2}+\frac{1}{r}\frac{\partial u_z}{\partial r}\right)+\rho\, g_z \tag{3}$$

Conservation of Enthalpy:

$$\frac{\partial}{\partial z}(\rho\, u_z\, \Phi)+\frac{1}{r}\frac{\partial}{\partial r}(\rho\, u_r\, \Phi\, r)= \frac{\partial}{\partial z}\left\{\frac{k}{c_p}\left(\frac{\partial \Phi}{\partial z}\right)\right\}+\frac{1}{r}\frac{\partial}{\partial r}\left\{\frac{k}{c_p}\left(r\frac{\partial \Phi}{\partial z}\right)\right\}+S_\Phi(r) \tag{4}$$

where u is the velocity; r and z are the radial and the axial direction indicators, respectively; p is the density; μ is the viscosity; p is the pressure; c_p is the specific heat; k is the thermal conductivity; Φ is the enthalpy and $S_\Phi(r)$ is the source of enthalpy and represents the absorption of energy from the laser beam. The power density distribution of the laser beam, J_Φ, is assumed to be Gaussian in nature and is given by the following equation:

$$J_\Phi(r)=\frac{3Q}{\pi r_b^{\,2}}e^{\left(-\frac{3r^2}{r_b^{\,2}}\right)} \tag{5}$$

where Q is the power input and r_b is the beam radius. The local values of the source of enthalpy, $S_\Phi(r)$, are obtained from laser power distribution.

The calculations were performed for two-dimensional, steady, incompressible flow. The boundary conditions included the prescription of the heat exchange between the surface of the sample and the laser beam by Equation 5. At the bottom and the sides of the plate, the conduction heat flux was equated to the convection flux. At the surface of the weld pool, the Marangoni effect was incorporated by equating the shear stress to the spatial gradient of surface tension. At the solid-liquid interface, the curved weld pool boundary was approximated by a series of steps, and the velocities were prescribed to be zero, which amounts to an assumption of no-slip between the liquid and the solid surface. At the axis of the pool, the velocity and the enthalpy gradients were taken to be zero on the basis of geometric symmetry. Since the objective of this part of the work is to investigate the role of thermophysical properties, free surface deformation was not considered for simplification. Furthermore, all densimetric effects were ignored.

The governing equations were represented in a finite difference form and solved iteratively on a line-by-line basis utilizing a Tri-Diagonal Matrix Algorithm (TDMA). The Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) algorithm was employed for the discretization of the equations. The details of the procedure are described elsewhere (Ref. 23). Due to symmetry with respect to the center plane, the calculations were done only for one side of the plane. The model used a 40 X 40 fixed rectangular grid system for the calculation of the enthalpies and velocities. A steady state was assumed to have been reached when the differences in the amount of heat inflow at the surface and the heat outflow at the walls was less than 1%. When this condition was satisfied, the difference between the successive iterated values of enthalpies and the velocities was very small.

Results and Discussion

Values of several important thermophysical properties are necessary to simulate heat transfer and fluid flow in the weld pool. The density and viscosity data are required for the solution of the equations of conservation of mass and momentum. Similarly, values of thermal conductivity, specific heat and density are necessary for the solution of the equation of conservation of enthalpy. However, the thermal conductivity and the specific heat appear as a single variable, k/C_p. The values of energy absorption coefficient and the laser beam power density distribution are needed to define the energy influx at the surface. Furthermore, one needs to know the temperature dependence of surface ten-

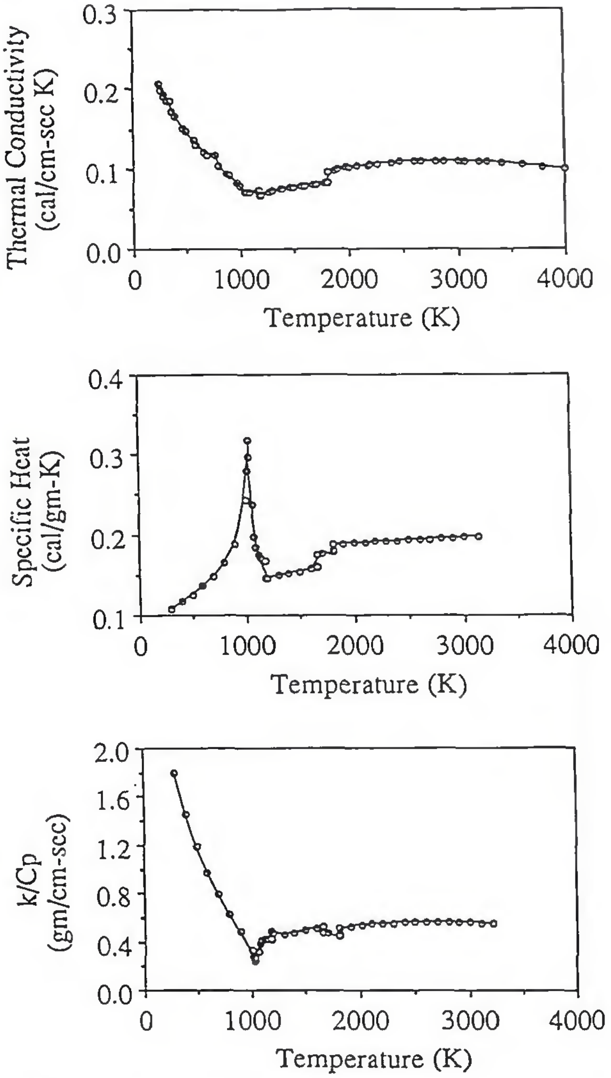

Fig. 1 — Variation of thermal conductivity, k, specific heat, C_p, and k/C_p as a function of temperature for iron.

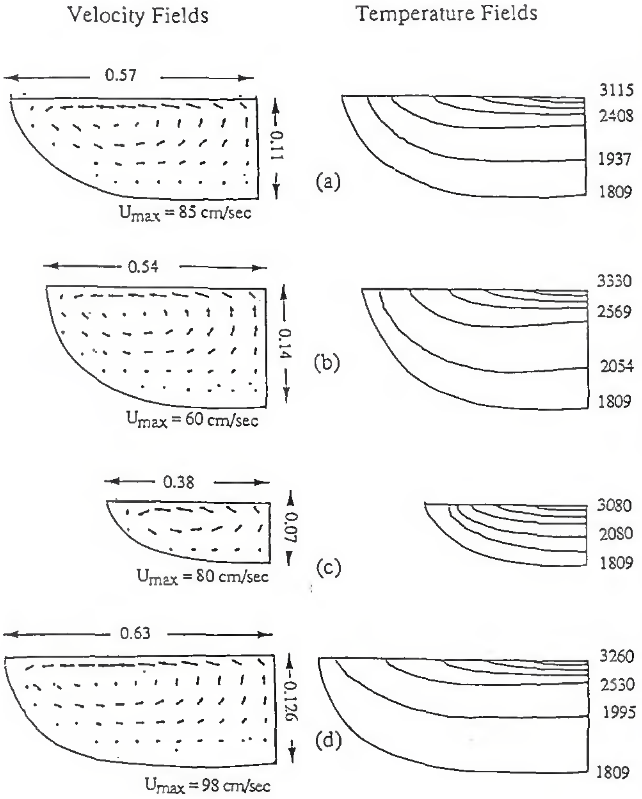

Fig. 2 — Velocity and temperature fields for four different cases. A — Data used from Table 1; B — viscosity used is 1.0 gm/cm-s; C — k/C_p of solid used is 0.48 gm/cm-s; D — absorption coefficient used is 0.18. All dimensions are in mm and temperatures in K.

sion, $d\gamma/dT$, to calculate the shear stress at the weld pool surface. Thus, for a constant density and given laser beam power density distribution, the important properties required for the calculations are the absorption coefficient, the temperature coefficient of surface tension, viscosity of the molten metal, the ratio of thermal conductivity and the specific heat for both the solid and the liquid phases. The plots of specific heat, C_p, thermal conductivity, k, and their ratio, k/C_p for iron as functions of temperature are presented in Fig. 1. It is observed from Fig. 1 that for solid iron, the values of k/C_p vary from 0.24 gm/cm-s to 1.8 gm/cm-s. However, since temperature-independent constant values of k/C_p of solid are frequently used in the literature, it is important to understand the consequences of such practice.

Figure 2 shows the velocity and temperature fields for four different cases. The enthalpies were converted to temperatures using data presented in Fig. 3. The values of the thermophysical properties used for the calculations are indicated in Table 1. It is observed from the computed results that depending on the values of the thermophysical properties used, the pool geometry, the temperature and the velocity fields can vary significantly.

In heat transfer and fluid flow calculations, enhanced values of viscosities are commonly used to simulate the effects of turbulence. Depending on the particular turbulence model adapted, the computed values of effective viscosity and its spatial distribution vary significantly. Furthermore, high values of viscosity are also utilized to achieve numerical stability in computations. In fact, for the welding of a given material, a wide range of viscosity values have been used by various investigators for weld pool modeling. The computed values of width, depth and aspect ratio of the weld pool, the maximum velocity and peak temperature, and the Peclet number for heat transport are plotted as a function of viscosity in Fig. 4. The Peclet number is a measure of the relative magnitudes of convective and diffusive heat trans-

Table 1—Data Used for Calculations

Property/Parameter	Value
Density (gm/cm^3)	7.80
Melting Point (K)	1809.0
Laser Power (watts)	500.0
Radius of the Beam (cm)	0.02
Viscosity (gm/cm-s)	0.40
k/Cp of Solid (gm/cm-s)	0.24
k/Cp of Liquid (gm/cm-s)	0.54
Absorption Coefficient	0.15
Temperature Coefficient of Surface Tension (dyne/cm-s)	−0.50

port and is given by: Pe = $U_{max}L/\kappa$, where U_{max} is the maximum velocity, L is the characteristic length that can be taken as the radius of the laser beam and κ is the thermal diffusivity of the liquid metal given by $k/\rho C_p$.

The role of viscosity can be investigated from its effect on the Peclet number. Since the Marangoni flow boundary condition is implemented at the weld pool surface, choice of high viscosity values in the computations leads to weak surface velocities and, consequently, low Peclet numbers. Therefore, the convective heat transfer becomes less important when a high value of viscosity is used. A direct consequence of the diminished role of convection is manifested in the rise of the peak temperature at the surface of the weld pool. The computed results indicate a peak temperature rise by more than 200 K when the viscosity is increased from 0.1 to 1.0 gm/cm-s. A high value of viscosity im-

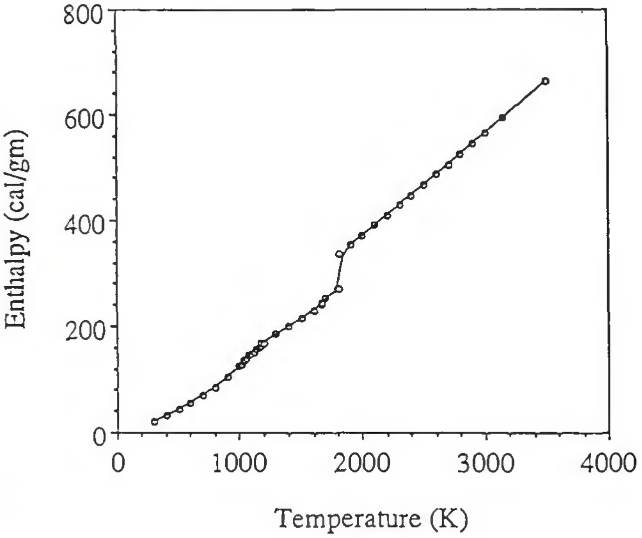

Fig. 3 — Enthalpy vs. temperature curve for iron.

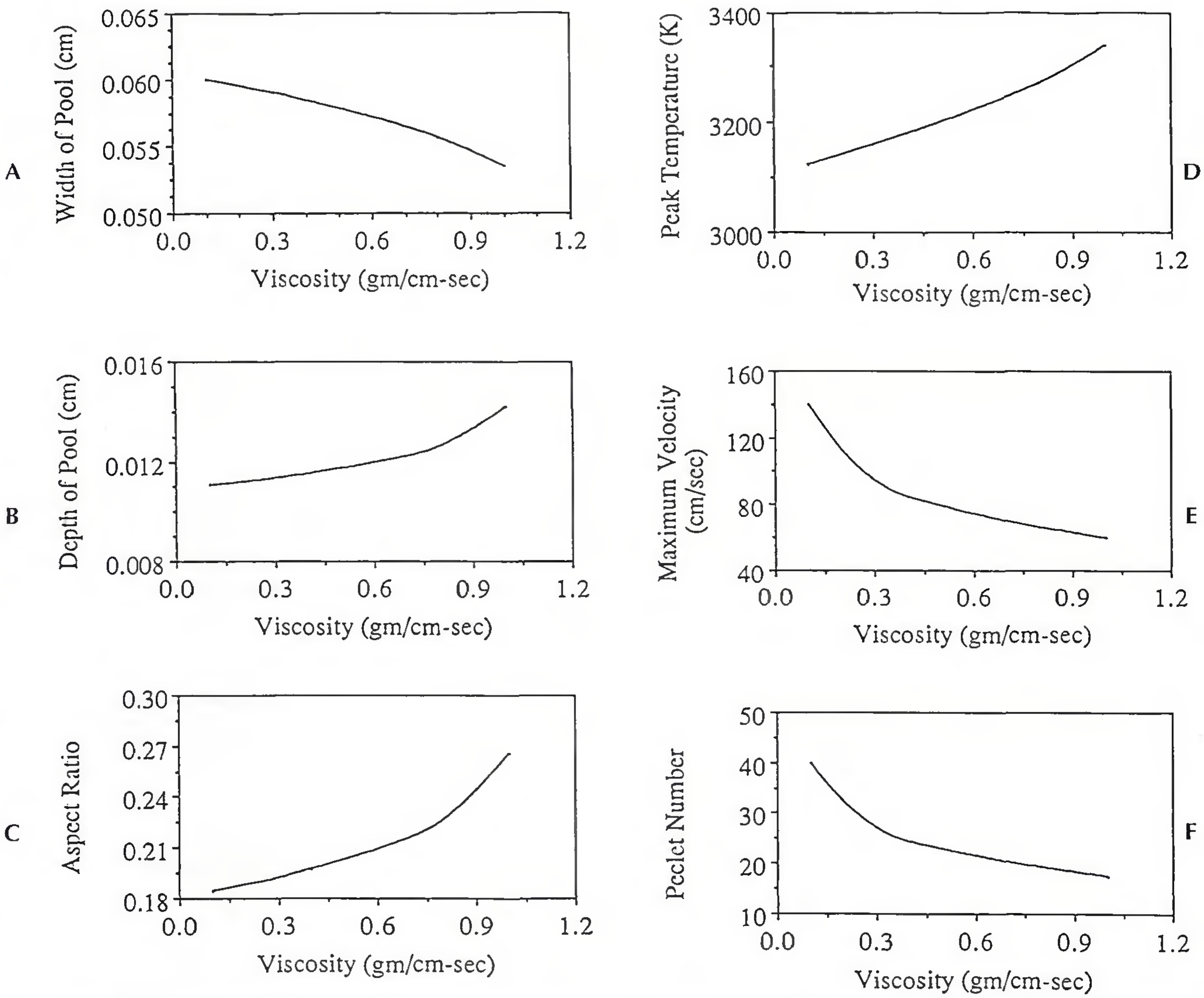

Fig. 4 — Effect of viscosity on: A — diameter; B — depth; C — aspect ratio of the weld pool; D — the peak temperature; E — maximum surface velocity; F — the Peclet number for heat transfer.

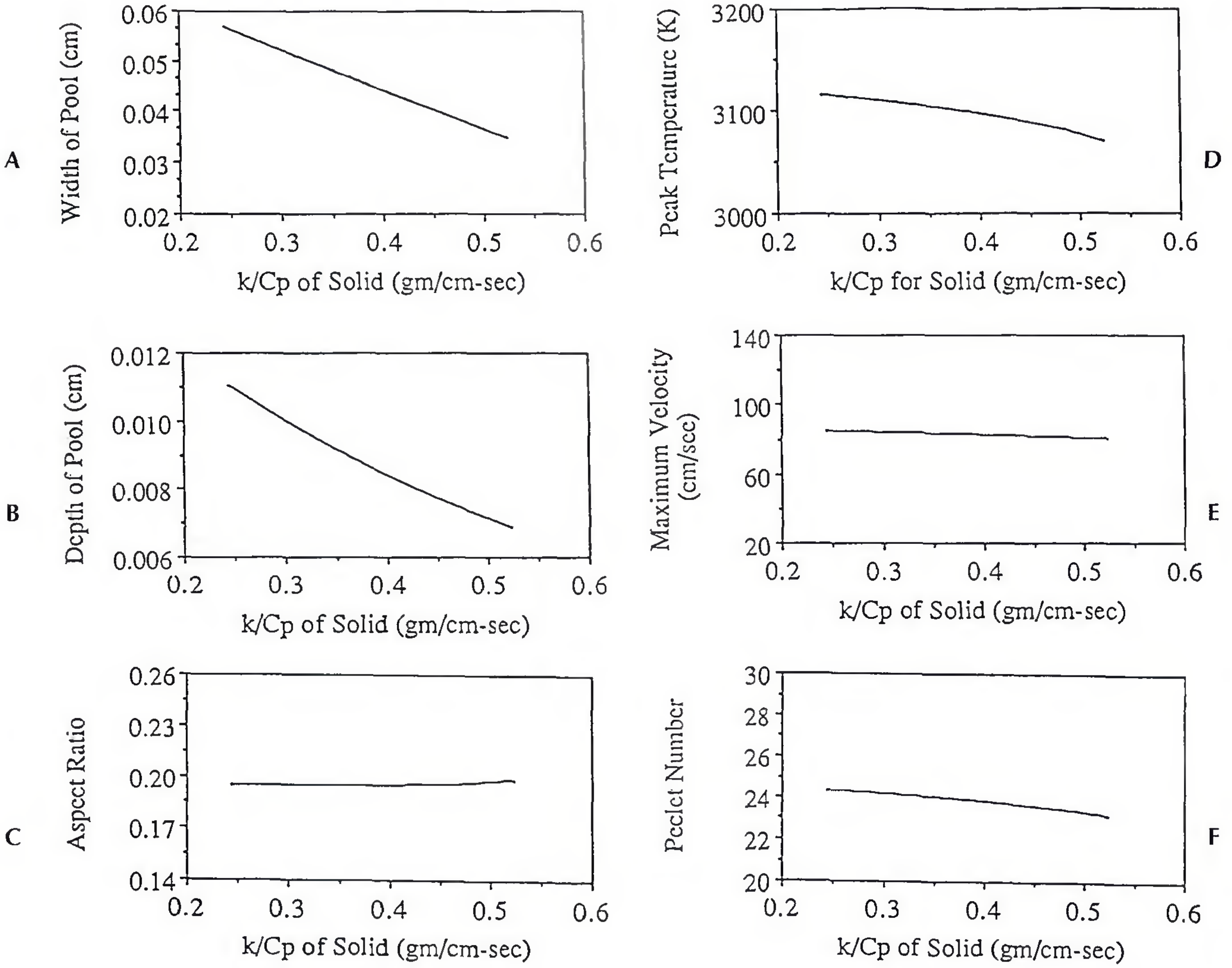

Fig. 5 — Effects of k/C_p of solid on: A — diameter; B — depth; C — aspect ratio of the weld pool; D — the peak temperature; E — maximum surface velocity; F — the Peclet number for heat transfer.

plies a major role of conduction heat transfer. For example, the use of an infinitely large viscosity amounts to solving heat conduction equation in the weld pool. Lancaster (Ref. 24) has demonstrated that the use of conduction models always results in high peak temperatures. When high values of viscosity are used, the weak surface velocities and negative value of the temperature dependence of surface tension lead to smaller width and larger depth of the weld pool and, consequently, higher depth-to-width ratio, commonly described as the aspect ratio. The variation in the viscosity from 0.1 to 1.0 gm/cm-s results in the increase in aspect ratio by 30%. However, it is to be pointed out here that the trends in the variation of the various simulated results will change when one considers positive temperature coefficient of surface tension. For example, when the temperature coefficient of surface tension is positive, an increase in the viscosity will result in a decrease in radially inward-directed velocity, a decreased depth and increased width, and as a consequence, a decreased aspect ratio. However, since the purpose of the investigation is to bring out the sensitivity of the properties used on the calculated results, the trends in the variation of the results are explained only for the case when the temperature coefficient of surface tension is negative.

The spatial distribution of viscosity in strongly agitated turbulent systems is computed using an appropriate turbulence model. The currently available turbulence models were formulated to deal with mainly parabolic flows in large systems where the physical dimensions were much larger than the width of the weld pool. In laser melted weld pools, the dimensions are often of the order of milimeters and the velocities can reach up to about a meter a second. The occurrence of large recirculating velocities in a small region in the weld pool makes the structure of the flow in laser melted weld pools very different from the flow structure encountered in most other materials processing systems. The validity of the currently available turbulence models for the modeling of the weld pool is therefore open to question. Thus, in the absence of adequate knowledge about the structure of fluid flow in weld pools, the values of viscosity are currently prescribed somewhat arbitrarily.

Thermal diffusivity of solid is an important thermophysical property which influences the geometry of the weld pool. In the literature, widely different values of k/C_p of solid have been used for the same material. The effects of k/C_p on the weld pool geometry, peak temperature and the maximum surface velocity are presented in Fig. 5. Both the width and the depth of the pool decrease with an increase in the k/C_p value. For example, when the value of k/C_p is increased from 0.24 to 0.52 gm/cm-s, both

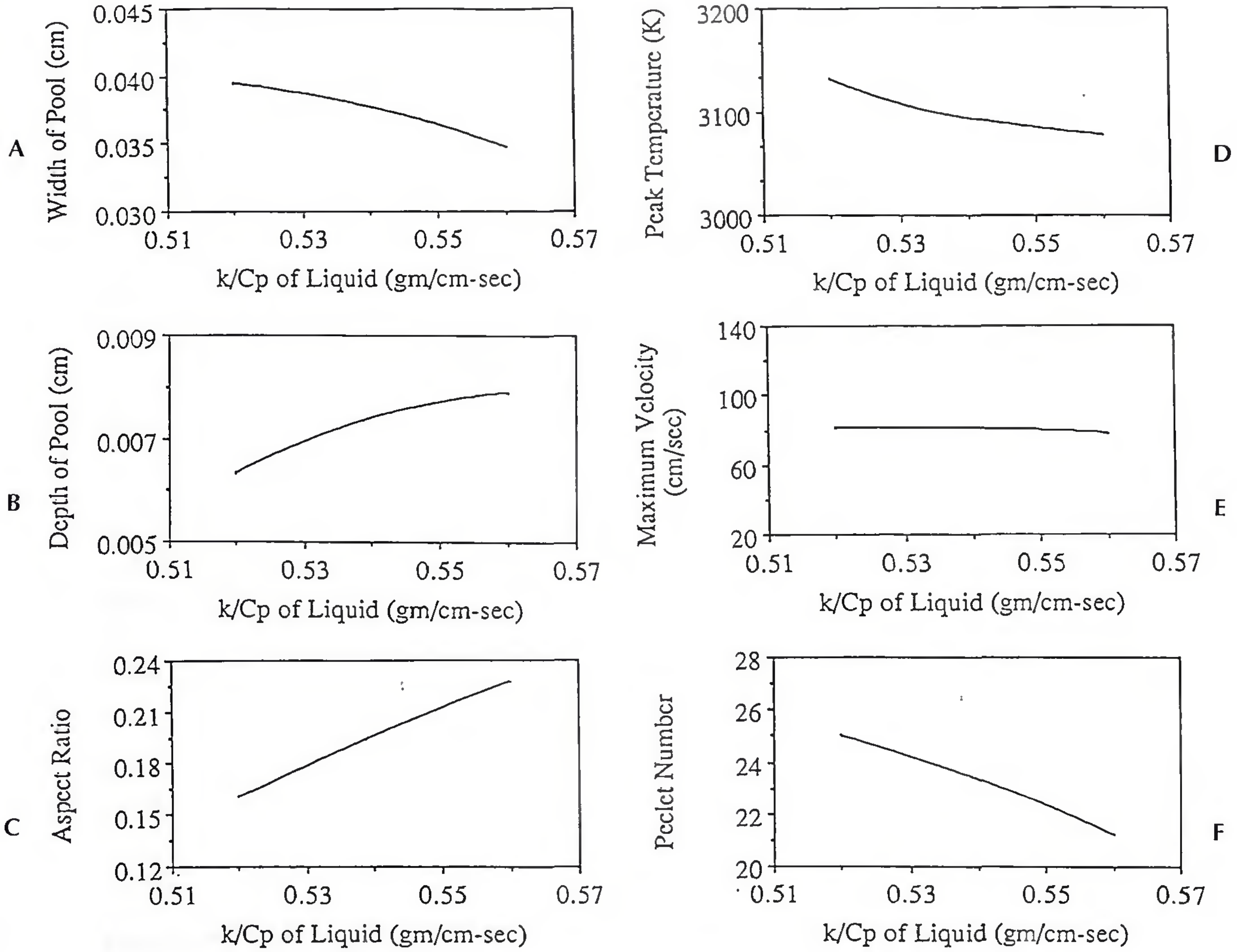

Fig. 6— Effects of k/C_p of liquid on: A — diameter; B — depth; C — aspect ratio of the weld pool; D — the peak temperature; E — maximum surface velocity; F — the Peclet number for heat transfer. The value of k/C_p of solid used was 0.5 gm/cm-s.

parameters decrease by more than 35%. The trend is consistent with faster heat conduction in the solid, and since the heat influx at the surface is constant, the heat is more rapidly conducted away from the weld pool. Furthermore, with the increase in k/C_p, the total enthalpy of the pool decreases, and this results in low peak temperatures on the surface of the molten pool. However, the maximum velocity at the pool surface is not significantly affected, since the decreased temperature is accompanied by lower weld pool width, and consequently, the temperature gradient induced Marangoni stress does not change significantly. Thus, it is evident that the choice of k/C_p can significantly change the depth and the width of the pool and the peak temperature. However, no significant change in either the maximum velocity or the aspect ratio is observed.

For a given material, a wide range of values of thermal conductivity of liquid have been reported for the calculations of heat transfer and fluid flow in the weld pool. The effects of k/C_p of liquid on the various parameters are indicated in Fig. 6. The role of this parameter can be understood from the way it influences the heat distribution in the molten pool. A high value of k/C_p implies that there is less resistance to heat flow in the pool and the heat absorbed at the surface reaches the liquid-solid interface easily. For high values of k/C_p, a given amount of heat is more uniformly distributed in the pool, resulting in low peak temperatures, as can be observed from the figure. Since the thermal diffusivity of the solid at low temperatures is higher than the thermal diffusivity of the liquid, the heat is rapidly conducted away from the interface. The higher diffusivity also results in a smaller weld pool as is evident from the figure. Although the maximum surface velocity is insensitive to the thermal diffusivity of the liquid, the Peclet number decreases with the increase in thermal diffusivity of the solid. The decrease in the Peclet number is reflected in the decrease in width and increase in the depth of the weld pool, and as a consequence, in the increased aspect ratio of the pool. The aspect ratio changes by more than 30% when the k/C_p changes by less than 10%. Thus, it is evident that the value of thermal diffusivity of the liquid has a significant influence on the results of numerical simulation.

For a given power density distribution on the substrate surface, the absorption coefficient of the material determines the amount of the energy that is absorbed by the material. For a given material, its value depends on the temperature, wavelength of the laser and the nature of the surface finish of the material (Ref. 25). Traditionally, a time- and temperature-independent constant value of absorption coefficient has been used in the modeling of the weld pool. The effects of the absorption coefficient in determining weld pool width, depth, peak temperature, maximum surface velocity and Peclet number are presented in Fig. 7. An increase in the absorption coefficient results in an increase in both

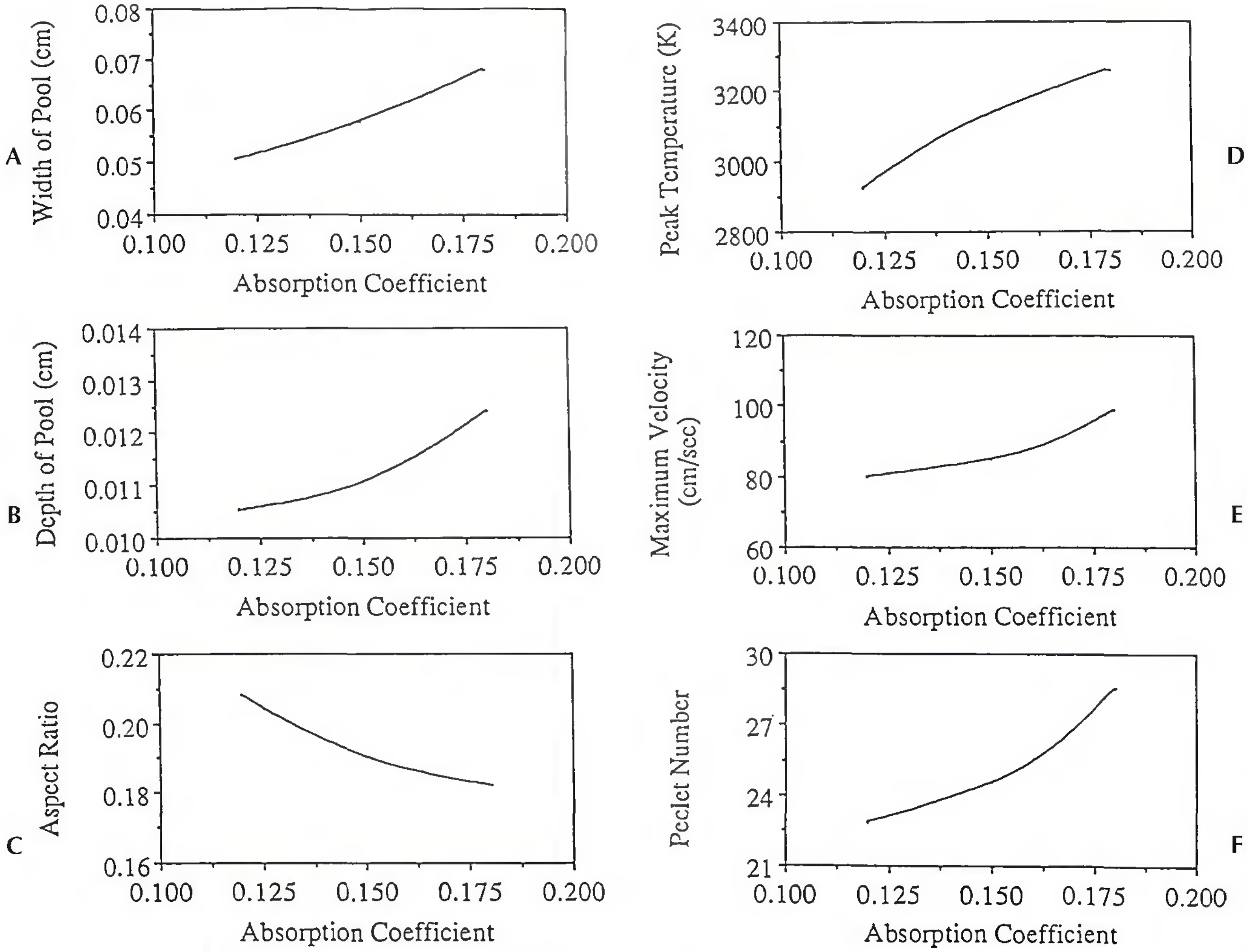

Fig. 7 — Effects of absorption coefficient on: A — diameter; B — depth; C — aspect ratio of the weld pool; D — the peak temperature; E — maximum surface velocity; F — the Peclet number for heat transfer.

the depth and width as a consequence of high power. The aspect ratio of the pool shows a modest decrease. Furthermore, the peak temperature, the velocity and the Peclet number are increased.

The temperature coefficient of surface tension is an important parameter in defining the geometry of the weld pool. The Marangoni stress, the main driving force for fluid flow in laser melted weld pools, is directly related to the temperature coefficient of surface tension, dγ/dT. In the literature, there is a wide discrepancy in the reported values of surface tension and its temperature coefficient for most metals, especially at high temperatures. In addition, the presence of a small amount of surface active impurity in metals results in significant changes in the values of dγ/dT. The effects of dγ/dT on the weld pool geometry, peak temperature and maximum surface velocity are presented in Fig. 8. The effect of an increase in dγ/dT is very similar to the effect of decrease in viscosity. An increase in dγ/dT results in an increased shear stress and surface velocities. The Peclet number increases, resulting in increased width and decreased depth of the weld pool. Thus, the aspect ratio decreases. The increased Peclet number also results in lower peak temperatures at the center of the pool due to enhanced convective heat transfer.

From the computed results presented in this paper, it is possible to examine what choice of material properties can produce a particular effect in the computed results. For example, a combination of high values of energy absorption coefficient, viscosity, thermal diffusivity of the liquid and low values of the thermal diffusivity of the solid leads to prediction of a large weld pool size. Similarly, low values of energy absorption coefficient, viscosity, thermal diffusivity of the liquid and high values of the thermal diffusivity of the solid leads to prediction of small weld pool size. Similarly, a given aspect ratio of the weld pool can result from other suitable combinations of thermophysical properties. Since there is significant discrepancy in the reported values of thermophysical properties in the literature, special care is needed to select accurate values of these properties.

Summary and Conclusions

The effects of thermophysical properties such as viscosity, thermal diffusivities of both the liquid and solid, temperature coefficient of surface tension and power absorption coefficient on important welding parameters such as the weld pool geometry, the maximum surface velocity and the peak temperature were determined. The results indicate that the viscosity, thermal diffusivity and the temperature coefficient of surface tension are the most crucial parameters. Thus, temperature-dependent values of thermal diffusivity and accurate values of the temperature coefficient of surface tension are crucial for realistic simulation of weld pool behavior. Although the need for accurate prescription of the viscosity data cannot be overemphasized, such need can only be met with new in-

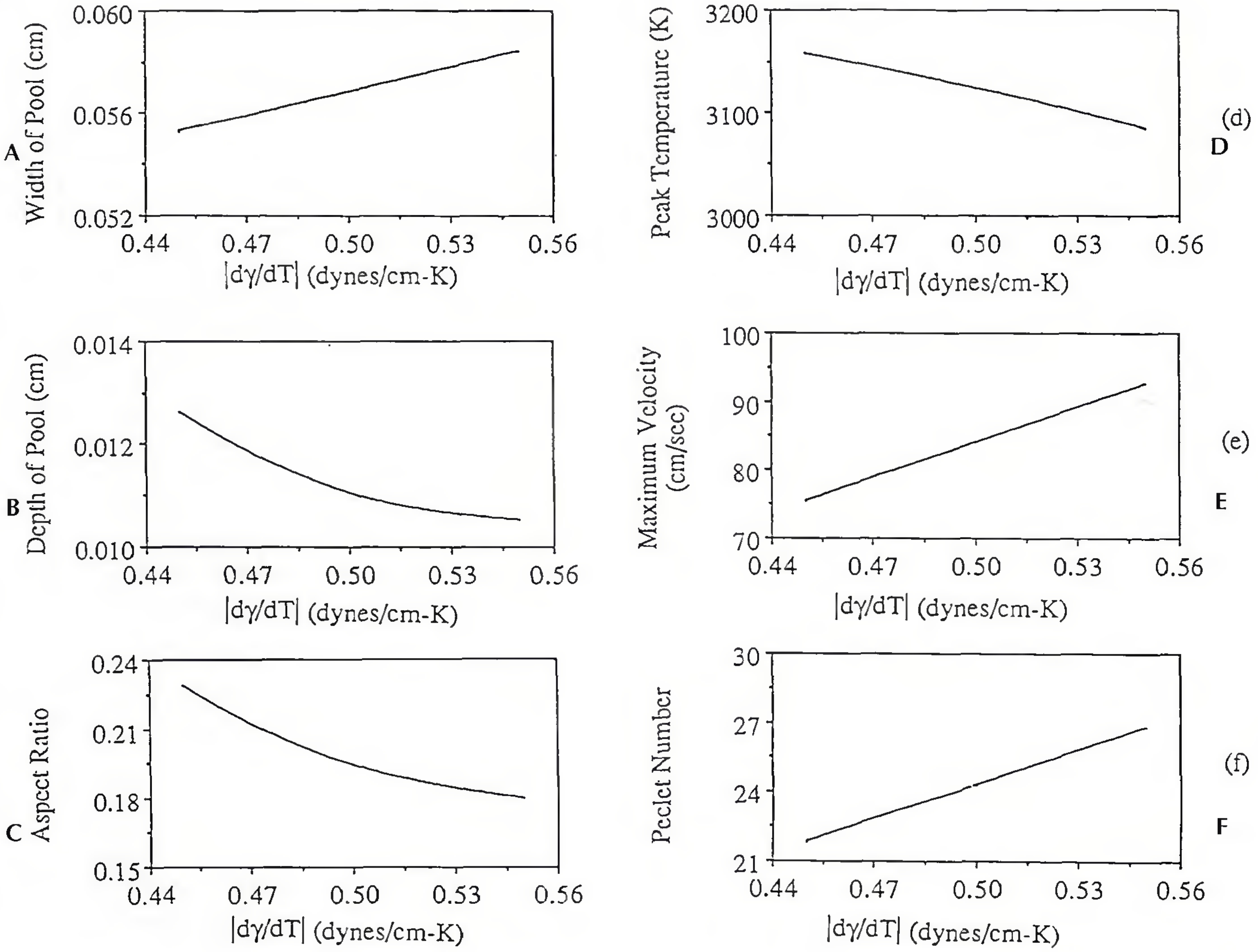

Fig. 8 — Effects of temperature coefficient of surface tension on: A — diameter; B — depth; C — aspect ratio of the weld pool; D — the peak temperature; E — maximum surface velocity; F — the Peclet number for heat transfer.

depth experimental and theoretical research on the structure of fluid flow in the weld pool.

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