A SMART BI-DIRECTIONAL MODEL OF HEAT TRANSFER AND FREE SURFACE FLOW IN GAS-METAL-ARC FILLET WELDING FOR PRACTISING ENGINEERS

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ABSTRACT

In recent years, numerical heat transfer and fluid flow models have provided significant insight about fusion welding processes and welded materials. A major problem in their practical utility is that several input parameters cannot be easily prescribed from fundamental principles. Available inverse models of fusion welding for the determination of these unknown parameters have ignored important physical processes such as convection in the weld pool to make computational tasks tractable. As a result, these models are not very different from the neural network type models that are not required to obey any physical law. A smart, bi-directional, numerical model has been developed to determine three-dimensional temperature and velocity profiles, weld geometry and the shape of the solidified weld reinforcement surface during gas metal arc (GMA) welding of fillet joints. Apart from the transition of heat from the welding arc, additional heat from the metal droplets was also considered in the model. The model is capable of estimating unknown parameters such as the arc efficiency, effective thermal conductivity and effective viscosity from a limited number of data on weld geometry based on multivariable optimisation. Alternative strategies for the optimisation are examined. The calculated shape and size of the fusion zone, finger penetration characteristic of the GMA welds and the solidified free surface profile were in fair agreement with the experimental results for various welding conditions. In particular, the computed values of the leg length, the penetration depth and the actual throat agreed well with those measured experimentally for various heat inputs. The weld thermal cycles and the cooling rates were also in good agreement with the independent experimental data. The research presented here shows that advances in computational hardware and software have now made construction of smart, bi-directional, large transport phenomena based phenomenological models a useful undertaking.

IIW-Thesaurus keywords: Arc welding; Gas shielded arc welding; GMA welding; Fillet welds; Mathematical models; Computation; Optimisation; Heat flow; Viscosity; Physical properties; Thermal conductivity; Thermal properties; Thermal cycling; Process conditions; Leg length; Dimensions; Sizes; Statistical methods; Reference lists.

1 INTRODUCTION

In the previous two decades, application of transport phenomena has resulted in improved understanding of complex fusion welding processes and welded materials. For example, numerical calculation of heat transfer and fluid flow in welding have enabled accurate quantitative calculations of thermal cycles and fusion zone geometry [1-5]. In many simple systems, the co-rotated thermal cycles have been used to quantitatively understand weld metal composition and phase composition, grain structure and inclusion structure. Capabilities to quantitatively understand geometry, composition and structure of welds in simple systems have provided hope that that one day welding engineers may be able to use numerical models to tailor weldment characteristics [5-10] to meet specificities. In reality, the numerical heat transfer and fluid flow codes for fusion welding have so far been used mostly as a research tool rather than in the industry. There are several reasons for the restricted use of these advanced tools. An important difficulty is the need for very few input parameters that cannot be easily specified.

Current computer models for calculation of heat transfer and fluid flow in fusion welding require many input parameters to define the welding system such as the system geometry, welding variables, and thermophysical data. Several of these parameters such as the welding current, voltage and welding speed can be easily specified with a reasonable degree of certainty. However, the arc efficiency, effective thermal conductivity and the effective viscosity of the liquid metal in weld pool are the three important examples which are required for weld pool modelling [1, 11]. Values of these parameters are important, since they allow accurate modelling of the high rates
of transport of heat and mass in systems with strong fluctuating velocities that are inevitable in small weld pools with very strong convection currents [11-13]. Since fluctuating components of velocities exist in small weld pools with strong mean recirculating velocities, a regular practice has been to consider an enhancement in the values of liquid thermal conductivity and viscosity above their corresponding molecular values. Alternatively, the two-equation k-ε turbulence model [11-14] has also been applied in estimating effective thermal conductivity and thermal con- ductivity in weld pool. However, the application of the two-equation k-ε turbulence model and the associated empirical constants, which was originally developed to model parabolic fluid flow in large systems (such as pipes), in small scale weld pools with elliptic flow is open to question. Thus, no unified basis to confidently pre- script the enhancements been for thermal conductivity and viscosity in weld pool based on scientific principles are available [15] to date. The present work attempts to outline a modeling procedure utilizing the power of a phenomenological field transfer and fluid flow model and an optimisation algorithm to estimate these parameters as a function of power input. Due to narrow range of experimental data set, variation of arc efficiency, effective thermal conductivity and effective viscosity is consid- ered to be linear with input power. So, now we need six variables i.e. constant terms and the slopes of the linear functions to define the arc efficiency, effective ther- mal conductivity and effective viscosity. These unknown values can then be used in a numerical heat transfer and fluid flow model under similar welding conditions. Two interactive computational modules are embedded into the present smart model - one for the analysis of heat transfer and fluid flow in fusion welding and the other for the optimisation of the unknown parameters. The optimisation procedure attempts to estimate the unknown parameters by learning the sensitivity of the known variables with respect to the unknown parama- ters. The sensitivity terms have to be calculated by run- ning the heat transfer and fluid flow model several times for small changes in the unknown parameters. The mod- eling procedure can be computationally very intensive and so far have been based on rather simple heat con- duction equation, often utilizing Rosenthal's analytical solution that completely ignored convection in the weld pool. Furthermore, the primary focus of these works was to determine the distribution of heat flux at the work- piece surface exposed to an arc or a laser beam from measured temperatures at several monitoring locations in the solid region. It seems that the adaptation of the simplified heat-conduction equation in the present work was mandated, at least to a large extent, because of the lack of fast computers and advanced software neces- sary to rigorously analyse heat and fluid flow in the weldment. With the advances in the computational hard- ware and software in recent years, it is now possible to undertake computationally intensive optimisation schemes that embody realistic three-dimensional numer- ical heat transfer and fluid flow calculations. Since the optimisation routine principally learns from the results obtained from the actual weld pool modeling calcula- tions, any simplification in the latter will have a strong influence on the accuracy and reliability of the estimated results of unknown parameters. Thus, the inclusion of a three-dimensional heat transfer and fluid flow model for weld pool simulation in the present work is certainly desirable if not necessary. Furthermore, the approach adopted here is inherently different from the neural net- work technique where its input and output variables are related through a set of hidden nodes and their rela- tionships do not have to comply with any physical law. In contrast, when the optimisation algorithm embodies a heat transfer and fluid flow model, as adopted in the research reported in this paper, the input welding param- eters and the output weld pool geometry are dictated by a phenomenological framework of the equations of conservation of mass, momentum and energy. In effect, the complete procedural scheme acts as a smart model that identifies important unknown parameters in an itera- tive manner starting from a set of their initial guessed values exploiting the phenomenological framework. The goal of the present work is to estimate the variation of efficiency, effective thermal conductivity and effective viscosity with input power through an inverse modelling approach which includes a combination of an optimisation algorithm, a heat transfer and fluid flow model and, a set of experimentally measured weld pool penetrat- ion, throat and the leg length. Table 1 presents the

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Contact tube to workplace distance (CTWD) (mm)</th>
<th>Wire feeding rate (mm/s)</th>
<th>Travel speed (mm/s)</th>
<th>Voltage (V)</th>
<th>Estimated current (A)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>22.2</td>
<td>211.7</td>
<td>42</td>
<td>31</td>
<td>312.0</td>
</tr>
<tr>
<td>2</td>
<td>22.2</td>
<td>169.3</td>
<td>42</td>
<td>31</td>
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<tr>
<td>3</td>
<td>22.2</td>
<td>169.3</td>
<td>42</td>
<td>33</td>
<td>312.0</td>
</tr>
<tr>
<td>4</td>
<td>22.2</td>
<td>211.7</td>
<td>4.2</td>
<td>33</td>
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</tr>
<tr>
<td>5</td>
<td>28.6</td>
<td>211.7</td>
<td>4.2</td>
<td>31</td>
<td>306.6</td>
</tr>
<tr>
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<td>28.6</td>
<td>169.3</td>
<td>4.2</td>
<td>33</td>
<td>306.6</td>
</tr>
<tr>
<td>7</td>
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<td>211.7</td>
<td>4.2</td>
<td>31</td>
<td>331.4</td>
</tr>
<tr>
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<td>28.6</td>
<td>211.7</td>
<td>4.2</td>
<td>33</td>
<td>331.4</td>
</tr>
</tbody>
</table>

Polarity: direct current electrode positive (DCEP).
Joint type: flat joint, flat position, 90 degree joint angle, and no root gap.
Electrode type: 1.32 mm (0.052 inch) diameter stick weld.
Base metal: A/SA X-36 mild steel.
Shielding gas: Ar + 16 % CO2.
experimentally measured values used in this work. The
optimization algorithm minimizes the error between the
predicted and the experimentally observed penetration,
threshold and the leg length during the GMAW process by
considering the sensitivity of the weld penetration, threshold
and the leg length to each of the unknown parameters.
The Levenberg-Marquardt and two versions of conjuga
gradient methods (i.e., Fletcher-Reeves and Polak-
Ribiere) of non-linear parameter optimization are used to
estimate these unknown parameters with a well tested
three-dimensional numerical heat and fluid flow model.

2 MODEL DESCRIPTION

2.1 Modelling of heat transfer and fluid flow
during GMA fillet welding

The heat transfer and fluid flow model takes into account
the liquid metal convection in the weld pool, the complex
fillet joint geometry, the deformation of the weld pool top
surface, additions of the filler metal, and the heat
transfer by metal droplets. The driving forces for weld
pool convection include the surface tension gradient, the
electromagnetic force and the buoyancy force (gravita-
tional) force. The complicated physical domain is trans-
formed into a simple rectangular computational domain.
The transformed governing equations are then dis-
cretized and solved in the computational domain using
control volume method and a modified SIMPLE algo-
rithm. The output from the model includes temperature
and velocity fields, thermal cycles, fusion zone geome-
try and the solidified geometry of the weld reinforce-
ment. More details about the numerical model are avail-
able in the literature [1, 16]. Only salient features are
summarized below.

2.1.1 Governing equations

By using a coordinate system attached to the heat
source, the welding problem is assumed to be at steady
state [1]. Therefore, the heat transfer and fluid flow dur-
ing welding can be calculated by solving the following
governing equations [1, 16].

\[
\frac{\partial \phi}{\partial t} + \frac{\partial}{\partial x} \left( \rho u \phi \right) + \frac{\partial}{\partial y} \left( \rho v \phi \right) = \nabla \cdot (\mathbf{k} \nabla \phi) + S
\]

(1)

(2)

(3)

Equations (1), (2) and (3) are the continuity, momentum
conservation and energy conservation equations,
respectively.

In these equations:

- subscripts \( i \) and \( j \) indicate the coordinate direction
  \( (i, j = 1, 2 \) and \( 3) \),
- \( x \) is the distance,
- \( u \) is the melt velocity,
- \( \rho \) is the density,
- \( \mu \) is the viscosity,
- \( S_i \) is the source term for \( j \)-th momentum equation,
- \( h \) is the sensible heat,
- \( \alpha \) is the thermal diffusion coefficient defined as \( \alpha = \frac{k}{C_p} \),
where \( k \) is the thermal conductivity and \( C_p \) is the spe-
cific heat,
- \( U_i \) is the material moving speed (parallel to the positive
  \( x \) direction, i.e., \( i = 1 \) direction),
- \( L \) is the latent heat of fusion,
- \( S_i \) is a source term accounting for the additional heat
from metal droplets.

In equation (2), the source term \( S_i \) is given as:

\[
S_i = - \frac{\partial P}{\partial x} - \rho \frac{\partial u}{\partial x} \frac{\partial \phi}{\partial x} - C_i \left( \frac{1}{2} - f \right) \frac{\partial u}{\partial x} F_i + F_i^* P_i^*
\]

(4)

where \( P \) represents pressure, \( f \) is the liquid metal fraction, and
\( F_i \) and \( F_i^* \) correspond to the electromagnetic and buoy-
ancy forces in the \( j \)-th direction, respectively.

Details about the calculation of the electromagnetic and
buoyancy source terms are available in the literature [1, 16, 17]. In equation (4), the third term represents the
fractional dissipation in the mushy zone according to the
Carnan-Kozeny approximation [18], where \( B \) and \( C \) are
two constants. The liquid metal fraction, \( f \), is assumed
to vary linearly with temperature:

\[
\begin{align*}
T &\geq T_c \\
T &< T_c \\
\frac{f}{T - T_c} &< f < 1
\end{align*}
\]

(5)

where \( T_c \) and \( T_f \) are the liquidus and solidus tempera-
ture of the material, respectively.

2.1.2 Coordinate transformation

Much of previous research to understand welding
processes through numerical heat transfer and fluid flow
calculations have focused mainly on simple systems
such as butt welds. Regular Cartesian or Cylindrical grid
system is conveniently employed in the numerical solu-
tion of governing equations. For fillet welds, accurate
solution of heat transfer and fluid flow with a deformable
weld pool surface and complex joint geometry desires the
use of non-orthogonal deformable curvilinear grid
system. Therefore, in the present work, the governing
equations are transformed from the Cartesian to curvi-
linear coordinate system. Figure 1 shows the transfor-
mation from the \( L \)-shape physical domain denoted by \( (x, y, z) \)
to a simple rectangular computational domain rep-
resented by \( (\zeta, \eta, \xi) \), where the transformed governing
equations were discretized and numerically solved. As
shown in this figure, only the \( \zeta \) coordinate in the physi-

cal domain is transformed into the \( \zeta \) coordinate in the
computational domain, while \( \eta \) and \( \xi \) coordinates remain
the same as \( x \) and \( y \) coordinates, respectively. For clar-
ity, subscripts \( x, y, z, \xi, \zeta, \) and \( \eta \) are used to represent
corresponding partial derivatives in the following dis-
cussion. For example, symbols \( \xi_x \) and \( \eta_x \) represent the
partial derivatives \( \partial / \partial x \) and \( \partial / \partial x \) respectively. Using the
Chain rule [19, 20], the governing equations (1), (2)
The shadowed area, $A_{\text{shad}}$, is equal to the amount of test wire per unit length.

Figure 1 – Schematic plot showing the coordinate transformation from the physical $(x, y, z)$ to the computational domain $(\xi, \eta, \zeta)$

(a) Physical domain, and (b) Computational domain

and (3) are transformed into equations (6), (7) and (8), respectively, in the curvilinear coordinates [1, 16].

$$\frac{\partial U_p}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial U_p}{\partial \eta} \frac{\partial \eta}{\partial x} + \frac{\partial U_p}{\partial \zeta} \frac{\partial \zeta}{\partial x} = 0$$

(6)

$$\begin{align*}
\frac{\partial}{\partial \xi} \left[ \frac{1}{\rho} \frac{\partial (\rho U_p)}{\partial \xi} \right] &+ \frac{\partial}{\partial \eta} \left[ \frac{1}{\rho} \frac{\partial (\rho U_p)}{\partial \eta} \right] \nonumber \\
&\quad+ \frac{\partial}{\partial \zeta} \left[ \frac{1}{\rho} \frac{\partial (\rho U_p)}{\partial \zeta} \right] = \frac{\partial}{\partial \xi} \left[ -\frac{1}{\rho} \frac{\partial (\rho U_p)}{\partial \xi} \right] \nonumber \\
&\quad+ \frac{\partial}{\partial \eta} \left[ -\frac{1}{\rho} \frac{\partial (\rho U_p)}{\partial \eta} \right] \nonumber \\
&\quad+ \frac{\partial}{\partial \zeta} \left[ -\frac{1}{\rho} \frac{\partial (\rho U_p)}{\partial \zeta} \right] - \rho \left( \frac{\partial \xi}{\partial x} \frac{\partial \zeta}{\partial \eta} - \frac{\partial \zeta}{\partial x} \frac{\partial \xi}{\partial \eta} \right) \nonumber \\
&\quad- \rho \left( \frac{\partial \eta}{\partial x} \frac{\partial \xi}{\partial \zeta} - \frac{\partial \xi}{\partial x} \frac{\partial \eta}{\partial \zeta} \right) - c_f \left( \frac{1}{\rho} \frac{\partial (\rho U_p)}{\partial \xi} \right) + \frac{1}{2} \rho \frac{\partial (\rho U_p)}{\partial \xi} = 0
\end{align*}$$

(7)

$$\begin{align*}
\frac{\partial}{\partial \xi} \left[ \frac{1}{\rho} \frac{\partial (\rho V_p)}{\partial \xi} \right] &+ \frac{\partial}{\partial \eta} \left[ \frac{1}{\rho} \frac{\partial (\rho V_p)}{\partial \eta} \right] \nonumber \\
&\quad+ \frac{\partial}{\partial \zeta} \left[ \frac{1}{\rho} \frac{\partial (\rho V_p)}{\partial \zeta} \right] = \frac{\partial}{\partial \xi} \left[ -\frac{1}{\rho} \frac{\partial (\rho V_p)}{\partial \xi} \right] \nonumber \\
&\quad+ \frac{\partial}{\partial \eta} \left[ -\frac{1}{\rho} \frac{\partial (\rho V_p)}{\partial \eta} \right] \nonumber \\
&\quad+ \frac{\partial}{\partial \zeta} \left[ -\frac{1}{\rho} \frac{\partial (\rho V_p)}{\partial \zeta} \right] - \rho \left( \frac{\partial \xi}{\partial x} \frac{\partial \eta}{\partial \eta} - \frac{\partial \zeta}{\partial x} \frac{\partial \xi}{\partial \eta} \right) \nonumber \\
&\quad- \rho \left( \frac{\partial \eta}{\partial x} \frac{\partial \zeta}{\partial \eta} - \frac{\partial \xi}{\partial x} \frac{\partial \eta}{\partial \zeta} \right) - c_f \left( \frac{1}{\rho} \frac{\partial (\rho V_p)}{\partial \xi} \right) + \frac{1}{2} \rho \frac{\partial (\rho V_p)}{\partial \xi} = 0
\end{align*}$$

(8)

where $u, v$ and $w$ are Cartesian velocity components along the $x$, $y$ and $z$ directions, respectively, and $U, V$ and $W$ are the contravariant velocity components in the $\xi, \eta$ and $\zeta$ directions, respectively.

The transformation coefficients are expressed as [1, 16]:

$$\begin{align*}
\xi &= x \\
\eta &= y \\
\zeta &= z
\end{align*}$$

(9)

where $J$ is the Jacobian of the transformation and is given as $J = 1 / \zeta$.

Coefficient $q_{11}$ is defined as $q_{11} = J (J^2 + z^2 + \xi^2 + \eta^2 + \zeta^2)$. The contravariant velocity components $U, V$ and $W$ are related to the Cartesian velocity components $u, v$ and $w$ by the following equation:

$$U = \frac{\partial x}{\partial \xi} U + \frac{\partial x}{\partial \eta} V + \frac{\partial x}{\partial \zeta} W = z u$$

(10)

$$V = \frac{\partial y}{\partial \xi} U + \frac{\partial y}{\partial \eta} V + \frac{\partial y}{\partial \zeta} W = z v$$

(11)

$$W = \frac{\partial z}{\partial \xi} U + \frac{\partial z}{\partial \eta} V + \frac{\partial z}{\partial \zeta} W = -z u - z v + z w$$

2.1.3 Boundary conditions

The velocities at the weld pool top surface are given as:

$$u, v = 0$$

(11a)

$$\mu \frac{\partial v}{\partial T} |_{z=0} = t_1 \frac{\partial T}{\partial N}$$

(11b)

$$\mu \frac{\partial v}{\partial T} |_{\xi=0} = t_1 \frac{\partial T}{\partial \xi}$$

(11c)

where $V$ is the liquid metal velocity, $\mu$ is the temperature coefficient of surface tension, $t_1$ is the local unit normal vector to the $x$-$y$ surface, and $t_1$ and $t_1$ are local unit tangential vectors to the top surface along the $\xi$ and $\eta$ directions, respectively.

Equation (11a) indicates that the normal velocity to the weld pool top surface is zero, while equations (11b) and (11c) represent the Marangoni shear stress at the top surface. As shown in Figure 1 (b), the normal and tangential vectors to the weld pool top surface are given as:

$$t_1 = \frac{x}{\sqrt{x^2 + y^2 + z^2}}$$

(12a)

$$t_1 = \frac{y}{\sqrt{x^2 + y^2 + z^2}}$$

(12b)

$$t_1 = \frac{z}{\sqrt{x^2 + y^2 + z^2}}$$

(12c)
where \( i \) and \( j \) are the unit vectors along \( x \), \( y \), and \( z \) directions, respectively.

The liquid metal velocity at all other surfaces, i.e., bottom, east, west, south and north surfaces, are equal to zero.

The heat flux from the arc is assumed to be a Gaussian distribution at the weld top surface. As shown in Figure 1(a), the heat flux at the top surface, \( F_v \), is given as [1, 15]:

\[
\alpha \nabla H \cdot n_1 = F_v = \frac{B}{2 \pi} \exp \left(-\frac{x^2 + y^2}{2 \xi^2}\right) (\mathbf{x} \cdot \mathbf{n}_1) - \alpha \left(T_a - T_g\right)
\]

(13)

where

- \( L \) is the current,
- \( V \) is the voltage,
- \( \eta \) is the power efficiency,
- \( \xi \) is the heat distribution parameter,
- \( x_n \) and \( y_n \) are the \( x \) and \( y \) distances to the arc axis, respectively,
- \( \sigma \) is the Stefan-Boltzmann constant,
- \( \xi \) is the emissivity,
- \( h_n \) is the convective heat transfer coefficient, and
- \( T_g \) is the ambient temperature (a value of 298 K is used).

For the bottom surface, the heat flux, \( F_v \), is given as:

\[
\alpha \nabla H \cdot n_0 = h_b (T_p - T_o)
\]

(14)

where

- \( n_0 \) is a unit normal vector to the bottom surface.

The temperatures at other surfaces, i.e., east, west, south, and north surfaces, are set to the ambient temperature.

2.1.4. Grid system and discretization of the governing equations

The transformed governing equations, i.e., (6), (7) and (8), are discretized using the control volume method, where the computational domain is divided into small rectangular control volumes, as shown in Figure 2. A scalar grid point is located at the centre of each control volume, storing the values of scalar quantities such as pressure and enthalpy. Velocity components lie at the control volume faces, staggered with respect to scalar locations. For example, both Cartesian \( v \) and contravariant \( V \) velocity are placed at the south and north faces of a control volume \( P \), as shown in Figure 2. Thus, the control volumes for vectors are different than those for scalars. Such an arrangement is extensively used in orthogonal coordinates to prevent the decoupling of the velocity and pressure fields [21]. Discretized equations for a variable are formulated by integrating the corresponding governing equation over the control volumes in the computational domain. A power-law based scheme is used to describe the convective flux at the control volume faces. The final expression can be written in the following general form as [21]:

\[
\alpha_{i} \Delta V_{i} = \alpha_{i} \Delta V_{i} + \alpha_{i} \Delta V_{i} + \alpha_{i} \Delta V_{i} + \alpha_{i} \Delta V_{i} + \alpha_{i} \Delta V_{i} + b
\]

(15)

where

- \( \alpha_{i} \), \( \Delta V_{i} \), etc., denote the combined convection-diffusion coefficients, and
- \( b \) includes all the source terms.

A modified Semi-Implicit Algorithm for Pressure Linked Equations (SIMPLE) is used to solve the discretized equations [16]. The modification takes into account the main feature in the transformed governing equations in the curvilinear coordinate system, i.e., a mixed Cartesian-contravariant velocity components.

2.1.5 Heat transfer from metal droplets

An important feature of the GMA welding is the finger penetration which is mainly caused by the transversal heat from the superheated metal droplets into the weld pool. In the present work, the droplet heat transfer is effectively simulated by incorporating a time-averaged volumetric heat source term \( \Delta E_{v} \) in the energy conservation equation. This volumetric heat source is characterized by its radius, height and power density. Details about the calculation of the volumetric heat source based on the available knowledge base of the interaction between metal droplets and the weld pool for various welding conditions are available in reference [1].

2.1.6 Calculation of the weld pool top surface profile

During GMA fillet welding, the weld pool top surface under the electrode is depressed by the arc force. Furthermore, the addition of filler metal also deforms the weld pool. Therefore, the weld pool top surface is not flat and the profile needs to be determined. In the present work, an energy minimization method was used. The total energy to be minimized includes the surface energy due to the change in area of the pool surface.
the potential energy in the gravitational field and the work performed by the arc pressure displacing the pool surface. Detailed procedure for the calculation of the free surface profile is available in the literature [1], and only salient features are presented here.

The following two equations are solved to obtain the weld pool surface profile:

\[
\left( \frac{1 - \alpha_2}{1 + \alpha_1} \right) \beta_0 = \frac{2 \alpha_2 \alpha_1 (1 + \alpha_1)^2 \beta_0}{(1 + \alpha_1)^2} \quad \text{e}^{\alpha_1} + \frac{1}{\alpha_1} \left( \frac{1 - \alpha_2}{1 + \alpha_1} \right)^{\alpha_1} \beta_0 = 0 \\
\frac{1}{U_s} = \frac{2 W_c}{U_p} = 0
\]

In equation (16):
- \( \gamma \) is the surface tension,
- \( P_s \) is the arc pressure distribution at the pool top surface, and
- \( \lambda \) is the Lagrange multiplier.

In equation (17):
- \( r_a \), \( w_c \), and \( U_s \) are the wire radius, wire feeding rate and the welding speed, respectively, and
- \( \beta_0 \) is the solidified surface profile.
- \( \alpha_1 \) is the z location of the workpiece top surface, as shown in Figure 1.

Equation (16) represents the static force balance at the pool top surface, while equation (17) defines a constraint condition that the deformed area, \( A_{deform} \), at a solidified cross section of the weld pool is equal to the amount of fed wire per unit length, as shown in Figure 1.

The pressure distribution at the top surface, \( P_s \), is given as:

\[
P_s = \frac{F}{2 \pi r_a^2} \exp \left( -\frac{x_2^4 + y_2^4}{2 \sigma_c^2} \right)
\]

where
- \( F \) is the total arc force,
- \( \sigma_c \) is the distribution parameter for arc pressure, and
- \( x_2 \) and \( y_2 \) are the x and y distances to the arc axis, respectively.

The values of \( F \) and \( \sigma_c \) were calculated based on the experimental work of Lin and Eagers [22] as:

\[
F = -0.04791 + 0.0003447 \times 1 (N) \quad \text{and} \quad \sigma_c = 1.4875 + 0.00123 \times 1 (mm)
\]

where
- \( I_1 \) is the welding current in Amperes.

2.1.7 Overall solution procedure

The governing equations are solved "simultaneously" to obtain the temperature and velocity fields and the free surface profile. First, the modified SIMPLE algorithm is used to calculate the temperature and velocity fields. Then, the free surface profile is calculated based on the temperature field obtained in the previous step. After the solution of the free surface profile, the x locations of grid points are adjusted to fit the surface profile, and the temperature and velocity fields are then re-calculated in the fitted grid system. The calculation procedure is repeated until converged temperature and velocity fields and free surface profile are obtained.

A 72 x 66 x 47 grid system was used and the corresponding solution domain had dimensions of 450 mm in length, 108 mm in width and 18 mm in depth. Spatially non-uniform grids with finer grids near the heat source were used for maximum resolution of variables. The calculations normally converged within 5,000 iterations, which took about 50 minutes in a PC with 2.8 GHz Intel CPU and 512 MB PC2700 DDR-SDRAM memory. Comparing with the heat transfer model [1] which converges in 4,000 iterations (about 6 minutes), the heat transfer and fluid flow calculation is much more computationally intensive.

2.2 Inverse modeling

Inverse modeling provides the estimation of unknown welding parameters using the measured weld features like, the actual throat, leg length and penetration in the filled weld. The inverse problem is often difficult to solve because it is a mathematically ill-posed problem [23-26], and small perturbations in the observed parameter functions may result into large changes in the corresponding solutions and requires special numerical techniques to stabilize [23-24] the results of the calculations. In general, inverse problems require more computation time than the corresponding direct approaches as it usually involves an iterative procedure involving multiple computations of the direct problem.

Inverse model involves the minimization of an objective function that depicts the difference between the computed and measured values. For example, if the penetration, throat and the leg length of the fusion zone are of interest, an objective function, \( O(f) \), can be defined as follows:

\[
O(f) = \frac{1}{2} \left( p_{21}^2 - p_{21}^2 \right) + \frac{1}{2} \left( l_{21}^2 - l_{21}^2 \right) + \frac{1}{2} \left( l_{21} - l_{21} \right)
\]

where
- \( p_{21} \), \( l_{21} \) and \( l_{21} \) are the penetration, actual throat and the leg length of the weld pool calculated by the numerical heat transfer and fluid flow model, respectively and
- \( p_{21} \), \( l_{21} \) and \( l_{21} \) are the corresponding experimentally determined values of these two variables.

The penetration, actual throat and leg length in a GMAW filled weld are defined in Figure 3. The subscript m in equation (21) corresponds to a specific weld in a set of M welds. Equation (21) bears a strong resemblance to the functional form of least square technique for the minimization of error.

Often an experiment is repeated to determine the standard deviation, \( \sigma_c \), in measurements. These standard deviations can be included in the objective function such that more reliable measurements with small standard deviations get a higher weight than less reliable measurements that are characterized by relatively large standard deviations. A weight factor can also be assigned with the measured quantities if they represent different measurement scale or the physical dimension. The
Objective function, \( Q(t) \), can now be defined as follows where every weld is lubricated a multiple number of times.

\[
Q(t) = \frac{W}{\psi} \left( \frac{d_{l} - d_{e}}{d_{l} - d_{e}} \right)^{p} + \frac{W}{\psi} \left( \frac{d_{l} - d_{e}}{d_{l} - d_{e}} \right)^{p} \left( \frac{L - L_{0}}{L - L_{0}} \right)^{q} + \frac{W}{\psi} \left( \frac{d_{l} - d_{e}}{d_{l} - d_{e}} \right)^{p} \left( \frac{L - L_{0}}{L - L_{0}} \right)^{q}
\]

Where

\( W \), \( \psi \), and \( \psi \) represent the weight factor assigned to penetration, throat and leg length respectively.

In equations (21) and (22), \( f \) refers to a set of six unknown non-dimensional parameters, \( f_{1}, f_{2}, f_{3}, f_{4}, f_{5}, \) and \( f_{6} \) of the constant terms (i.e. \( A, B, C, D, E \) and \( F \)) of the assumed linear functions of efficiency, \( \eta \), effective thermal conductivity, \( \kappa_{\text{eff}} \), and effective viscosity, \( \mu_{\text{eff}} \), with the non-dimensional input power, \( P_{\text{in}} \), in the following manner:

\[
(f_{1}, f_{2}, f_{3}, f_{4}, f_{5}, f_{6}) = (A, B, C, D, E, F, f_{\text{in}})
\]

\( \eta = A + B \cdot P_{\text{in}} \) \hspace{1cm} (24)
\( \kappa_{\text{eff}} = C + D \cdot P_{\text{in}} \) \hspace{1cm} (25)
\( \mu_{\text{eff}} = E + P_{\text{in}} \) \hspace{1cm} (26)

\( P_{\text{in}} = \frac{W}{(\varepsilon_{w} d_{w}^{2})} + \frac{W}{(\varepsilon_{w} d_{w}^{2})} \) \hspace{1cm} (27)

where

\( \varepsilon_{w} \) is the conductivity of the liquid metal,
\( d_{w} \) is the viscosity of the liquid material,
\( l \) is the current,
\( V \) is the voltage,
\( r_{a} \) is the wire radius,
\( w_{f} \) is the wire feeding rate,
\( \rho \) is the density,
\( C_{s} \) is the specific heat,
\( T_{a} \) is the ambient temperature,
\( L \) is the latent heat of the alloy,
\( r_{a} \) is the arc radius and
\( U_{w} \) is the welding speed.

In equation (24), input power is non-dimensionalised with wire feeding rate and wire radius because if any of these two parameters is large, more power will be consumed in melting the wire. Therefore, less power will go to the workplace in the form of arc. While, in case of effective thermal conductivity and effective viscosity, input power is non-dimensionalised with respect to the welding speed and the arc radius. The reason is that with high torch speed or the arc radius, the input power will be distributed in a larger area which will reduce the effect of input power on the turbulence behaviour in the weld pool. This reduction in turbulence behaviour will lead to less increase in effective thermal conductivity and viscosity.

Evidently, \( Q(t) \) is a function of \( f \) since \( Q(t) \) contains variables \( p_{1}, t_{p} \), and \( L_{0} \) which are dependent on the parameters included in \( f \). Assuming that \( Q(t) \) is continuous and has a minimum value, the optimum values of the six unknowns are obtained by differentiating equation (21) with respect to the six unknown parameters and equating each derivative to zero:

\[
\nabla Q(t)_{f_{1,6}} = \sum_{i=1}^{6} \frac{\partial Q(t)}{\partial f_{i}} \frac{\partial f_{i}}{\partial f_{i}} = 0
\]

where

\( f_{1} \) represents any one of the six unknowns in \( f \).

Equation (29) contains partial derivatives of weld penetration, actual throat and leg length with respect to all six unknown parameters. These partial derivatives are generally referred as sensitivity of the computed weld penetration, actual throat and leg length with respect to the unknown parameters. The values of these sensitivity terms are computed numerically by running the numerical heat transfer and fluid flow codes and subsequently calculating the derivatives. For example, the sensitivity of non-dimensional penetration, \( p_{j} \), with respect to variable \( j_{i} \) is calculated from the following relation:

\[
\delta p_{j} = \frac{p_{j} (l_{j}, t_{f}, t_{p}, t_{1} + \delta t_{1}, t_{2} + \delta t_{2}, \ldots)}{p_{j} (l_{j}, t_{f}, t_{p}, t_{1}, t_{2}, \ldots)} - 1
\]

where

\( \delta t_{1} \) is very small compared to \( t_{1} \).

The equation (29) depicts that each sensitivity term need two executions of the direct numerical analysis. Now, equation (28) calls for the calculated values of \( p_{j} \), \( t_{f} \) and \( t_{p} \) to be very close to the corresponding experimental values of \( p_{j} \), \( t_{f} \) and \( t_{p} \) for all M sample welds. Since \( p_{j} \), \( t_{f} \) and \( t_{p} \) in equation (28) are obtained from the solution of the direct numerical heat and fluid flow model for a certain set of six unknown parameters, and these unknown parameters do not explicitly appear in equation (28), this equation cannot provide a direct solution for the desired unknown parameters. These sensitivity terms can be written in a matrix form, known as sensitivity matrix, \( J_{ij} \). The elements of the sensitivity matrix, i.e. sensitivity coefficients, \( J_{ij} \) are defined as:

\[
J_{ij} = \frac{\partial q_{j}}{\partial f_{i}} = \frac{\delta q_{j}}{\delta f_{i}} * \frac{1}{Q(t)_{n}}\hspace{1cm} \frac{\delta q_{j}}{\delta f_{i}} \hspace{2cm} \frac{\delta q_{j}}{\delta f_{i}} \hspace{2cm} \frac{\delta q_{j}}{\delta f_{i}}
\]

where

\( i = 1 \) to \( M \) and
\( j = 1 \) to \( 6 \).

For the minimization of least-square objective function [i.e. equation (22)], Levenberg-Marquardt (LMA) method
and two different modifications of the conjugate gradient method suggested by Fletcher-Reeves and Polak-Ribiere are used for the analysis. These methods differ in calculation of step size (i.e., increment in the unknown parameters) and direction of descent which is physical representation of the relative change in the unknown parameters.

2.2.1 Levenberg-Marguardt method

To calculate the step size in LM method, the dependent variables $p_i$, $q_i$, and $l_i$ can be expanded using the Taylor's series to explicitly contain values of increments and unknown parameters i.e., $f_i$, $t_i$, $f_i$, $t_i$, and $l_i$. The higher derivative terms in the Taylor's series can be dismissed because these are very small compared to the term involving the first derivative. So, for the variable $p_i$, the expansion takes the following form:

$$p_i^{(k+1)} = p_i^{(k)} + 2p_i^{(k)} \frac{\partial p_i}{\partial f_i} \Delta f_i + 2p_i^{(k)} \frac{\partial p_i}{\partial t_i} \Delta t_i + 2p_i^{(k)} \frac{\partial p_i}{\partial l_i} \Delta l_i$$

$$+ \frac{\partial^2 p_i}{\partial f_i^2} (\Delta f_i)^2 + \frac{\partial^2 p_i}{\partial t_i^2} (\Delta t_i)^2 + \frac{\partial^2 p_i}{\partial l_i^2} (\Delta l_i)^2$$

(31)

where \(\Delta f_i, \Delta t_i, \Delta f_i, \Delta t_i, \Delta l_i\) and \(\Delta l_i\) are the unknown increments in $f_i$, $t_i$, $f_i$, $t_i$, and $l_i$.

Superscripts $k$ and $k+1$ represent the values at the $k$th and $(k+1)$th iterations, respectively. All other terms on the right-hand side of equation (31) are considered to be known. The value of $p_i^{(k)}$ at the end of $(k+1)$th iteration i.e., $p_i^{(k+1)}$, is unknown since $\Delta f_i, \Delta t_i, \Delta f_i, \Delta t_i, \Delta l_i$, and $\Delta l_i$ and hence, $f_i, t_i, f_i, t_i$, and $l_i$ after $(k+1)$th iteration are unknown. It should be noted here that $p_i^{(k+1)}$ is always considered to be evaluated through a direct numerical solution using a corresponding set of $f_i, t_i, f_i, t_i$, and $l_i$ and other known parameters. The terms in equation (29) represents the $k + 1$ iteration terms which are unknown. So, these terms can be rewritten as $k$th iteration terms using equation (31). Substituting equation (30) in equation (28) and removing the second derivative terms will convert equation (28) to following form:

$$[S][\Delta f_i] = [S]^{(k+1)}$$

(32)

with $[S]$ as an $N \times N$ matrix containing sensitivity terms, $\Delta f_i$ as an $N \times 1$ matrix and $[S]^{(k+1)}$ as an $N \times 1$ matrix where $N$ represents the number of unknown variables i.e., 5. The elements of matrix [S], i.e.,

$$[S] = \begin{bmatrix}
S_{11} & S_{12} & S_{13} & S_{14} & S_{15} \\
S_{21} & S_{22} & S_{23} & S_{24} & S_{25} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
S_{N1} & S_{N2} & S_{N3} & S_{N4} & S_{N5}
\end{bmatrix}$$

(33)

can be written as:

$$S_{ij} = \frac{1}{w_{ij}} \left[ \frac{\partial S_{ij}}{\partial f_i} \frac{\partial S_{ij}}{\partial t_i} \frac{\partial S_{ij}}{\partial l_i} \right]$$

for i = 1 to 6

(34)

The indices $i$ and $j$ refer to the number of unknown parameters. Furthermore,

$$[S]^{\dagger} = \begin{bmatrix}
S_{11}^{\dagger} & S_{12}^{\dagger} & S_{13}^{\dagger} & S_{14}^{\dagger} & S_{15}^{\dagger} \\
S_{21}^{\dagger} & S_{22}^{\dagger} & S_{23}^{\dagger} & S_{24}^{\dagger} & S_{25}^{\dagger} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
S_{N1}^{\dagger} & S_{N2}^{\dagger} & S_{N3}^{\dagger} & S_{N4}^{\dagger} & S_{N5}^{\dagger}
\end{bmatrix}$$

(35)

$$[S]^{\dagger} = \begin{bmatrix}
S_{11}^{\dagger} & S_{12}^{\dagger} & S_{13}^{\dagger} & S_{14}^{\dagger} & S_{15}^{\dagger} \\
S_{21}^{\dagger} & S_{22}^{\dagger} & S_{23}^{\dagger} & S_{24}^{\dagger} & S_{25}^{\dagger} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
S_{N1}^{\dagger} & S_{N2}^{\dagger} & S_{N3}^{\dagger} & S_{N4}^{\dagger} & S_{N5}^{\dagger}
\end{bmatrix}$$

(36)

The unknown matrix $([\Delta f_i])$ in equation (32) has also to be modified as:

$$[\Delta f_i] = \begin{bmatrix}
\Delta f_i^{\dagger} \\
\Delta t_i^{\dagger} \\
\Delta f_i^{\dagger} \\
\Delta t_i^{\dagger} \\
\Delta l_i^{\dagger} \\
\Delta l_i^{\dagger}
\end{bmatrix}$$

(37)

The expression in equation (37) should now be treated as,

$$[S]^{\dagger} = \begin{bmatrix}
[S]^{\dagger} & \Delta f_i^{\dagger} \\
[S]^{\dagger} & \Delta t_i^{\dagger} \\
[S]^{\dagger} & \Delta f_i^{\dagger} \\
[S]^{\dagger} & \Delta t_i^{\dagger} \\
[S]^{\dagger} & \Delta l_i^{\dagger} \\
[S]^{\dagger} & \Delta l_i^{\dagger}
\end{bmatrix}$$

(36)

Further, the sensitivity terms such as

$$\frac{\partial S_{ij}}{\partial f_i} \frac{\partial S_{ij}}{\partial t_i} \frac{\partial S_{ij}}{\partial l_i}$$

for i = 1 to 6 in the equations (34) as well as in (36) often tend to be very small as the values of the unknown parameters $f_i, t_i, f_i, t_i$, and $l_i$ move close to the optimum values. As the optimum combination of the unknown parameters are reached, the individual influence of a specific parameter on the dependent variables, manifested by the sensitivity terms, may become very small or zero. Subsequently, the matrix [S] may tend to become a singular matrix and the inverse problem may become ill-conditioned. The matrix [S] can be null if any column of [S] can be expressed as a linear combination of other columns. To avoid any numerical instability, equation (32) is further modified following Levenberg-Marguardt method as:

$$[S] + \lambda^2 [I] [\Delta f_i] = [S]^{\dagger}$$

(39)

where $\lambda$ is a scalar damping coefficient and usually taken as 0.001 and $[I]$ is the diagonal matrix.

The order of $[I]$ is same as that of the matrix [S] and is defined as $[I] = \text{diag}([3])$. Thus the product $\lambda^2 [I]$ in equa-
tion (39) ensures that the left-hand term in equation (39) will remain non-zero even if the determinant of the matrix [S] is zero. The damping parameter is generally made large at the beginning of the iterations, since the problem is generally ill-conditioned in the region around the initial guess in the iterative procedure, which can be quite far from the final solution. The parameter $\lambda$ is then gradually decreased as the iteration procedure advances to the solution of the parametric estimation problem.

**Algorithm:**

1. Guess initial values of unknown variables set 1.
2. Compute objective function, $O(1)$.  
3. Choose a most favorable damping factor ($\lambda$), say $\lambda = 0.001$.  
4. Solve for increment in unknown variables, $\Delta$.  
5. Evaluate $O(1) + \Delta$.  
6. If $O(1) + \Delta > O(1)$, increase $\lambda$ by a factor of 10 (or any other substantial factor) and go back to step 2.  
7. If $O(1) + \Delta < O(1)$, decrease $\lambda$ by a factor of 10 (or any other substantial factor). Update $\lambda$.
8. Exit if stopping criterion is satisfied, otherwise go back to step 4.

The following stopping criteria suggested by Dennis and Schnelle [27] to stop the iterative procedure of the LM method is used in this paper.

1. $O^{(n)} < \epsilon_0$.  
2. $\parallel \Delta \parallel < \epsilon_0$.  
3. $\parallel x^{(n)} - P \parallel < \epsilon_0$.  

where $r$, $c$, and $v$, are user prescribed tolerances, and $\parallel \parallel$ is the vector Euclidean norm, i.e., $\parallel x \parallel = (x^T x)^{1/2}$, where the superscript $T$ denotes the transpose.

The first criteria tests if the objective function is sufficiently small, which is going to be the neighborhood of the solution for the problem. Similarly, second criteria checks if the norm of the gradient of $O(1)$ is sufficiently small, since it is expected to vanish at the point where $O(1)$ is minimum. Although such a condition of vanishing gradient is also valid for maximum and saddle points of the $O(1)$, the LM method is very unlikely to converge to such points [25, 30]. The third stopping criteria result from the fact that changes in the vector of parameters are very small when the method has converged. The use of a stopping criteria based on small changes of the least squares norm $O(1)$ could also be used, but with extreme caution. It may happen that the method stagnates for a few iterations and then starts advancing to the point of minimum afterwards [26, 27].

### 2.2.2 Conjugate gradient method

Conjugate gradient method differs from LM method principally in the calculation of search step size and the direction of descent. In the iterative procedure of the conjugate gradient method, at each iteration a suitable step size is taken along a direction of descent, in order to minimize the objective function. The direction of descent is obtained as a linear combination of the negative gradient direction at the current iteration with the direction of the descent of the previous iteration [31, 32]. This linear combination is such that the resulting angle between the direction of descent and the negative gradient direction is less than 90° and the minimization of the objective function is assured.

The iterative procedure of the Conjugate Gradient method for the minimization of the objective function is given by:

$$f^{(n)} = e - P \Delta$$

for $i = 1$ to 6

(40)

where $P$ is the search step size, $k$ is the number of iterations and $\Delta$ is the direction of descent for the $k$th variable.

The direction of descent for variable $i$, $\Delta_i$, is a conjugate of its gradient direction, $\nabla O(h_i)$, and its direction of the descent of the previous iteration, $\Delta_i^{(n-1)}$, and is given as:

$$\Delta_i = [\nabla O(h_i)]_{[\nabla O(h_i)]_{[\nabla O(h_i)]}}$$

for $i = 1$ to 6

(41)

where $\gamma$ is the conjugation coefficient.

Different expressions are available in the literature for the conjugate coefficient, $\gamma$. Fletcher and Reeves [30] suggested $\gamma$ as:

$$\gamma = \frac{N}{N+1} \frac{[\nabla O(h_i)]^2}{[\nabla O(h_i)]_{[\nabla O(h_i)]}}$$

for $k = 1, 2, ...$ and $\gamma = 0$

(42)

where $N$ is the number of unknown variables, i.e., 8, Polak-Ribiere [31] suggested expression for $\gamma$ as:

$$\gamma = \frac{N}{N+1} \frac{[\nabla O(h_i)]^2}{[\nabla O(h_i)]_{[\nabla O(h_i)]}}$$

for $k = 1, 2, ...$ and $\gamma = 0$

(43)

Here $\nabla O(h_i)$ is the gradient direction of variable $i$ evaluated at iteration $k$ evaluated in equation (29). Either expression [equations (42) and (43)] for the computation of the conjugation coefficient $\gamma$ assure that the angle between the direction of descent and the negative gradient direction is less than 90° so that the objective function is minimized.

If $\gamma = 0$ for all iterations $k$, the direction of descent becomes the gradient direction in equation (41), and the steepest-descent method is obtained.

The search step size, $P$, is obtained as the one which minimizes the objective function. Substituting the values of Taylor series expansion of the unknown parameters at iteration $k+1$ i.e., equation (40) in equation (29), and minimizing with respect to $P$, we get:
After computing the sensitivity terms, the gradient direction, the conjugation coefficient and the search step size, the iterative procedure given by equation (40) is implemented until a stopping criterion is satisfied.

Algorithm:
1. Calculate the objective function, O(t) for the initial guesses of unknown variables, \( \mathbf{f} \).
2. Check the stopping criteria. Continue if not satisfied.
3. Compute the sensitivity matrix, \( \mathbf{J}(t) \).
4. Compute the gradient direction, \( \mathbf{g}(t) \).
5. Evaluate the conjugate coefficient, \( \rho(t) \).
6. Compute the direction of descent, \( \mathbf{d}(t) \).
7. Compute the search step size, \( \Delta(t) \).
8. Compute the new estimates for the unknown variables, \( \mathbf{f}(t+1) \).
9. Increase the iteration no. and return to step 1.

In "chi-square objective function" the uncertainties associated with each data are required. If these values are not known in advance then it is assumed that all measurements have the same standard deviation, \( \sigma_i = \sigma \), and the model does fit well with the data, then we can proceed by assigning an arbitrary constant value \( \sigma = 1 \) to all points [32]. It converts the objective function from chi-square function to a least square function.

3 RESULTS AND DISCUSSION

3.1 Calculations of heat transfer and fluid flow

As discussed in previously, the numerical heat transfer and fluid flow model was used as the direct model. The physical properties of the A-36 mild steel workpiece used in the calculations are given in Table 2. The numerical model provides detailed information of heat temperature distribution, velocity field in the weld pool and surface profile for a given set of input parameters. Some salient findings of heat transfer and fluid flow calculations are briefly discussed below and more details are available in the reference [16].

3.1.1 Heat transfer and fluid flow in the fillet weld pool

The calculated temperature and velocity fields in a fillet weld are shown in Figure 4. The welding conditions used are those in case #4 shown in Table 1. For clarity, only half of the weld pool is shown, since the weld is symmetric about the central longitudinal plane containing the welding direction. As shown in this figure, the liquid metal motion is quite complicated due to the combined effect of the driving forces. The electromagnetic force plays a dominant role in driving the liquid metal flow in the weld pool. In the middle of the weld pool, the liquid metal is driven downwards by the electromagnetic forces, and a major anticlockwise circulation loop is formed along the central longitudinal plane. On the other hand, at the top surface of the weld pool, the Marangoni shear stress drives the melt from the centre to the edge of the pool in the region close to the heat source, where the spatial variation of the surface temperature is relatively high. In the rear part of the weld pool, where the temperature gradient is relatively low, the effect of Marangoni shear stress is less strong than that of elect.
3.1.2 Relative importance of convection and conduction in the heat transfer in the weld pool

During welding, the arc energy is carried away from the top surface of the weld pool to the surrounding solid region by both heat conduction and liquid metal convection. The rate of the heat flow determines not only the peak temperature and shape of the weld pool but also the temperature distribution in the heat-affected zone (HAZ). Therefore, it is of importance to understand the effect of conduction and convection on the heat dissipation in the weld pool. The relative importance of convection and conduction in the transfer of heat in the weld pool can be accessed from the value of the Peclet number (Pe), which is given by:

$$Pe = \frac{u_n C_n L_n}{k}$$  \hspace{1cm} (45)

where \( u_n \) and \( L_n \) are the characteristic velocity and length of the weld pool, respectively, and the symbols \( p, C_n \) and \( k \) have been defined earlier.

When \( Pe \) is large, which in practical terms means large liquid metal velocity, large weld pool, and poor thermal conductivity, the liquid metal convection significantly affects heat transfer in the weld pool. On the other hand, when \( Pe \) is small, say much less than unity, the conduction plays an important role in the heat dissipation in the weld pool.

For the fillet weld shown in Figure 4, if the average velocity and the pool width are used as the characteristic velocity and length of the weld pool, respectively, the Peclet number is then calculated to be 120. Since the Peclet number is much larger than unity, the liquid metal convection plays a dominant role in the dissipation of heat in the weld pool.

3.1.3 Weld thermal cycles

The temperature field obtained from the calculation is in quasi-steady state, since the coordinate system is attached to the heat source moving at a constant welding speed. Therefore, the thermal cycles can be calculated by considering the distance into time using the welding speed. Figure 5 shows the thermal cycles at the top surface of the weld for case #2. Curve 1 is located in the FZ and curves 2 and 3 are located in the HAZ. As shown in Figure 5, the heating rates are much higher than the cooling rates. This is due to the following two reasons. One is that the isotherms in front of the heat source are compressed whereas those behind it are largely elongated due to the high welding speed. The other is that the existence of the volumetric heat source also contributes to the high heating rates. As expected, the peak temperatures are higher at locations close to the weld centre, and decrease as the monitoring location moves outward. The calculated average cooling rate between 1.073 to 773 K (800 to 500 °C)

3.2 Estimation of unknown parameters using inverse modelling

The evolution of weld pool involves complex interaction of physical processes such as application of welding arc, metal droplet transfer, heat transfer through conduction and convection, free surface deformation and the fluid flow inside the weld pool. To simulate these simultaneous processes in the numerical heat transfer and fluid flow analysis, several input parameters are treated as unknowns whereas the values of \( n, k_{w, f} \) and \( \rho_{mf} \) are not known beforehand.

3.2.1 Effect of the effective thermal conductivity and viscosity on weld geometry

The effects of variation of effective thermal conductivity and effective viscosity on the weld geometry i.e. actual throat, penetration and leg length are presented in Figures 6 to 8 for case #1 in Table 1. Actual throat, penetration and leg length are non-dimensionalized by dividing the numerically obtained values with the corresponding experimental values. Figures 6 and 7 show that non-dimensional value of actual throat and penetration decreases with increase in the value of \( y_{w, f} \). This is due to the fact that at higher values of \( y_{w, f} \), the liquid metal velocities are low. As a result, the rate of convective heat transfer is diminished and the weld pool size is reduced. Figure 8 shows that the non-dimensional leg length decreases with increase in \( y_{w, f} \). The higher values of the effective thermal conductivity lower
Figure 6 – Contour plot of the non-dimensional actual throat value for case #1 given in Table 1

Figure 7 – Contour plot of the non-dimensional penetration value for case #1 given in Table 1

Figure 8 – Contour plot of the non-dimensional leg length value for case #1 in Table 1

Figure 9 – Computed values of non-dimensional actual throat, penetration and leg length using $\eta = 0.98$, $k_w = 209.0 \text{ J m}^{-1} \text{s}^{-1} \text{K}^{-1}$, and $\mu_w = 0.12 \text{ kg m}^{-1} \text{s}^{-1}$ for all the eight measurement cases listed in Table 1.

The resulting temperature gradient. The lower temperature gradient, in turn, decreases the convective heat transport and results in smaller leg length at high values of $k_w$.

Figure 9 shows the non-dimensional penetration, actual throat and leg length obtained by using the values of arc efficiency as 0.54, $k_w = 209.0 \text{ J m}^{-1} \text{s}^{-1} \text{K}^{-1}$ and $\mu_w = 0.12 \text{ kg m}^{-1} \text{s}^{-1}$ as suggested in the literature [11, 13, 14]. The non-dimensional penetration value obtained using these values is more than 1.0 for most of the cases. Therefore, the suggested combination of $\mu_w$ and $k_w$ will not lead to optimum prediction of geometry for the weld conditions studied here and a set of optimised values of $\eta$, $\mu_w$ and $k_w$ is needed.

3.2.2 Estimation of the unknown parameters

Table 3 shows the calculated values of these unknown parameters obtained by using different techniques. The progress in the optimisation of the two unknown parameters related to arc efficiency is shown in Figures 10 and 11. The values of these two parameters related to arc efficiency decrease slightly and finally reach almost same optimised values by different techniques. All the other unknown variables also show a similar trend and finally attain optimised values. Figure 12 depicts the variation in least square error (i.e. O(f)) with number of iterations. The objective function decays rapidly in the first 4 iterations in the LM method and both versions of CG. After that the objective function becomes almost constant for some iterations and then starts fluctuating.

Table 3 shows that the Fletcher and Reeves's CG method gives somewhat better convergence of the objective function compared to other two methods. By using this method, the minimum value of the objective function obtained is 0.22 after 13 iterations while LM and Petkak-Ribiere's CG method produced the value as 0.27 and 0.26 in 13 and 14 iterations, respectively.
Table 3 - Comparison of results obtained by using LM method and the two CG methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Parameters</th>
<th>Estimates</th>
<th>O(f)</th>
<th>Iterations</th>
<th>Probability</th>
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<td>13</td>
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<td></td>
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<td></td>
</tr>
<tr>
<td></td>
<td>b5</td>
<td>2.82</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CG method- Fletcher and Reeves</td>
<td>b1</td>
<td>0.31</td>
<td>0.22</td>
<td>13</td>
<td>0.99</td>
</tr>
<tr>
<td></td>
<td>b2</td>
<td>5.97</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>b3</td>
<td>2.10</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>b4</td>
<td>1.96</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>b5</td>
<td>2.46</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>b6</td>
<td>2.02</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CG method-Polak and Ribiere</td>
<td>b1</td>
<td>0.34</td>
<td>0.26</td>
<td>14</td>
<td>0.99</td>
</tr>
<tr>
<td></td>
<td>b2</td>
<td>5.75</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>b3</td>
<td>2.09</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>b4</td>
<td>2.08</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>b5</td>
<td>3.66</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>b6</td>
<td>4.14</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

3.2.3 Arc efficiency, effective thermal conductivity and viscosity

As the optimum combination of the unknown parameters are reached, the individual influence of a specific parameter on the dependent variables, contained in the sensitivity terms, may become very small or zero. The maximization of sensitivity matrix is generally aimed in order to estimate the optimum values [24-26, 32] of these unknown parameters. Figure 13 shows the variation of the determinant of the sensitivity matrix with iteration. The determinant of the sensitivity matrix does not significantly change with number of iterations after 12 iterations. The figure also shows that the values obtained by Fletcher-Reeves’s CG method are the best optimal values because this method gives the highest value of the sensitivity matrix. The sensitivity coefficients and correlation coefficients of the matrix $J/J$ are given in Tables 4 and 5. The correlations coefficients $C_j$ given in
Table 5 are computed from Table 4 using the following relation:

\[ C_i = \frac{A_i}{\sum A_j A_j} \]

where

\[ A_i \] is the \( i^{th} \) component of the \( J^*U \) matrix.

The correlations given in Table 5 indicate a large correlation between \( f_i \), \( f_j \), \( f_k \), and \( f_l \), while \( f_m \) and \( f_n \) have very low correlations with \( f_p \). \( f_q \) and \( f_r \). It shows that values of effective thermal conductivity and effective viscosity depend significantly on the value of the efficiency. It also shows that the values of arc efficiency, effective thermal conductivity and effective viscosity are inter-dependent and vary with change in any value of these parameters.

A rational way to describe the optimum combination of the six unknown parameters is as a set of system properties that is inherent within the eight measured weld samples governed by the optimisation calculation. Using the model, the optimal values of these unknown parameters for the welding conditions listed in Table 1 can be expressed as:

\[ \eta = 0.31 + 4.65 \times 10^{-4} \frac{V}{\nu} \]

\[ k_{\text{eff}} = 41.80 + 3.17 \times 10^{-4} \frac{N}{U_c} \text{ (W/m - K)} \]

\[ \mu_{\text{eff}} = 0.016 + 1.05 \times 10^{-4} \frac{V}{U_c} \text{ (kg/m - s)} \]

where \( I \) is the current (A), \( V \) is voltage (V), \( \nu \) is the wire feeding speed (m/s) and \( U_c \) is the welding speed (m/s).

The values of \( \eta \), \( k_{\text{eff}} \) and \( \mu_{\text{eff}} \) are calculated by using equations (47), (48) and (49), for the experimental conditions given in Table 1. Table 6 shows that the efficiency increases slightly with the increase in input power and decreases in the wire feeding rate (case #3 and case #7 of Table 1). Table e also shows that there can be 50% variation in the value of effective thermal conductivity depending on the experimental conditions. The optimised values give enhancement factors of 5 and 7 for thermal conductivity and viscosity, respectively. Hong and Weckman [11, 13] suggested an enhancement factor between 12 to 15 for the Hall conductivity and a factor more than 10 for the viscosity for 150A current and 25 V power supply. Choo and Szekely suggested an enhancement factor of more than 8 times for the thermal conductivity and a factor of 30 for the viscosity for a current of 100A. But the values available in the literature [11, 13, 14] are independent of each other. There is no guidance available about the selection of the values of these parameters for specific welding conditions.

The computed \( k_{\text{eff}} \) and \( \mu_{\text{eff}} \) indicate that the rates of transport of momentum and heat are higher than that from laminar flow. The relation between the two variables is

Table 4 – Sensitivity matrix, \( JU \), obtained for the six unknown parameters estimated by using Fletcher-Reeves’s CG method

<table>
<thead>
<tr>
<th>Non-dimensional parameters</th>
<th>( f_1 )</th>
<th>( f_2 )</th>
<th>( f_3 )</th>
<th>( f_4 )</th>
<th>( f_5 )</th>
<th>( f_6 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( f_1 )</td>
<td>668.58</td>
<td>15.45</td>
<td>18.84</td>
<td>22.43</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( f_2 )</td>
<td>20.21</td>
<td>45.45</td>
<td>0.89</td>
<td>1.14</td>
<td>1.03</td>
<td></td>
</tr>
<tr>
<td>( f_3 )</td>
<td>20.57</td>
<td>0.89</td>
<td>1.14</td>
<td>1.03</td>
<td>1.03</td>
<td></td>
</tr>
<tr>
<td>( f_4 )</td>
<td>18.84</td>
<td>0.89</td>
<td>1.14</td>
<td>1.03</td>
<td>1.03</td>
<td></td>
</tr>
<tr>
<td>( f_5 )</td>
<td>15.45</td>
<td>0.89</td>
<td>1.14</td>
<td>1.03</td>
<td>1.03</td>
<td></td>
</tr>
<tr>
<td>( f_6 )</td>
<td>22.43</td>
<td>1.14</td>
<td>1.30</td>
<td>1.34</td>
<td>1.72</td>
<td></td>
</tr>
</tbody>
</table>

Table 5 – Correlation matrix obtained for the sensitivity coefficients in \( J^*U \) from Table 4

<table>
<thead>
<tr>
<th>Non-dimensional parameters</th>
<th>( f_1 )</th>
<th>( f_2 )</th>
<th>( f_3 )</th>
<th>( f_4 )</th>
<th>( f_5 )</th>
<th>( f_6 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( f_1 )</td>
<td>1.00</td>
<td>0.95</td>
<td>0.79</td>
<td>0.69</td>
<td>0.66</td>
<td>0.60</td>
</tr>
<tr>
<td>( f_2 )</td>
<td>0.95</td>
<td>1.00</td>
<td>1.00</td>
<td>0.96</td>
<td>0.94</td>
<td>0.93</td>
</tr>
<tr>
<td>( f_3 )</td>
<td>0.79</td>
<td>1.00</td>
<td>1.00</td>
<td>0.96</td>
<td>0.94</td>
<td>0.93</td>
</tr>
<tr>
<td>( f_4 )</td>
<td>0.69</td>
<td>0.96</td>
<td>0.96</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>( f_5 )</td>
<td>0.66</td>
<td>0.94</td>
<td>0.94</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>( f_6 )</td>
<td>0.60</td>
<td>0.93</td>
<td>0.93</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
</tbody>
</table>
Table 6 – Comparison of optimized values of arc efficiency, effective thermal conductivity and viscosity for eight test cases

<table>
<thead>
<tr>
<th>Test</th>
<th>LM method</th>
<th>CG method- Fletcher and Reeves</th>
<th>CG method- Polak and Ribiere</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\eta$</td>
<td>$\mu_{\text{eff}}$ (kg/m-s)</td>
<td>$\mu_{\text{eff}}$ (kg/m-s)</td>
</tr>
<tr>
<td>1</td>
<td>0.61</td>
<td>112.87</td>
<td>0.05</td>
</tr>
<tr>
<td>2</td>
<td>0.59</td>
<td>96.15</td>
<td>0.04</td>
</tr>
<tr>
<td>3</td>
<td>0.62</td>
<td>91.97</td>
<td>0.04</td>
</tr>
<tr>
<td>4</td>
<td>0.60</td>
<td>133.77</td>
<td>0.05</td>
</tr>
<tr>
<td>5</td>
<td>0.58</td>
<td>87.79</td>
<td>0.04</td>
</tr>
<tr>
<td>6</td>
<td>0.60</td>
<td>112.87</td>
<td>0.05</td>
</tr>
<tr>
<td>7</td>
<td>0.47</td>
<td>121.22</td>
<td>0.05</td>
</tr>
<tr>
<td>8</td>
<td>0.58</td>
<td>96.15</td>
<td>0.05</td>
</tr>
</tbody>
</table>

Figure 14 depicts $p_{\text{iso}}^*$, $\tau_{\text{iso}}$, and $\tau_{\text{iso}}$, as calculated using these optimised values of the unknown parameters. The welding process parameters and material properties such as welding current, voltage and weld speed corresponding to the measurements referred in Figure 14 are given in Tables 1 and 2, respectively. The non-dimensional values of actual throat and leg length obtained using these optimised parameters are much better than those obtained in Figure 9 for all the eight cases. Figure 15 shows a satisfactory agreement between the computed and the experimentally obtained weld geometry. The calculated geometric features of the fillet weld could be satisfactorily predicted by the using the optimised values of parameters in the numerical heat transfer and fluid flow model.

4 SUMMARY AND CONCLUSIONS

A smart phenomenological model for GMA fillet welding involving numerical calculation of heat transfer and fluid flow and parameter optimisation was developed. The

![Graph](image-url)
REFERENCES


