Mathematical Modelling of Heat and Fluid Flow Phenomena

in A Mutually Coupled Welding Arc and Weld Pool

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Abstract

A mathematical model was developed to simulate the heat and fluid flow phenomena in a mutually coupled welding arc and weld pool. Through the statements of continuity, momentum, energy, and Maxwell's electromagnetic equations, the velocity profile, temperature distribution, anode heat and current fluxes in the arc can be determined. These in turn serve as boundary conditions for the weld pool and from which the weld pool characteristics such as surface temperature and weld bead geometry can be predicted from an identical set of transport equations. In this manner, a comprehensive mathematical model of the arc welding process is obtained whereby the final weldment characteristics are described primarily from the input process parameters through the mutual coupling of the arc with the weld pool.

Stationary gas tungsten arc welding operation with argon shielding is modelled as a two-dimensional axi-symmetric system. The workpiece consists of AISI 304 stainless steel and a flat cathode tip is assumed. The weld pool was solved using the PHOENICS numerical package while the welding arc was solved using 2/E/FIX, a public domain code.

This study focused specifically on three phenomena occurring at the free surface; evaporative heat losses, Marangoni shear, and gas shear stress of the plasma in driving weld pool convection. A parametric analysis was performed on the variations of the arc power distribution, material composition, and material transport properties on weld pool characteristics (pool size, shape, surface temperature, pool velocity) to examine their sensitivities.

A mixed control vaporization model due to the combined mechanisms of Langmuir kinetics and mass diffusion across the anode solute boundary layer was developed to account for evaporative heat losses. Marangoni shear due to the surface active element sulphur was examined using a correlation by Sahoo et al [69] which relates the surface tension coefficient, \( \partial \gamma / \partial T \), to sulphur content and surface temperature. Finally, the gas shear stress, \( \tau_{gas} \), is calculated directly from the arc model and serves as an additional boundary condition for the weld pool surface.

The heat loss due to vaporization does not control the surface temperature as this heat loss accounts for less than 10% of the input heat flux. The mixed control vaporization model predicts a heat loss which is about 1/15th that due to Langmuir vaporization.
Marangoni shear is seen to be the more dominant factor governing both the peak surface temperature and surface temperature distribution. In particular, the Marangoni shear or the surface tension shear stress, which is expressed by $\partial / \partial T$ and $\partial T / \partial r$ (the temperature gradient), are both temperature dependent. As the magnitude of $\partial / \partial T$ increases, the surface tension shear stress, $\tau_{s,t}$, also increases and so does the resulting surface velocity. This will cause more thermal energy to be transported away from the free surface and so the surface temperature distribution drops. $\partial / \partial T$ is seen to have a stronger influence on surface temperature than $\partial T / \partial r$.

The gas shear stress (the fourth driving force responsible for weld pool convection) is not an important factor for controlling weld pool convection, and thus weld pool shape. This is because $\tau_{g,s}$ due to $(\partial / \partial T) \ast (\partial T / \partial r)$ is much larger (> 5 times) than that due to $\tau_{g,s}$. With a 200 A arc, the addition of $\tau_{g,s}$ expands the pool radius by less than 0.1 mm. $\tau_{g,s}$ influences the weld pool by strengthening the flow field if the fluid flow direction is the same as the direction of the gas shear stress such as that due to a negative $\partial / \partial T$ driven flow.

Examination of the weld pool profiles indicates substantial differences between the calculated results and the experimental results when the simulations were performed using molecular transport properties. On introducing turbulence by two separate methods: (a) using a constant effective viscosity that is ten times the molecular value, and (b) using the two-equation K-ε turbulence model, the calculated results yield pool shapes and sizes that resemble the experimental data. It is proposed in this study that the flow field in the weld pool is in fact turbulent.

In summary, a methodology has been proposed to calculate the free surface temperature in weld pool which takes into account of the mutual interaction between the arc and the weld pool. This study allows a more fundamental approach into addressing the transport phenomena in arc welding operations by considering the entire process from the electrode down to the plasma, onto the workpiece and to the final solidification of the weld.

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NOMENCLATURE

\( a \)  
Effective radius of heat flux (m)

\( a_{Fe} \)  
Activity of Fe (-)

\( a_{Fe(T)} \)  
Activity of Fe at temperature T (-)

\( a_{Fe(T_{ref})} \)  
Activity of Fe at reference temperature \( T_{ref} \) for thermodynamic calculation (-)

\( a_{i} \)  
Activity of specie i (-)

\( a_{Mn} \)  
Activity of Mn (-)

\( a_{Mn(T)} \)  
Activity of Mn at temperature T (-)

\( a_{Mn(T_{ref})} \)  
Activity of Mn at reference temperature \( T_{ref} \) for thermodynamic calculation (-)

\( a_{s} \)  
Activity of sulphur (-)

\( A \)  
Constant in surface tension coefficient (N/m-K)

\( b \)  
Effective radius of current flux (m)

\( B \)  
Magnetic flux density (Wb/m²)

\( \mathcal{B} \)  
Magnetic flux density [vector quantity] (Wb/m²)

\( B_{θ} \)  
Azimuthal magnetic field (Wb/m²)

\( C \)  
Constant used in electromagnetic stream function (~10 for cathode spot mode)

\( C_{o} \)  
Initial solute content (mole)

\( C_{p} \)  
Heat capacity (J/kg)

\( \overline{C}_{p} \)  
Integral mean heat capacity (J/kg)

\( C_{Fe}^a \)  
Concentration of Fe at surface of workpiece (kg/m³)

\( \overline{C}_{Fe} \)  
Concentration of Fe in the bulk of shielding gas (kg/m³)

\( C_{Mn} \)  
Concentration of Mn (kg/m³)

\( C_{Mn}^a \)  
Concentration of Mn at surface of workpiece (kg/m³)

\( \overline{C}_{Mn} \)  
Concentration of Mn in the bulk of shielding gas (kg/m³)

\( d \)  
Distance (m)

\( D_{Fe-Ar} \)  
Binary diffusion coefficient of Fe in Ar gas (m²/s)

\( D_{Mn-Ar} \)  
Binary diffusion coefficient of Mn in Ar gas (m²/s)

\( e \)  
Electronic charge (C)

\( E \)  
Electric potential field [vector quantity] (V/m)

\( \mathcal{E} \)  
Electric potential field (V/m)

\( f_{L} \)  
Fraction of fluid in mushy zone(-)

\( g \)  
Gravitational acceleration (m/s²)

\( G \)  
Temperature gradient of solid-liquid interface (K/m)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$G_{xs}$</td>
<td>Partial excess free energy (cal/mole)</td>
</tr>
<tr>
<td>$G_{Fe}$</td>
<td>Partial excess free energy of Fe in binary Fe-Mn alloy (cal/mole)</td>
</tr>
<tr>
<td>$G_{Mn}$</td>
<td>Partial excess free energy of Mn in binary Fe-Mn alloy (cal/mole)</td>
</tr>
<tr>
<td>$h$</td>
<td>Plasma enthalpy (J/kg)</td>
</tr>
<tr>
<td>$h_e$</td>
<td>Plasma enthalpy at the edge of the anode boundary layer (J/kg)</td>
</tr>
<tr>
<td>$h_h$</td>
<td>Heat transfer coefficient of workpiece (W/m²-K)</td>
</tr>
<tr>
<td>$h_{h(bot)}$</td>
<td>Heat transfer coefficient at bottom of workpiece (W/m²-K)</td>
</tr>
<tr>
<td>$h_{h(side)}$</td>
<td>Heat transfer coefficient at side of workpiece (W/m²-K)</td>
</tr>
<tr>
<td>$h_{heat}$</td>
<td>Heat transfer coefficient of workpiece (W/m²-K)</td>
</tr>
<tr>
<td>$h_{L,vap}$</td>
<td>Heat transfer coefficient due Langmuir vaporization (m/s)</td>
</tr>
<tr>
<td>$h_{m(efi)}$</td>
<td>Effective mass transfer coefficient (m/s)</td>
</tr>
<tr>
<td>$h_{m(efi),Fe}$</td>
<td>Effective mass transfer coefficient due to Fe (m/s)</td>
</tr>
<tr>
<td>$h_{m(efi),i}$</td>
<td>Effective mass transfer coefficient due to species i (m/s)</td>
</tr>
<tr>
<td>$h_{m(efi),Mn}$</td>
<td>Effective mass transfer coefficient due to Mn (m/s)</td>
</tr>
<tr>
<td>$h_{mass}$</td>
<td>Mass transfer coefficient due to diffusion across solute boundary layer (m/s)</td>
</tr>
<tr>
<td>$h_{vap}$</td>
<td>Mass transfer coefficient due to vaporization (m/s)</td>
</tr>
<tr>
<td>$h_w$</td>
<td>Plasma enthalpy at the anode wall (J/kg)</td>
</tr>
<tr>
<td>I</td>
<td>Arc current (A)</td>
</tr>
<tr>
<td>J</td>
<td>Current density (A/m²)</td>
</tr>
<tr>
<td>J</td>
<td>Current density [vector quantity] (A/m²)</td>
</tr>
<tr>
<td>$J_a$</td>
<td>Anode current density (A/m²)</td>
</tr>
<tr>
<td>$J_{a,max}$</td>
<td>Maximum anode current density (A/m²)</td>
</tr>
<tr>
<td>$J_c$</td>
<td>Cathode spot current density (A/m²)</td>
</tr>
<tr>
<td>$J_0$</td>
<td>Anode current density at $r = 0$ (A/m²)</td>
</tr>
<tr>
<td>$J_r$</td>
<td>Radial current density (A/m²)</td>
</tr>
<tr>
<td>$J_z$</td>
<td>Axial current density (A/m²)</td>
</tr>
<tr>
<td>k</td>
<td>Molecular thermal conductivity (W/m-K)</td>
</tr>
<tr>
<td>$k_1$</td>
<td>Function of entropy of segregation (-)</td>
</tr>
<tr>
<td>$k_b$</td>
<td>Boltzmann constant (J/K)</td>
</tr>
<tr>
<td>$k_{eff}$</td>
<td>Effective thermal conductivity (W/m-K)</td>
</tr>
<tr>
<td>$k_l$</td>
<td>Thermal conductivity of liquid steel (W/m-K)</td>
</tr>
<tr>
<td>$k_s$</td>
<td>Thermal conductivity of solid steel (W/m-K)</td>
</tr>
<tr>
<td>$k_t$</td>
<td>Turbulent thermal conductivity (W/m-K)</td>
</tr>
<tr>
<td>K</td>
<td>Drag coefficient in source term for phase change source term (kg/m³s)</td>
</tr>
<tr>
<td>K</td>
<td>Stability parameter used by Atthey [43] and Sozou [39] for weld pool</td>
</tr>
<tr>
<td>Symbol</td>
<td>Definition</td>
</tr>
<tr>
<td>--------</td>
<td>------------</td>
</tr>
<tr>
<td>$K_{\text{max}}$</td>
<td>Maximum drag coefficient in phase change source term (kg/m$^3$s)</td>
</tr>
<tr>
<td>$K_{\text{seg}}$</td>
<td>Equilibrium constant for segregation (-)</td>
</tr>
<tr>
<td>$L$</td>
<td>Characteristic length (m)</td>
</tr>
<tr>
<td>$L_r$</td>
<td>Radius of plate (m)</td>
</tr>
<tr>
<td>$L_z$</td>
<td>Thickness of plate (m)</td>
</tr>
<tr>
<td>$L_{\text{vap,Fe}}$</td>
<td>Heat of vaporization of Fe (J/kg)</td>
</tr>
<tr>
<td>$L_{\text{vap,i}}$</td>
<td>Heat of vaporization of specie i (J/kg)</td>
</tr>
<tr>
<td>$L_{\text{vap,Mn}}$</td>
<td>Heat of vaporization of Mn (J/kg)</td>
</tr>
<tr>
<td>$m_{\text{Fe}}$</td>
<td>Mass flux of Fe due to vaporization (kg/m$^2$s)</td>
</tr>
<tr>
<td>$m_i$</td>
<td>Mass flux of specie i due to vaporization (kg/m$^2$s)</td>
</tr>
<tr>
<td>$m_{k,\text{Fe}}$</td>
<td>Mass flux of Fe due to vaporization by kinetic theory (kg/m$^2$s)</td>
</tr>
<tr>
<td>$m_{k,Mn}$</td>
<td>Mass flux of Mn due to vaporization by kinetic theory (kg/m$^2$s)</td>
</tr>
<tr>
<td>$m_{\text{L,Fe}}$</td>
<td>Mass flux of Fe due to vaporization by Langmuir theory (kg/m$^2$s)</td>
</tr>
<tr>
<td>$m_{\text{L,Mn}}$</td>
<td>Mass flux of Mn due to vaporization by Langmuir theory (kg/m$^2$s)</td>
</tr>
<tr>
<td>$m_{\text{Mn}}$</td>
<td>Mass flux of Mn due to vaporization (kg/m$^2$s)</td>
</tr>
<tr>
<td>$M(_{\text{Ar}})$</td>
<td>Atomic weight of Argon (g/mole)</td>
</tr>
<tr>
<td>$M(_{\text{Fe}})$</td>
<td>Atomic weight of Iron (g/mole)</td>
</tr>
<tr>
<td>$M(_{\text{Mn}})$</td>
<td>Atomic weight of Manganese (g/mole)</td>
</tr>
<tr>
<td>$M_{\text{Ar}}$</td>
<td>Atomic weight of Argon (kg/mole)</td>
</tr>
<tr>
<td>$M_{\text{Fe}}$</td>
<td>Atomic weight of Iron (kg/mole)</td>
</tr>
<tr>
<td>$M_{\text{Mn}}$</td>
<td>Atomic weight of Manganese (kg/mole)</td>
</tr>
<tr>
<td>$n$</td>
<td>Normal direction to anode surface (-)</td>
</tr>
<tr>
<td>$n_{Fe}$</td>
<td>Coefficient in Lewis number (-)</td>
</tr>
<tr>
<td>$n_{\theta}$</td>
<td>Unit vector in the azimuthal direction (m)</td>
</tr>
<tr>
<td>$Nu_{\text{w}}$</td>
<td>Nusselt number at the anode wall (-)</td>
</tr>
<tr>
<td>$P$</td>
<td>Pressure (Pa)</td>
</tr>
<tr>
<td>$P_{s,\text{max}}$</td>
<td>Maximum anode over-pressure at anode surface (Pa)</td>
</tr>
<tr>
<td>$P_{\text{atm}}$</td>
<td>Ambient pressure of shielding gas (atm)</td>
</tr>
<tr>
<td>$P_{\text{Fe}}$</td>
<td>Partial pressure of Fe (Pa)</td>
</tr>
<tr>
<td>$P_{\text{Fe(T)}}$</td>
<td>Partial pressure of Fe at temperature T (Pa)</td>
</tr>
<tr>
<td>$P_{\text{Fe}}$</td>
<td>Vapor pressure of pure Fe (Pa)</td>
</tr>
<tr>
<td>$P_{\text{Fe}}^*$</td>
<td>Partial pressure of Fe in the bulk of shielding gas (Pa)</td>
</tr>
<tr>
<td>$P_i$</td>
<td>Partial pressure of species i (atm)</td>
</tr>
<tr>
<td>$P_{\text{Mn}}$</td>
<td>Partial pressure of Mn (Pa)</td>
</tr>
<tr>
<td>$P_{\text{Mn(T)}}$</td>
<td>Partial pressure of Mn at temperature T (Pa)</td>
</tr>
</tbody>
</table>
\( P_{Mn}^0 \)  
Vapor pressure of pure Mn (Pa)

\( P_{Mn}^w \)  
Partial pressure of Mn in the bulk of shielding gas (Pa)

\( Pr \)  
Prandtl number, \( C_p \mu / k \) (-)

\( Pr_t \)  
Turbulent Prandtl number, \( C_p \mu_t / k_t \) (-)

\( Pr_w \)  
Plasma Prandtl number at the anode wall temperature (-)

\( q_a \)  
Anode heat flux (W/m²)

\( q_{a,\text{conv}} \)  
Convective contribution to anode by plasma arc (W/m²)

\( q_{\text{arc}} \)  
Reference anode heat flux due to welding arc (W/m²)

\( q'_{\text{arc}} \)  
Revised anode heat flux with constant source, \( q_{\text{cons}} \) added (W/m²)

\( q''_{\text{arc}} \)  
Revised anode heat flux with relative source added (W/m²)

\( q_{\text{const}} \)  
Constant heat flux added to reference heat source (W/m²)

\( q_{\text{conv}} \)  
Convective heat loss from surface of workpiece (W/m²)

\( q_{\text{net}} \)  
Net heat input into workpiece (W/m²)

\( q_0 \)  
Anode heat flux at \( r = 0 \) (W/m²)

\( q_{\text{rad}} \)  
Radiative heat loss from surface of workpiece (W/m²)

\( q_{\text{tot}} \)  
Total heat gained by anode (W/m²)

\( q_{\text{vap,Fe}} \)  
Heat loss due to vaporization of Fe (W/m²)

\( q_{\text{vap,i}} \)  
Heat loss due to vaporization of species i (W/m²)

\( q_{\text{vap,Mn}} \)  
Heat loss due to vaporization of Mn (W/m²)

\( q_{\text{vap,tot}} \)  
Total heat loss due to vaporization (W/m²)

\( Q_{a,\text{conv}} \)  
Convective heat gained by anode in anode boundary layer (W/m²)

\( Q_{e,\text{elec}} \)  
Electron contribution of the anode heat flux (W/m²)

\( Q_{a,\text{max}} \)  
Maximum anode heat flux (W/m²)

\( Q_{a,\text{rad}} \)  
Radiative contribution to the anode heat flux (W/m²)

\( Q_{c,\text{ionic}} \)  
Heat source from ionic contribution in the cathode fall region (W/m²)

\( Q_{\text{conv}} \)  
Convective heat gained by anode in anode boundary layer (W/m²)

\( Q_{r,l,j} \)  
Heat flux received at surface \( S_i \) from volume \( V_j \) located the distance \( r_{i,j} \) away (W/m²)

\( Q_{\text{total}} \)  
Total power received by workpiece (W)

\( Q'_{\text{total}} \)  
Revised total power received by workpiece due to additional heat source (W)

\( r \)  
Radial coordinate (m)

\( r' \)  
Anode spot size (m)

\( r_{i,j} \)  
The direction vector from surface, \( S_i \) to volume element, \( V_j \) (m)

\( R \)  
Gas constant (J/mole)

\( R_c \)  
Cathode spot radius (m)

\( R_c' \)  
Radius of electrode (m)
\( R_g \)  
Gas constant (J/kg-mole)

\( R_{s-l} \)  
Growth rate of solid-liquid interface (m/s)

\( Re \)  
Reynolds number, \( \rho u L / \mu \) (-)

\( Re_w \)  
Reynolds number at the anode wall (-)

\( S_R \)  
Radiation source (W/m³)

\( S_{R,i,j} \)  
View factor from anode surface \( i \) to volume element \( V_j \)

\( Sc \)  
Schmidt number, \( \nu / D_{Mn-Ar} \) (-)

\( t \)  
Time (s)

\( T \)  
Temperature (K)

\( T_{amb} \)  
Ambient temperature (K)

\( T_{bp(Ar)} \)  
Boiling point of argon (K)

\( T_{Cu} \)  
Temperature of copper plate for cooling workpiece (K)

\( T_e \)  
Plasma temperature at the edge of the anode boundary layer (K)

\( T_{a,elec} \)  
Electron temperature adjacent to anode (K)

\( T_{e,elec} \)  
Electron temperature adjacent to cathode (K)

\( T_f \)  
Film temperature (K)

\( T_{Fe,ref} \)  
Reference temperature for Fe in activity calculations (K)

\( T_{liq} \)  
Liquidus temperature (K)

\( T_{max} \)  
Maximum temperature in plasma arc or weld pool (K)

\( T_{mp(Fe)} \)  
Melting point of Fe (K)

\( T_{mp(Mn)} \)  
Melting point of Mn (K)

\( T_{Mn,ref} \)  
Reference temperature for Mn in activity calculations (K)

\( T_r \)  
Reference temperature for Boussinesq approximation (\( T_{\text{sol}} \) K)

\( T_{s,max} \)  
Maximum weld pool surface temperature (K)

\( T_s \)  
Surface temperature of workpiece/weld pool (K)

\( T_{sol} \)  
Solidus temperature (K)

\( T_w \)  
Anode wall temperature (K)

\( u \)  
Radial velocity (m/s)

\( u_e \)  
Plasma velocity parallel to the anode surface at the edge of the boundary layer (m/s)

\( u_{max} \)  
Maximum velocity in plasma arc or weld pool (m/s)

\( u_{wall} \)  
Plasma velocity at anode wall (m/s)

\( U_0 \)  
Characteristic velocity (m/s)

\( V \)  
Arc voltage (V)

\( V_{arc} \)  
Calculated arc voltage (includes approximate cathode fall voltage) (V)

\( V_c \)  
Cathode fall voltage (V)

\( V_{col} \)  
Arc column voltage (V)
$V_j$ The differential volume element in the radiation view factor relation (m$^3$)
$V_{Ar,liq}$ Molar volume of Ar at boiling point (cm$^3$/g-mole)
$V_{Fe,soln}$ Molar volume of Fe at melting point (cm$^3$/g-mole)
$V_{Mn,soln}$ Molar volume of Mn at melting point (cm$^3$/g-mole)
$w$ Axial velocity (m/s)
$x$ Fraction increment of heat source (-)
$X_{Fe}$ Mole fraction of Fe (-)
$X_{Mn}$ Mole fraction of Mn (-)
$z$ Axial coordinate (m)

Greek Symbols

$\alpha$ Thermal diffusivity (m$^2$/s)
$\alpha_j$ Current distribution parameter (m$^{-1}$)
$\alpha_q$ Heat distribution parameter (m$^2$)
$\alpha_s$ Sticking coefficient (-)
$\beta$ Volume coefficient of thermal expansion (K$^{-1}$)
$\gamma$ Surface tension (N/m)
$\Gamma_s$ Surface excess at saturation (kg/(kg-mole-m$^2$))
$\partial \gamma / \partial T$ Surface tension coefficient (N/m-K)
$\Delta H$ Latent heat of fusion of steel (J/kg)
$\Delta H_{mix,Fe}$ Partial heat of mixing of Fe in binary Fe-Mn alloy (cal/mole)
$\Delta H_{mix,Mn}$ Partial heat of mixing of Mn in binary Fe-Mn alloy (cal/mole)
$\Delta r$ Radial grid size (m)
$\Delta t$ Time step (s)
$\Delta z$ Axial grid size (m)
$\Delta C_{Fe}$ Concentration difference of Mn between surface and bulk, $C_{Fe}^s - C_{Fe}^\infty$ (kg/m$^3$)
$\Delta C_i$ Concentration difference of Fe between surface and bulk, $C_i^s - C_i^\infty$ (kg/m$^3$)
$\Delta C_{Mn}$ Concentration difference of Mn between surface and bulk, $C_{Mn}^s - C_{Mn}^\infty$ (kg/m$^3$)
$\Delta H^o$ Standard heat of adsorption (J/kg-mole)
$\Delta H^o_{304}$ Standard heat of adsorption of SS 304 (J/kg-mole)
$\Delta H^o_{FeS}$ Standard heat of adsorption of binary FeS (J/kg-mole)
$\Delta T$ Temperature difference between surface and ambient condition, $T_{surf} - T_{amb}$ (K)
$\Delta T^4$ Temperature difference between surface and ambient condition, $T_{surf}^4 - T_{amb}^4$ (K)
\( \nabla \) Del operator (m\(^{-1}\))

\( \nabla^2 \) Laplacian operator (m\(^{-2}\))

\( \varepsilon \) Emissivity (-)

\( \varepsilon_{Fe} \) Characteristic energy of interaction between Fe molecules (K)

\( \varepsilon_{Fe-Ar} \) Characteristic energy of interaction between Fe and Ar (K)

\( \varepsilon_{Mn} \) Characteristic energy of interaction between Mn molecules (K)

\( \varepsilon_{Mn-Ar} \) Characteristic energy of interaction between Mn and Ar (K)

\( \eta \) Arc efficiency (%)

\( \theta \) Azimuthal direction (radian)

\( \mu \) Molecular dynamic viscosity (kg/m-s)

\( \mu_e \) Dynamic viscosity of shielding gas at the edge of the boundary layer (kg/m-s)

\( \mu_{eff} \) Effective dynamic viscosity (kg/m-s)

\( \mu_{gas} \) Dynamic viscosity of shielding gas (kg/m-s)

\( \mu_{liq} \) Dynamic viscosity of liquid steel (kg/m-s)

\( \mu_0 \) Magnetic permeability of free space (H/m)

\( \mu_t \) Turbulent dynamic viscosity (kg/m-s)

\( \mu_w \) Dynamic viscosity of shielding gas at the anode wall (kg/m-s)

\( \nu \) Kinematic viscosity (m\(^2\)/s)

\( \rho \) Density (kg/m\(^3\))

\( \rho_{(Ar)} \) Density of Ar at boiling point (g/cm\(^3\))

\( \rho_{(Fe)} \) Density of Fe at melting point (g/cm\(^3\))

\( \rho_{(Mn)} \) Density of Mn at melting point (g/cm\(^3\))

\( \rho_{(Ar)} \) Density of argon at boiling point (K)

\( \rho_e \) Charge density (C/m\(^3\))

\( \rho_{e} \) Density of shielding gas at the edge of the boundary layer (kg/m\(^3\))

\( \rho_{w} \) Density of shielding gas at the anode wall (kg/m\(^3\))

\( \sigma_{Ar} \) Characteristic diameter of Ar molecule (Angstrom)

\( \sigma_{H} \) Heat distribution parameter (m\(^2\))

\( \sigma_e \) Electrical conductivity (ohm-m\(^{-1}\))

\( \sigma_{Fe} \) Characteristic diameter of Fe molecule (Angstrom)

\( \sigma_{Fe-Ar} \) Characteristic diameter of Fe–Ar molecule (Angstrom)

\( \tau_{gas} \) Gas shear stress (Pa)

\( \sigma_l \) Current distribution parameter (m\(^2\))

\( \sigma_{Mn} \) Characteristic diameter of Mn molecule (Angstrom)

\( \sigma_{Mn-Ar} \) Characteristic diameter of Mn–Ar molecule (Angstrom)

\( \sigma_{ab} \) Stefan-Boltzmann constant (W/m\(^2\)-K\(^4\))
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau_{st}$</td>
<td>Surface tension shear stress (Pa)</td>
</tr>
<tr>
<td>$\phi$</td>
<td>Electric potential (V)</td>
</tr>
<tr>
<td>$\Phi_{c(max)}$</td>
<td>Maximum electric potential in the vicinity of cathode (V)</td>
</tr>
<tr>
<td>$\Phi_{a(min)}$</td>
<td>Minimum electric potential in the vicinity of anode (V)</td>
</tr>
<tr>
<td>$\phi_d$</td>
<td>Thermal diffusion coefficient for electrons (A/m-K)</td>
</tr>
<tr>
<td>$\Phi_a$</td>
<td>Work function of the anode material (V)</td>
</tr>
<tr>
<td>$\Phi_c$</td>
<td>Work function of the cathode material/cathode surface (V)</td>
</tr>
<tr>
<td>$\Phi_{Cu}$</td>
<td>Work function of the copper anode (V)</td>
</tr>
<tr>
<td>$\Phi_{Fe}$</td>
<td>Work function of the iron (steel) anode (V)</td>
</tr>
<tr>
<td>$\psi$</td>
<td>Solid angle $r_{i,j}$ makes with the normal to surface $S_i$ (radian)</td>
</tr>
<tr>
<td>$\psi_e$</td>
<td>Electromagnetic stream function (-)</td>
</tr>
<tr>
<td>$\Omega_{Fe-Ar}$</td>
<td>Function of $k_B T/\epsilon_{Fe-Ar}$ (-)</td>
</tr>
<tr>
<td>$\Omega_{Mn-Ar}$</td>
<td>Function of $k_B T/\epsilon_{Mn-Ar}$ (-)</td>
</tr>
<tr>
<td>$\Omega$</td>
<td>Function obtained from Bird et al [131]</td>
</tr>
</tbody>
</table>
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Finally, all efforts go to God Almighty.
1. INTRODUCTION

It is generally accepted that conventional welding can be improved by computer control and robotic technology for automated process control of welding parameters [1]. Automated welding systems, for example, using expert systems are becoming more frequent and have been commercially marketed [2]. The success of such an automated manufacturing process requires a data base from which optimum process parameters can be selected. This data base can be efficiently developed through a basic understanding of the physical and chemical interaction between the heat and mass sources of the arc and the base metal.

The objective of this investigation is to develop a fundamental understanding of the fluid flow and heat transfer in autogeneous gas tungsten arc welding (GTAW) operations through mathematical modelling efforts. The present investigation is part of an overall objective sponsored by the U.S. Department of Energy (Basic Energy Sciences Section Welding Program) aimed at relating welding process parameters to the structure and properties of the resultant weld.

This chapter describes the importance of mathematical models in the welding operation, reviews previous work in this area, and presents the objectives of this dissertation.

1.1 Importance of Fluid Flow and Heat Transfer in Gas Tungsten Arc Welding

There are ample evidence to suggest that weld pool convection can strongly affect the structure and properties of the resultant weld [3-6]. The role convection plays is by defining the heat transfer and the position of the isotherms within the melt, and this has significant effect in determining the shape of the weld pool and its associated solidification phenomena. Some of the weld characteristics affected include surface smoothness, weld pool geometry, fume formation, macro-segregation, grain structure, and the gas porosity of the resultant weld bead. Convection is also primarily responsible for mixing and, therefore, affects the composition profile of the weld pool. Thus, an understanding of these variations in weld characteristics caused by convective flows, which could well determine the integrity of the weldment, is fundamental to welding technology.
1.2 Role of Convection on Weld Bead Characteristics

The principal driving forces controlling convection have been identified as buoyancy, electromagnetic, surface tension, and the plasma arc. Each of these forces produces different degrees of convection and at different locations in the pool, thus resulting in different weld bead configurations.

Buoyancy driven flow is caused by the temperature dependence of density. When the weld pool is formed by the welding arc, the lighter liquid at the high temperature region will rise while the heavier liquid at the lower temperature region will sink. A convective loop is thus established (Fig. 1(a)) with a characteristic velocity of the order of mm/s.

Electromagnetically driven flow is caused by the interaction between the divergent current flux from the electrode and the magnetic field induced within the melt. This interaction produces the Lorentz force \((J \times B)\), shown in Fig. 1(b), and has a characteristic velocity of the order of several cm/s.

Surface tension driven flows is caused by the temperature dependence of surface tension and this is defined in part by the surface tension coefficient, \(\partial \gamma / \partial T\). In general, liquid metals have negative \(\partial \gamma / \partial T\) but surface active elements such as N, P, As, and Sb (Group V) and O, Se, S, and Te (Group VI) can alter \(\partial \gamma / \partial T\) substantially [7], and thus the weld pool geometry. Their net effect are shown schematically in Figs. 1(c) and (d). Their characteristic velocity is in the 0.5–1.0 m/s range with \(\partial \gamma / \partial T = 10^{-4} \text{ N/m-K}\). The change in the pool shape with the sign of \(\partial \gamma / \partial T\) is especially significant.

The role of arc force as a contributing factor to weld pool convection is generally significant at arc currents above 250 A. Lin and Eagar [8] have calculated and measured the surface depression as a function of arc current. At arc currents below 200 A, depression is shallow and does not significantly influence the pool shape. At higher currents (> 250 A), however, surface depression can alter both the flow within the pool and the geometry (Fig. 1(e)). With travelling welds in excess of 2 mm/s, the effect of convection was even more pronounced, producing vortex flows which were determined to be responsible for weld defects like undercutting, humped beads, and piping [9].
(a) Buoyancy-driven flow
Velocity ~ few mm/s

(b) Electromagnetically-driven flow
Velocity ~ few cm/s

(c) Surface tension driven flow
\(\frac{d\gamma}{dT} < 0\) : Velocity ~ m/s

(d) Surface tension driven flow
\(\frac{d\gamma}{dT} > 0\) : Velocity ~ m/s

(e) High currents arcs (> 260 A)
Cross-section of moving weld [5]

Figure 1. Schematic flow profiles produced by the various driving forces. The arc is located directly above the middle of the pool.
It can be seen that the arc force can significantly affect pool shape and this has important consequences on the solidified substructure as discussed in the next section.

In summary, the driving forces, so described, can affect the flow field and thus the weld bead shape. It seems apparent that by proper control of welding parameters such as welding speed and arc current, one can control the final shape of the weld and the type of defects produced.

1.3 Role of Convection on the Solidified Substructure

In the mid-60's, Savage et al [10-12] did some pioneering studies in relating solidification substructure of fusion welds to welding parameters. Much of their work have been summarized in a later paper [13]. Employing concepts from solidification technology, their principal findings are that welding speed and arc current are the 2 major controlling factors for a specific binary alloy composition. For instance, at high welding speeds, a tear-drop weld pool is produced with straight columnar grains (Fig. 2) [14] which are susceptible to center line cracking whereas at low welding speeds, where an almost elliptical pool is formed, "curved" columnar grains are produced. They reasoned that the competitive, epitaxial growth of these substructures can be determined from the shape of the weld pool and the maximum temperature gradient at the melt-solid interface. We note that these two factors are inherently related to the convective flows in the pool.

In addition, the solidification modes and substructures were explained from the concepts of constitutional supercooling. The extent of constitutional supercooling has a pronounced effect on the solidification mode and resulting substructure. Figure 3, adapted from Tiller and Rutter [15], summarized the effect of the temperature gradient, growth rate, and solute content on the solidification mode. Savage et al [13] employed this diagram to assist in the explanation of microstructures that they found. Thus, depending upon process parameters, various grains can form due to the temperature gradient (G) and the rate of growth of the solid-liquid interface (R_+). It is relevant to state that convection can alter the shape of the weld pool, the temperature profile within the pool, and also the solidification rate. Therefore, a direct link exists between the microstructural development, convection, and process parameters.
Figure 2 Comparison of weld pool shapes due to varying travel speeds [14].
(a) Slow (b) Intermediate (c) Fast
Figure 3. Schematic summary of factors controlling growth mode during solidification [15]. Various substructures can form depending upon the initial solute content and the G/R ratio.
1.4 Role of Free Surface in Weld Pool Behavior

In the past, virtually all modelling studies assumed for a flat workpiece. We now know that this is an over-simplification. The following lists some of the effect of free surface in welding.

Sorensen and Eagar [16] reported the existence of an oscillatory weld pool surface with direct current straight polarity gas GTAW (Fig. 4 (a)). In travelling welds, rippling effect of the solidified weldment is common (Fig. 4 (b)) [17]. At arc currents above 250 A, significant surface depression (> 2 mm) can occur which can give rise to weld defects (bubble entrapment) on extinguishing the arc (Fig. 4 (c)) [5]. Finally, even with low currents GTAW (< 100 A), the final solidified structure is generally non-planar (Fig. 4 (d)) [18].

The free surface represents the interface by which the workpiece receives its heat and current sources. It is also the region where the most dominant convective driving force exists. Furthermore, this surface is deformable and represents a moving and free boundary problem. Thus, the free surface is a critical component in any weld modelling effort. The Gaussian-type heat and current flux distributions that are frequently assumed in all previous studies may not be appropriate. It has been shown by Choo et al [19] that deformed pools (≥ 1 mm) can lead to non-Gaussian distributions. Thus, a comprehensive representation of the arc welding operation may need to involve a dynamic coupling of the welding arc and weld pool in order to reflect the physical processes occurring at the free surface. These physical processes (vaporization and surface tension) will be described in greater detail in Chapter 3.

1.5 Difficulties in Arc-Weld Pool Experiments

The interaction of the heat source with the weld pool, which has been previously described, is a complex physical phenomenon. Experimental investigations of flow conditions in weld pool are generally limited to the measurement of surface velocities and temperatures. Direct observation of flow velocities in the small, intensely heated pool is usually complicated by the presence of the arc over the weld surface. Besides, information such as solidification rate, bulk flow velocity, and bulk temperature profile are not readily obtainable. In addition, the interactive
Figure 4 Free surface effect in welding
(a) Oscillating free surface in direct current electrode negative GTAW [16]
(b) Solidified ripples in moving welds [17]
(c) Deep surface depression in high arc current welding [5]
(d) Solidified structure is non-planar [18]
nature of the entire process makes it difficult to determine the relative importance of each welding parameter in affecting weld quality.

Studies of the arc include measuring the temperatures of the arc [20,21], heat and current flux distributions [22-24], near anode cross-section [25], arc voltage [26], and arc efficiency [27,28]. These results are generally obtained for water-cooled Cu plate with a flat surface. Such studies do not truly reflect the actual welding process of steel. For instance, since vaporization is ignored, this can lead to higher arc efficiencies. In addition, fluctuating surfaces which are observed at low current (100 A) welding are not considered.

Studies of the weld pool include surface temperature measurements [29,30], surface profile shape and arc pressure [8], and arc force [31,32]. Except for the studies of Kraus [29,30] which employed an optical spectral radiometric/laser reflectance method for measuring the surface temperature, most of the measurements entail a high degree of uncertainty in the reported values due to the difficult and tedious experimental work involved in observing the welding process. Often, the experimental work involves substantial trials and errors to get a stable arc and reproducible results. It indicates the difficulty associated with arc welding work. Nevertheless, useful insight and trends can be obtained from such studies.

Mathematical models which can simulate convective heat flows in the weld pool can help address some of these difficulties. Through a systematic and parametric analyses of the various driving forces over a range of operating conditions, a fundamental understanding of the interactive nature of the welding parameters can be established. Also, numerical analyses performed in conjunction with experimental studies can be very helpful in understanding the processes occurring during welding.

1.6 Research Efforts in Mathematical Modelling of Weld Pool and Welding Arc

(a) Weld Pool Modelling Efforts

Figures 5 (a-c) [3,4,19,33-65] show primarily the state of modelling efforts for the weld pool in the past 20 years. It focussed mainly on the convective modelling efforts in the weld pool.
CONVECTIVE WELD POOL MODELLING EFFORTS

Rosenthal (1941, 1946) [33, 34]
- Analytical solutions to point, line, and plane sources

Carslaw & Jaeger (1955) [36]
- Conduction Heat Transfer

Ryakalin (1960) [35]
- Conductive Heat Transfer (Analytical)

Christensen, Davies, & Gjermundsen (1965) [37]
- Conduction Heat Transfer

\[
K = \frac{\mu_0^2}{2 \pi^2 \rho v^2}
\]

Sozou & Pickering (1976) [40]
- point source at centre of finite hemisphere
  - use free slip at free surface rather than fixed velocity
  - K reduced to 94

Sozou & Pickering (1978) [41]
- fluid flow in axisymmetric container with electrode in contact with liquid surface
- cylindrical electrode with uniform current density

Shercliff (1970) [38]
- semi-infinite inviscid fluid with point source
  - poses singularity at axis of symmetry

Sozou (1970) [39]
- added viscosity to the model but omitted the convective terms
  - singularity if K > 300.1

Andrew & Craine (1978) [42]
- flow in hemisphere with distributed current source
  - actually point source located a few mm above surface
  - direction of flow depends on location of current source

Atthe (1980) [43]
- isothermal MHD flow in hemispherical pool
  - distributed current source with inertia terms
  - extend parameter K further (singularity avoided)

Figure 5 (a) Convective Weld Pool Modelling Efforts (1970-1980)
### Convective Weld Pool Modelling Efforts (Cont.)

<table>
<thead>
<tr>
<th>Year</th>
<th>Authors</th>
<th>Description</th>
</tr>
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| 1983 | Oreper, Eagar, & Szekely (1983) [44] | - 2D steady convective flows with (buoyancy, MHD, Marangoni) in spot GTAW  
- predefined pool shape and distributed source |
| 1984 | Chan, Mazumder, & Chen (1984) [46] | - 2D transient laser weld with line source and calculated pool shape (free surface assumed flat) |
| 1985 | Kong & Sun (1985) [47] | - 2D steady state spot GTAW in Al with calculated pool shape  
- distributed heat & current sources |
| 1985 | Wei & Geidt (1985) [48] | 2D steady state EBW (analytical) with keyhole |
| 1985 | Fautrelle (1985) [49] | - 2D spot GTAW with predefined pool shape  
- emphasized on minor elements on free surface |
| 1986 | Oreper, Eagar & Szekely (1986) [50] | - 2D transient weldpool development (melting & freezing) for Al, Ti, steel |
| 1986 | Correa & Sundell (1986) [51] | - 2D steady-state spot GTAW with predefined pool shape (uniform heat source) |
- distributed heat & current sources (free surface assumed flat) |
| 1986 | Chan, Zehr, Mazumder, & Chen (1986) [53] | - 3D quasi-steady LW (analytical & numerical)  
- free surface assumed flat with line source  
- assume scanning speed < pool characteristic velocity |
| 1986 | Paul & DebRoy (1986) [54] | - 2D steady state LW (turbulence via increased viscosity) |
- pool penetration governed by arc length |
| 1987 | Oreper & Szekely (1987) [56] | - 2D transient solidification in spot GTAW |

Figure 5 (b) Convective weld pool modelling (1983-1987).
**CONVECTIVE WELD POOL MODELLING EFFORTS (CONT.)**

**Zacharia, Eraslan, Aidun, & David (1989) [62]**
- 2D and 3D transient model for spot/moving GTA
- free surface deformable (prescribed heat and current sources)

**Zacharia, David, Vitek, & Debroy (1989) [63,64]**
- 2D stationary GTAW/LW
- sign of $\gamma/\partial T$ function of $T$ and sulphur content in steel
- prescribed heat & current sources
- numerical and experimental results

**Tsao & Wu (1988) [59]**
- 2D GMAW/GTAW spot weld
- finger penetration observed in GMAW
- metal spray in GMAW modelled via thermal energy exchanged

**Paul & Debroy (1988) [60]**
- 2D transient LW with free surface effect
- effect of free surface is uncoupled from the heat source
  (Pool dimension ~ 0.2 mm)

**Tekriwal & Mazumder (1988) [61]**
- 3D finite element analysis
- conduction heat transfer
- Gaussian heat input with no vaporization

**Thompson & Szekely (1989) [65]**
- 2D transient spot GTA with a pre-deformed surface
- effect of Lorentz force is excluded

**Choo, Westhoff, & Szekely (1990) [19]**
- address free surface behavior (pool collapse)
- modelled heat & current fluxes for deformed pool surface
- semi-coupling of arc and weldpool

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Figure 5 (c) Convective weld pool modelling (1988-1990).
Solutions to the heat conduction equation can be found in the classical works of Rosenthal [33,34], Ryakalin [35], Christensen et al [37], and to some extent in Carslaw and Jaeger [36]. Instead of discussing the merits and dismerits of each paper, Fig. 5 will highlight the advances made. A discussion of the overall direction taken by the modelling efforts will also be given.

Prior to 1980's, much of the mathematical investigation were of an analytical nature providing analytical solutions to the heat conduction equation and the linearized momentum equation. After these classical studies, attempts were made to include the convective forces in the analyses. These stem from the experimental evidence that the weld pool is vigorously stirred [66]. Atthey [43] estimated that the ratio of the thermal to electromagnetic forces to be 0.06. Some of the initial problems encountered in these semi-infinite solutions were singularity in the velocity fields. In the early analysis (prior to Atthey's studies), the non-linear inertia terms were ignored and the linear momentum equation were solved for an isothermal system. The parameter $K$ (Fig. 5(a)) surfaces frequently and limits the solution to low current applications ($< 5$ A) [43]. Atthey [43] overcame the problem by solving semi-numerically the full unsteady Navier-Stokes equation and he described his solutions to be stable up to 100 A before the onset of turbulence caused his solution to break down. Incidentally, Lancaster [67] has a good collection of weld pool modelling papers prior to 1980 which discuss some of the analytical solution of both linear and non-linear momentum equations all the way back to 1934.

By the late 1970's, it was understood that convective flows were due primarily to the electromagnetic forces. In the early 1980's, surface tension was seen to an important force affecting weld pool geometry. Heiple and Roper [6] proposed the effect of Marangoni flows due to surface active elements and the effect of these minor elements on pool shape were very pronounced.

Oreper et al [3] were generally considered to be the first paper that accounts for the 3 major driving forces (buoyancy, electromagnetic, and surface tension) simultaneously and numerically solved the coupled momentum, energy, and continuity equations. Yokada and Matsunawa [45] were also solving similar equations numerically in 1983 but their pool geometry was less realistic (semi-cylindrical horizontal pool with semi-cylindrical heat source). Since then, there had been an
explosion of numerical studies on weld pool convection. An excellent review of the modelling efforts of these Marangoni flows is given by Keene [68] and the salient features of his review are also given in Figs. 5 (a-c).

It is evident from Figs. 5 (a-c) that there have been considerable advances in modelling the convective heat transfer in the weld pool. Currently, two-dimensional (2D) and three-dimensional (3D) modelling of spot and moving welds are possible. The results of these modelling studies have given useful insights as to the nature of convective flows in weld pool, some of which have been described earlier in Section 1.2.

Some of the ideas described by Keene’s review [68], written in 1988, on thermocapillary flow in weld pools are worthy of discussion. He called for further development of the mathematical model, in particular, that which addressed the free surface. This was in fact one of the objective of this work which was proposed in 1987. Secondly, Keene [68] called for the determination of the temperature and concentration dependance of surface tension, γ. Sahoo et al [69] have indeed began to address this γ dependance from a thermodynamic (equilibrium) viewpoint while Ishizaki [70] calls for a “dynamic” (kinetic) interaction of the surface tension. In addition, Keene [68] suggested the investigation of the effect of minor elements in affecting γ and ∂γ/∂T as well as the distribution of surface charges due to these elements. These, no doubt, represent some of the the problems that need to be resolved and further investigation of the γ dependance, which can assist in refining the mathematical models, is strongly recommended. These investigations, however, are beyond the scope of this study.

(b) Welding Arc Modelling Efforts

Equally important advances have also been made in modelling the welding arc. Figure 6 [20, 71-81] summarizes some of the important developments in arc modelling. A very recent review of the physics of the welding arc has been given by Lancaster [82,83]. In addition, Westhoff [84] had reviewed some of the numerical and experimental studies of the welding arc in his S.M. thesis. Here, only the general state of the arc modelling efforts will be highlighted.
WELDING ARC MODELLING EFFORTS

Glickstein (1979) [71]
- 1D analytical model with radial variations in temperature and current density

Lowke (1979) [72]
- 1D analytical expression for voltage, electric field, plasma velocity

Glickstein (1979) [73]
- 2D momentum & energy solved
- assuming flow driven by natural convection since low currents used (~ 10A)

Ramakrishnan & Nuon (1980) [74]
- 2D semi-analytical model with an assumed radial velocity profile
- radial isothermal arc column assumed

Lowke (1979) [75]
- 2D model with current and velocity in Gaussian profiles

Hsu, Etemadi, & Pfender (1983) [20]
- MHD equations solved using experimentally determined boundary conditions
- anode and cathode fall regions excluded
- J(cathode) assumed Gaussian shape

Hsu & Pfender (1983) [76]
- detailed modelling of the cathode region

McKelliget & Szekely (1986) [80]
- conservation equations solved using approximate b.c.
- J(cathode) = 65 MA per square meter

Tekriwal & Mazumder (1988) [81]
- analytical model for heat source (pointed tip)
- convection at anode by means of heat transfer coefficient
- gas properties assumed constant

Kovitya & Lowke (1985) [77]
- 2D conservation equations using theoretically calculated plasma properties
- J(cathode) = 100 MA per square meter

Kovitya & Cram (1986) [78]
- MHD equations using assumed boundary conditions
- steady state solutions obtained from transient equations

Goldak, Bibby, Moore et al (1986) [79]
- modelling heat source in GTAW
- finite element method resulting in a double-ellipsoid source

1979-1980
1982-1983
1985-1986
1988-1989

Figure 6 Welding arc modelling.
The arc is generally modelled in 2D, ignoring swirling, due to cylindrical symmetry. In most cases, the arc is assumed to be stable and diffuse. Important information that can be derived from modelling the arc includes heat flux, current flux, velocity profile, temperature profile, arc pressure distribution, arc efficiency, surface gas shear stress, and arc voltage, all of which are pertinent to weld pool modelling.

The basic observation is that the arc behavior is critically dependent upon the boundary conditions at the cathode and much less on the anode [20,76]. The specification of the boundary conditions at the cathode is approximate; but due to the stability of the GTAW relative to other arc welding process (thermionic versus non-thermionic), these approximate boundary conditions seem adequate. Probably, the most critical piece of information is the cathode spot radius or cathode spot current density which cannot be determined to a high degree of accuracy. However, this value is found to be relatively constant over a wide range of operating conditions and is adequate for the modelling efforts [80].

The computed results of temperature profiles show strong agreements with experiments [20,78,80]. In particular, the experimental results of Hsu et al [20] suggest that the electrode integrity (shape) deteriorates even though the arc remains stable; this can complicate the numerical simulation. Nevertheless, the strong and relatively good agreements do provide confidence to the mathematical model; which provide an alternative to experimental studies in addressing the fundamental understanding of the arc welding process.

(c) Simultaneous Arc and Weld Pool Modelling

In virtually all of these studies, the arc has been modelled independent of the pool and vice-versa. In the case of arc modelling, the anode (workpiece) is assumed to be a planar, isothermal surface. This is done to simulate a water-cooled Cu plate such that the arc model can be verified experimentally by measuring the heat flux on the Cu plate [22-24]. On the other hand, with the weld pool, some form of Gaussian heat and current flux distributions were applied as boundary conditions for the flat surface. Although surface deformation were permitted in certain
studies, these do not include the active coupling of the arc nor do they include the effect of the gas shear stress or the non-Gaussian sources. Zacharia et al [57,58,62] assumed a deformable surface due to convective flows in the pool. The effect of the plasma arc is not included. Such assumptions may be valid for low current welding (< 150 A) and that the arc behavior is not affected by surface shape changes. In addition, effect such as the arc length, gas mixtures, and tip angle cannot be modelled by these heat and current Gaussian sources which are usually functions of voltage, current, efficiency, and size of the plasma plume. Paul and DebRoy [60] also considered similar effect in laser welding as those studied by Zacharia et al [57,58,62] using a simple conduction model for the laser plasma plume. Similarly, the free surface is uncoupled from the heat source.

In a study by Choo et al [15], it was found that when the surface was depressed by even a mm, the Gaussian heat flux observed for a flat surface was changed to a bi-modal distribution. This distribution is due to the surface humping. The arc diverges more to the hump due to the shorter arc length. Also indicated in this study is that the resultant bi-modal distribution can generate multiple flow loops in the weld pool since the bi-modal flux will cause the hump to be heated at a different rate than the center of the pool; that is, the weld pool surface will no longer have a single temperature peak. The basic conclusion drawn in this study indicates that even with small fluctuations in the free surface shape, a phenomenon which is not uncommon in low currents welding, the heat and current flux distributions can be non-Gaussian, thus a dynamic coupling of the weld pool and welding arc is strongly recommended.

(d) Summary of Review

The literature review seems to point repeatedly to the importance of a dynamic coupling of the heat and current sources with the workpiece. In fact as early as 1986, Szekely et al [85] recommended the coupling of the arc and weld pool. Although their paper did not actually perform the coupling studies, they reported the consistency of the arc model relative to the weld pool model and vice-versa. There are of course other advances made in the numerical simulation of the weld pool besides the free surface but these can generally be classified as further refinement of the
mathematical model to simulate what are previously established. In fact, much of the published weld pool modelling results from 1983-88 have similar content; describing the importance of convective flows in weld pool for the three principal driving forces with a prescribed heat source over a flat anode.

It is felt that in this dissertation, an initial attempt can be made at coupling the welding arc to the weld pool. This approach is appealing for it allows the entire welding operation to be calculated from first principles since the boundary conditions at the weld pool free surface can be calculated and not prescribed. Secondly, this proposition deviates from the traditional modelling efforts in that by combining the two phenomena, there is a two-way interaction between them. The ultimate goal will be to predict the final shape and structure of the weld pool on the basis of just the input process parameters (such arc length, shielding gas, electrode material and diameter, workpiece material, and arc current).

1.7 Definition and Objective of Investigation

1.7.1 Definition of the Problem

On closer examination of the dynamic coupling between the welding arc and the weld pool, the interface (free surface) between the two domains represents a critical component of the modelling effort. As described above, this interface is not only deformable but also receives the heat source and encompasses the region with the most dominant driving force for the weld pool. The free surface problem can be categorically divided into two parts:

a) calculation of the free surface shape

b) calculation of the free surface temperature

The primary focus of this dissertation will be on the free surface temperature.
a) Free Surface Shape

The numerical simulation of the free surface shape is a relatively complex task and is beyond the scope of this dissertation. Briefly, the problem is due to several factors: i) the lack of an authoritative theory or model that can explain all the surface behavior, ii) the choice of a suitable numerical scheme to tackle the problem, and iii) the availability of a suitable numerical code for the problem.

In the first case, there are currently several models available to explain surface behavior ranging from steady-state deep penetrations [5] to oscillatory behavior in both stationary [16] and moving welds [8] to unstable surface fluctuations [86]. In the second case, there are many numerical schemes available [5,87-91] that can calculate the free surface shape; even though most are still under development and each one has its limitations. A comprehensive review of some of these schemes has been given by Floryan and Rasmussen [92]. Finally, there are currently two commercial codes**, FIDAP [88] and FLOW3D [95], and several public domain codes [89-91,96-100] that can approach, within their limitations, some of these free surface problems. The main conclusion is that although the tools are available, each of them can solve a very specific problem and there is no guarantee that these tools will be general enough to address the entire welding problem. In particular, the main difficulty in virtually all of these codes is the capacity to impose the Marangoni shear at the free surface.

b) Free Surface Temperature

The role of the free surface temperature on the weld pool has often been overlooked in spite of the fact that Marangoni shear has been identified as the most important driving force influencing weld pool shape and penetration. It is important to note that it is the same surface

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* It is not the intent of the author to discuss at length the nature of the free surface shape problems since these are not addressed within the thesis. Nevertheless, some highlights of the problem are useful to describe the scope of this task.

** At the writing of this thesis, PHOENICS v.1.5 [93] and NEKTON [94] are known to possess free surface capabilities on certain later versions of these codes. However, these versions are circulated on a limited basis.
temperature that gives Marangoni flow its driving force. The free surface temperature plays many important roles in the welding operation, such as:

i) The surface temperature controls the value of surface tension [69] and thus the surface tension coefficient, $\gamma/\partial T$. With the presence of surface active elements such as sulphur and oxygen, $\gamma/\partial T$ can change from a positive value to a negative value and the temperature where $\gamma/\partial T = 0$ is important since the flow direction can change [63,64].

ii) It also controls the temperature gradient, $\partial T/\partial r$, which is one of the two parameters responsible for Marangoni shear. It is well known that Marangoni shear is the dominant driving force and principally responsible for the type of weld pool shape that forms [3,4,44,52,63].

iii) It is frequently believed that the vaporization of gaseous species from the free surface is responsible for the surface temperature distribution as well as preventing the surface from reaching the boiling point of the workpiece [101,102]. This is due in part to the temperature dependance of the partial pressure of the gaseous species. Furthermore, this temperature distribution is governed in part by the heat flux distribution of the welding arc although the welding arc behavior is not so sensitive to the temperature of the weld pool [103].

iv) Finally, and perhaps most important, the surface temperature governs the net heat input into the workpiece. This is determined by an energy balance between the heat falling from the welding arc, the heat loss by vaporization, and the heat transferred into the workpiece by convective flows.

It seems clear that the type of pool that can be obtained is almost exclusively dependant upon the prediction of the surface temperature. Furthermore, the problem is inherently strongly coupled in that the temperature fields are required to calculate the strength of the Marangoni convective flows, and the convective flows in turn govern in part the surface temperature by determining the rate of heat transfer away from the free surface. Thus, the accurate representation of both velocity and thermal fields are important in the welding operation.
1.7.2 Objective of Investigation

In view of the overall goal of developing a fundamental understanding of the heat transfer and fluid flow phenomena in the welding arc and weld pool, this investigation will focus on the prediction of the free surface temperature for a two-dimensional (2D) spot weld with a planar surface, that is for low arc currents (< 200 A), on the basis of the input conditions calculated from the welding arc. This should provide the necessary groundwork for the fully three-dimensional moving weld with an asymmetrical pool shape. More specifically, the objectives are:

i) to establish a thermodynamic and kinetic model for predicting the vaporization rates and thus rate of heat loss from the weld pool free surface.

ii) to investigate the role of the various driving forces (buoyancy, electromagnetic, surface tension, and gas shear stress) in affecting weld pool surface temperature.

iii) to investigate the role of the arc (arc distribution, arc length, power levels) in affecting surface temperature.

iv) to compare the calculated results of the weld pool with experimental results.

By predicting the surface temperature, the shape of the pool will automatically follow since convection, which controls the pool shape, is governed by the most dominant driving force.

Figure 7 shows the sectional view of a typical water-cooled welding torch for manual GTAW [104]. The mathematical model, which is described in further details in chapters 2 and 3, will attempt to simulate the physical processes occurring in the vicinity of the electrode tip and the workpiece.

Chapters 2 and 3, which are common to subsequent chapters, will focus on the model development for the welding arc and the weld pool, respectively. Chapter 4 will describe the vaporization model and investigate the various effect of the driving forces on the surface temperature. Chapter 5 will compare the calculated results with experimental results.
Figure 7 Sectional views of a typical water-cooled welding torch for manual GTAW [104].
2. WELDING ARC MODELLING

This chapter highlights the development of the arc model, describes the refinements to it, and presents the implications of the calculated results to the weld pool model.

2.1 Introduction and Background Information

The coupling between the weld pool and the welding arc involves modelling the arc directly. The motivation for modelling the arc stems from the objective of providing boundary conditions for the weld pool through fundamental transport equations. Virtually all previous modelling studies [3,4,44,56-58,62-65] of the workpiece use either a Gaussian-type heat and current flux distributions such as:

\[
q_a = \frac{3\pi \nu I V}{\pi a^2} \exp \left[ -\frac{3r^2}{a^2} \right] \quad (1)
\]

\[
J_a = \frac{3I}{\pi b^2} \exp \left[ -\frac{3r^2}{b^2} \right] \quad (2)
\]

or experimentally determined boundary conditions [23]. It is well known that measuring the heat and current fluxes is not a trivial matter and measurements taken from a copper steel plate may not reflect those of steel since vaporization is not present. In addition, the measurements can be complicated if the free surface deforms. Equations (1) and (2) or similar forms of them have been used by many investigators [44,47,50-53,56-59,61-65] since it is assumed that the heat and current sources approximate a Gaussian function. Some of the pitfalls associated with this assumption include the estimation of input process parameter such as the arc efficiency and the selection of the empirical constants a and b. Besides, the deployment of these two equations automatically meant that a two-way coupling between the arc and weld pool will not be possible; the heat source is assumed unchanged and the free surface is assumed flat.

The more important implication is that changes in the weld pool behavior (particularly the free surface) will not be reflected in the arc and vice-versa. In order to avoid such empirical formulations of the heat source and to provide a mathematical model that would reflect the weld pool behavior more realistically, a more fundamental approach would be to model the arc directly.
using fundamental transport equations. Such analyses involved the simultaneous solution of the equations of continuity, momentum, energy, and Maxwell's electromagnetic equation. The end results will not only provide primary information such as heat and current distributions to the weld pool but also secondary information such as mass transfer rates, surface gas shear, and arc efficiency. The latter information are used to determine vaporization rates, free surface stability, and provide consistency checks, respectively, for the weld pool.

2.2 The Gas Tungsten Arc

Figure 8 shows a schematic representation of a gas tungsten arc. The detailed description of the arc model can be found in McKelliget and Szekely [80] and Westhoff's S.M. Thesis [84]. Here, only the essential features will be highlighted. For completeness, the governing equations and mathematical formulations are given in Appendix A. Several refinements have been made to the model to enable it to couple to the weld pool. These refinements as well as a discussion of some of the boundary conditions will be described in the following section.

The welding arc used in GTAW process at atmospheric pressure is a high current, low voltage discharge operating in the range of 10–2,000 A and 10–50 V [105]. In general, the arc constitutes a mechanism by which electrons are emitted from the cathode, transferred to the anode, and condensed there. These electrons are the predominant sources of heat and current to the workpiece. Structurally, the welding arc column can be divided into 5 parts (Fig. 8) [105]:

i) cathode spot - the part of the negative electrode from which electrons are emitted.

ii) cathode fall region - the gaseous region immediately adjacent to the cathode in which a sharp drop of potential drop occurs. This region can be divided into three zones: contraction, high luminosity, and space charge [106].

iii) arc column - the bright, visible portion of the arc, characterized by high temperature and low potential gradient. The column consists of plasma, a highly ionized gas which is electrically conductive. The divergent arc results in a JxB force that drives the flow. Joule heating, Thompson effect, and radiation losses are dominant in this region.

iv) anode fall region - the gaseous region immediately adjacent to the anode in which a further sharp drop of potential takes place. There are two zones: contraction and space charge [107].
Figure 8 Arc appearance and structure.
The thickness of the anode fall and cathode fall regions have been greatly exaggerated to show details. The various phenomena occurring in the arc column are shown schematically.
v) anode spot – the portion of the positive electrode within which the electrons are absorbed.

The following assumptions are employed in describing these 5 regions:

i) The arc is assumed to be axially symmetric.

ii) The operation of the arc is assumed to be in steady-state.

iii) The arc is assumed to be in local thermodynamic equilibrium (LTE), in that the electron and heavy particle temperatures are not significantly different. The studies by Hsu et al [20,108] show this assumption is accurate through most of the arc except in the fringes and very near the cathode and anode surfaces.

iv) The plasma arc is assumed to be pure argon at atmospheric pressure. The effect of other gases which may be entrained are neglected as are metal vapors from the electrode and workpiece.

v) The flow is assumed to be laminar. This assumption was justified by McKelliget and Szekely [80] on the basis of laminar-turbulent transition for a free jet.

vi) The plasma is assumed to be optically thin so that radiation may be accounted for using an optically thin radiation loss per unit volume.

vii) The heating effect of viscous dissipation and buoyancy forces due to gravity are neglected.

The mathematical model will simulate the cathode fall, the arc column, and the anode regions whose domains are divided according to the potential distribution shown in Fig. 8. The cathode spot and anode spot will act as boundary conditions. The physical processes occurring in these regions are cast into mathematical equations (App. A) and the solution of these simultaneous partial differential equations will provide a detailed description of the welding arc.

2.3 Boundary Conditions and Refinements of the Arc Model

Special considerations are given to the anode and cathode regions because these regions are not in LTE. Approximate boundary conditions are employed to describe these regions (Appendix A). It is perhaps interesting to note that the earlier studies by Hsu et al [20] and Kovitya and Cram [78] did not include these regions in their analyses. While the computed temperature plots of McKelliget and Szekely [80], with the anode fall and cathode fall regions included, showed some variations in the temperature profile in the arc when compared with Hsu et al’s model [20], the
trends are similar. Both models tend to overpredict the size of the temperature fields but McKelliget and Szekely's model [80] shows a slightly worse agreement with experimental results. The principal factor that will be affected when including both of these boundary layers is the arc efficiency which were not reported in all previous models. The arc efficiency, which is calculated theoretically from the net heat flux onto the anode and the sum of the potential drop in the cathode fall, anode fall, and arc column, is an important criterion in these models for it allows for consistency checks on the models with experimental results.

The cathode was assumed flat even though most welding operations were done with a pointed tip. It is also well known that depending upon the operating conditions, the pointed tip of the electrode changes shape with the onset of welding [109]. This model employs an effective cathode spot radius to model the hot spot. This radius is calculated from an experimentally determined cathode spot current density found in the literature [80,110]

Probably the major obstacle in this modelling study is the proper selection of the cathode boundary condition for the current. All previous models [20,78,80] had indicated difficulties in specifying the cathode spot radius and various modifications and assumptions were employed. This model employs a constant cathode spot current density which is quite realistic for thermionic cathodes. The current density generally has a range of $10^7 - 10^8$ A/m² and the arc is characteristically static and stable [111]. Table 1 shows the measured cathode spot current density [110]. The basic observation is that the current density decreases as the arc current increases. However, this variation is not large; 5.5x10⁷ A/m² at 150 A to 2.3x10⁷ A/m² at 800 A for tungsten electrode and 3.8x10⁷ A/m² at 300 A to 2.5x10⁷ A/m² at 700 A for thoriated-tungsten electrode. Incidentally, a rather large electrode is used (12.5 mm diameter) which may account for the lower current density as compared to the one employed in this study which is about 2.9–3.2 mm diameter. It would be highly desirable to be able to predict the cathode spot radius. This is not performed in this work. It is recommended that one way to obtain an estimate of the cathode spot radius is to model the heat transfer in the electrode itself.
<table>
<thead>
<tr>
<th>Cathode Material</th>
<th>Arc Current (Ampere)</th>
<th>Pressure (kPa)</th>
<th>Mean Current Density (A/m²)</th>
<th>Cathode Spot Temperature (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tungsten</td>
<td>150</td>
<td>80</td>
<td>$5.5 \times 10^7$</td>
<td>*</td>
</tr>
<tr>
<td>Tungsten</td>
<td>200</td>
<td>80</td>
<td>$3.8 \times 10^7$</td>
<td>*</td>
</tr>
<tr>
<td>Tungsten</td>
<td>300</td>
<td>80</td>
<td>$2.1 \times 10^7$</td>
<td>*</td>
</tr>
<tr>
<td>Tungsten</td>
<td>800</td>
<td>80</td>
<td>$2.3 \times 10^7$</td>
<td>*</td>
</tr>
<tr>
<td>Tungsten</td>
<td>500</td>
<td>13</td>
<td>$1.6 \times 10^7$</td>
<td>*</td>
</tr>
<tr>
<td>Tungsten</td>
<td>500</td>
<td>40</td>
<td>$2.7 \times 10^7$</td>
<td>*</td>
</tr>
<tr>
<td>Tungsten</td>
<td>500</td>
<td>80</td>
<td>$2.7 \times 10^7$</td>
<td>*</td>
</tr>
<tr>
<td>Thoriated-Tungsten</td>
<td>300</td>
<td>93</td>
<td>$3.8 \times 10^7$</td>
<td>*</td>
</tr>
<tr>
<td>Thoriated-Tungsten</td>
<td>500</td>
<td>93</td>
<td>$3.7 \times 10^7$</td>
<td>2,803</td>
</tr>
<tr>
<td>Thoriated-Tungsten</td>
<td>700</td>
<td>93</td>
<td>$2.5 \times 10^7$</td>
<td>2,973</td>
</tr>
</tbody>
</table>

Table 1. Experimental cathode spot current density in argon shielding gas [110].
* no value reported.

The model does not take into account of vaporization from the anode. The primary concern is the effect of the vapor species on the physical properties of the plasma. In the original study [80], the anode is assumed to be at 1,000 K (water-cooled) and so no vaporization occurs. However, in the welding of stainless steel, vaporization controls in part the surface temperature. Dunn et al [112,113] indicated that the transport properties (electrical and thermal conductivities) changes
substantially due to vapor species such as Al, Fe, and Ca. This observation was derived on the basis of theoretical calculations of binary and ternary mixtures of Fe, Ar, and Ca or Al.

The cathode was determined as a more important source of minor elements to the arc column than the anode. Vaporization of high vapor species (Mn,Fe,Cr) from the anode were not that critical in affecting arc properties since these metal vapors were mainly found to be localized at the anode surface at high currents (125 A) but were also detected near the cathode at low currents (20 A). The absence of vapor species in the high current operation may be explained by the fact that the plasma jet is travelling in excess of 100 m/s and will sweep the vapor species away from the anode such that the arc column is unaffected. The effect of these vapor species on the thin anode boundary layer is unknown. This region might not be a critical factor in influencing arc behavior; an observation confirmed by Hsu et al [20] who indicated that the boundary conditions at the anode were not very important in modifying arc behavior such as peak temperature, maximum axial velocity, column voltage, axial maximum current density, mass flow rate, and anode over-pressure. Hsu et al’s [20] findings indicated that the arc behavior was controlled primarily by the current (assuming tip angle, gas composition, and arc length are constant) which controls the boundary condition at the cathode. Thus, neglecting vaporization effect from the anode in the arc model may not pose a serious problem to the modelling effort.

As mentioned above, one of Dunn and Eagar’s [113] conclusions is that the effect of vaporization of minor elements such as Ca, Al, and Th from the tungsten electrode can have significant changes on the electrical and thermal conductivities in the upper regions of the arc column. The contamination of the shielding gas may affect the heat transfer to the anode. The significance of this contamination on thermal transport has yet to be investigated. This represents a limitation of this study rather than a limitation of the model. It is strongly recommended that the next study includes the effect of contamination on plasma properties. Nevertheless, useful insights can still be gained with the current model.

The anode temperature is assumed to be 1,000 K. It is felt that, in this instance, this assumption does not affect the arc substantially for the following reasons:
i) The arc temperature varies from 15,000 K at the center of the pool to 10,000 K at the edge of the pool; thus the film temperature changes only slightly.

ii) The pool temperature varies from 1,700 K to 2,800 K which is small relative to the arc temperature.

iii) The two main factors that are affected in the arc are the convective heat flux to the anode surface and the thermal and electrical conductivities near the vicinity of the anode. The convective contribution to the total heat flux is between 10-20% while the variation in electrical and thermal conductivities for the 1,000 K temperature difference is small relative to that of the arc temperature.

iv) As described above, studies have shown that the boundary conditions at the anode are not as sensitive as the cathode in determining arc behavior [20,107].

Westhoff’s [84] principal conclusion was that the heat and current flux distributions will be substantially modified when humping of the weld pool occurs. The humps were experimentally observed at arc currents above 250 A [8]. It was noted in Westhoff’s thesis [84] that the volume of the depression does not match the volume generated by the humps (sometimes by a factor of 3) thus not accounting for mass balance. Although the nature of the results does not change, the absolute value of the heat and current inputs may differ. In addition, if modelling of the pool collapse after the arc extinction is required, then this correction must be made and has been done in this study.

The refinements to the arc model are minor and should not pose serious problems to the model. These modifications have been incorporated into the current set of results with steel workpiece.

2.4 Results and Discussion

All the results presented in this chapter have flat tungsten cathode (2.9–3.2 mm diameter), argon gas shielding, and a copper electrode (ΦCu = 4.3 V) at 1,000 K. Incidentally, the work function for iron is 4.5 V. The computed results were first compared with experimental results to establish the confidence of the arc model and for consistency check. Figure 9 [84] shows both the computed and experimental temperature profiles of a 200 A arc (10 mm arc length). The computed results are in good agreement with the experiments. In addition, Figs. 10 (a) and (b) show the calculated anode heat and current fluxes as compared with experiments at 200 A (6.3 mm arc length). It should be
Figure 9 Comparison between experimental results and calculated values of the temperature profile in the welding arc [83]. The experimental results (200 A at 10 mm arc length) are from Hsu et al [20].
Figure 10 Comparison between experimental results and calculated values of the anode heat and current flux distributions [83]. The experimental results are from Nestor [24].
evident that there is good agreement between the numerical results and experimental data. Also, notice that there are three contributions to the anode heat flux. They are electronic, convective and radiative contributions. These two figures provide confidence to the arc model and we can now proceed to investigate other welding conditions.

Figures 11 (a) and (b) show the heat and current fluxes, respectively, when the anode surface is assumed to be 1,000 K and 2,000 K. It can be seen that the power distributions for the two different anode boundary conditions essentially overlap; indicating that the welding arc behavior is not very sensitive to the workpiece surface temperature. This observation confirms the reasonings given above (Section 2.3 : p. 51). The purpose of this exercise is that in the actual coupling, it is not necessary to alternate the numerical calculations between the welding arc and the weld pool when the weld pool surface temperature changes. By initially calculating for the arc characteristics and assuming steady-state conditions thereon, the transient behavior of the weld pool can proceed without interruption; thus saving tremendous computational time.

It is not the objective of this chapter to investigate the relative variations in the calculated arc parameters (such as maximum velocity, current density, peak temperature) with arc currents or arc lengths. This has been investigated elsewhere [20,84]. The primary concern is to explore the implications of the arc behavior relative to the weld pool and to identify key processes in the arc that will strongly affect weld pool behavior.

2.4.1 Cases Tested

A total of 11 cases was considered and they are listed in Table 2. Case A shows the effect of arc behavior with increasing current at constant arc length. Case B shows the effect of arc behavior with increasing arc length at constant arc current. Case C shows the effect of increasing surface depression with constant initial electrode to surface distance; that is, the effect at high arc currents (> 250 A).
Figure 11. Plot of (a) heat and (b) current flux distributions as a function of radial position with anode at 1,000 K and 2,000 K.

The two anode boundary conditions (1,000 K and 2,000 K) basically result in a heat and current flux distributions (star and symbol) that superimpose on one another.
<table>
<thead>
<tr>
<th></th>
<th>(A) 6.3 mm arc length</th>
<th>(B) 200 A arc</th>
<th>(C) 6.3 mm arc length</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>100 A</td>
<td>3.2 mm arc length</td>
<td>200 A (1.0 mm depression)</td>
</tr>
<tr>
<td>II</td>
<td>200 A</td>
<td>6.3 mm arc length</td>
<td>260 A (1.2 mm depression)</td>
</tr>
<tr>
<td>III</td>
<td>300 A</td>
<td>10.0 mm arc length</td>
<td>280 A (1.8 mm depression)</td>
</tr>
<tr>
<td>IV</td>
<td>–</td>
<td>12.2 mm arc length</td>
<td>300 A (4 mm depression)</td>
</tr>
</tbody>
</table>

Table 2. List of welding arc conditions examined. They are divided into three cases (A-C).

In the C cases, the 6.3 mm arc length represents the distance from the electrode to the flat surface prior to arc initiation. The pool shape had been assigned on the basis of the experimental results of Lin and Eagar [8]. The 1.0 mm case was extrapolated from the experimental results. Tables 4, 5, and 6 list the arc parameters obtained with respect to cases A, B, and C, respectively. The results are represented graphically in Figs. 12-16 for case A, Figs. 17-21 for case B, and Figs. 22-26 for case C. This is summarized below for easy reference (Table 3).

<table>
<thead>
<tr>
<th>Type of plot</th>
<th>Case A</th>
<th>Case B</th>
<th>Case C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Velocity</td>
<td>12</td>
<td>17</td>
<td>22</td>
</tr>
<tr>
<td>Temperature</td>
<td>13</td>
<td>18</td>
<td>23</td>
</tr>
<tr>
<td>Current Density</td>
<td>14</td>
<td>19</td>
<td>24</td>
</tr>
<tr>
<td>Lorentz Force</td>
<td>15</td>
<td>20</td>
<td>25</td>
</tr>
<tr>
<td>Anode Heat Flux, Current Flux, Gas Shear Stress, and Over-Pressure</td>
<td>16</td>
<td>21</td>
<td>26</td>
</tr>
</tbody>
</table>

Table 3. List of figures for the welding arc cases studied.
2.4.2.A Constant Arc Length With Increasing Arc Current (Case A)

Increasing current with a constant arc length has the effect of increasing the axial velocity and size of the plasma plume (Figs. 12 and 13). Table 4 indicates that most of the arc parameters increase as current increases, except for arc efficiency. The decreasing arc efficiency is caused by the higher plasma arc velocity resulting in more heat being convected away by the gas than being deposited on the anode.

Figures 14 and 15 show the current density and JxB plots, respectively. The current density essentially remain unchanged. The JxB plot is directly related to the current density plot. Note that the maximum Lorentz force occurs near the cathode since this is the region where the current path is most divergent and the pinch force strongest. However, from Fig. 12, the maximum velocity occurs a short distance from the cathode indicating that some displacement is required for the gas to accelerate to maximum velocity.

Figures 16 (a-d) show the computed heat flux, current flux, anode over-pressure, and gas shear stress, respectively. The trend shows increasing heat flux with increasing current. There is little need for discussing Fig. 16 in detail but this figure is important since it supplies the boundary conditions for the weld pool.

2.4.2.B Constant Current With Increasing Arc Length (Case B)

The velocity (Fig. 17), current density (Fig. 19), and body force (Fig. 20) remain relatively constant with increasing arc length. This is due to the constant current applied. However, the arc length has the most pronounced effect on the size of the plasma plume (Fig. 18) and the heat and current fluxes (Figs. 21 (a-b)). It can be seen that with a 200 A arc, the peak values change drastically with short arc lengths. Thus, previous Gaussian heat and current fluxes employed by other researchers which specified the source term as a function of \( \eta \), \( I \), \( V \), and effective cathode spot radius appeared to be rather empirical in that the effect of arc length was not included. In particular, the effective anode radius \( a \) and \( b \) can be modified to fit the peak value but the shape of the heat distribution may not be truly Gaussian. Lu and Kou [23] did report deviations from the
Figure 12  Velocity profile in the welding arc at 6.3 mm arc length for 100-300 A. The maximum velocity vector (m/s) is indicated by the arrow at right of figure.
Figure 13  Temperature contours in the welding arc at 6.3 mm arc length for 100-300 A.
Figure 14 Current density in the welding arc at 6.3 mm arc length for 100-300 A. The maximum current density vector (A/m²) is indicated by the arrow at right of figure.
Figure 15  Body force in the welding arc at 6.3 mm arc length for 100-300 A. The maximum body force vector (N/m²) is indicated by the arrow at right of figure.
Figure 16 Plot of (a) heat flux and (b) current flux distributions as a function of radial position at the anode at 6.3 mm arc length (100-300 A).
Figure 16 Plot of (c) arc pressure and (d) gas shear stress distribution as a function of radial position at the anode at 6.3 mm arc length (100-300 A).
Figure 17  Velocity profile in the welding arc at various arc lengths for a 200 A arc. The maximum velocity vector (m/s) is indicated by the arrow at right of figure.
Figure 18 Temperature contours in the welding arc at various arc lengths for a 200 A arc.
Figure 19 Current density in the welding arc at various arc lengths for a 200 A arc. The maximum current density vector (A/m²) is indicated by the arrow at right of figure.
Figure 20 Body force in the welding arc at various arc lengths for a 200 A arc. The maximum body force vector (N/m²) is indicated by the arrow at right of figure.
Figure 21. Plot of (a) heat flux and (b) current flux distributions as a function of radial position at the anode at various arc lengths (3.2-12.2 mm) for a 200 A arc.
Figure 21 Plot of (c) arc pressure and (d) gas shear stress distribution as a function of radial position at the anode at various arc lengths (3.2 - 12.2 mm) for a 200 A arc.
<table>
<thead>
<tr>
<th></th>
<th>100 A</th>
<th>200 A</th>
<th>300 A</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q_{a,\text{max}} (W/mm²)</td>
<td>21.3</td>
<td>63.1</td>
<td>105.1</td>
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<tr>
<td>J_{a,\text{max}} (A/mm²)</td>
<td>2.5</td>
<td>5.4</td>
<td>8.0</td>
</tr>
<tr>
<td>u_{\text{max}} (m/s)</td>
<td>151.5</td>
<td>277.5</td>
<td>391.4</td>
</tr>
<tr>
<td>T_{\text{max}} (K)</td>
<td>19,470</td>
<td>22,680</td>
<td>24,100</td>
</tr>
<tr>
<td>P_{a,\text{m, x}} (Pa)</td>
<td>104.9</td>
<td>518.7</td>
<td>1048.1</td>
</tr>
<tr>
<td>V_{\text{arc}} (V)</td>
<td>11.9</td>
<td>14.8</td>
<td>16.2</td>
</tr>
<tr>
<td>η (%)</td>
<td>68.5</td>
<td>64.0</td>
<td>63.9</td>
</tr>
<tr>
<td>R_{\text{c}} (mm)</td>
<td>0.7</td>
<td>1.0</td>
<td>1.22</td>
</tr>
<tr>
<td>Electrode radius (mm)</td>
<td>1.525</td>
<td>1.525</td>
<td>1.525</td>
</tr>
</tbody>
</table>

Table 4. Calculated arc parameters at various currents with J_{c} = 6.5 \times 10^7 A/m²

Gaussian distribution for both heat and current fluxes when compared with experimental results. In contrast, the weld pool boundary conditions in this study are predicted from fundamental conservation equations without the need for unnecessary empirical formulation.

On the practical level, in GTAW, the arc length is generally quite short (~ 1-3 mm). From Figs. 21 (a-b), we can see that as the arc length decreases, the distributions get slender and sharper. In particular, at very short arc lengths, the peak values are extremely sensitive. In an actual GTAW, the free surface is known to oscillate [16] even at low arc currents (100 A). Thus, the heat source to the weld pool can be a strong function of the arc length. Such modifications in heat source
will not be reflected in the empirical formulas given in eqns. (1-2). It indicates the necessity and importance of modelling the arc directly.

Another observation that is deduced from Figs. 21 (a-b) is that the heat and current distributions vary substantially at shorter arc length than longer ones. This observation reflects the sensitivity of the process and care must be exercised in the experimental work where the arc length distance can be determined to be no less than ± 0.1 mm accuracy. Thus, it may not be surprising that the weld pool penetration be different in two heats with the same arc current and duration of heating. The culprit could be that the arc length may have changed in the subsequent heats leading to a completely different heat distribution and content.

As expected, when the arc length increases, the voltage also increases in order to support the longer arc (Table 5). It also interesting to note that the arc efficiency decreases with a longer arc. This is because with a larger arc column, more heat is being loss to the environment by radiation and convection. The shorter arc length has a more constricted arc (Fig. 18) and the heat is transferred more effectively to the anode. Long arc lengths are generally not employed in welding for several reasons. Firstly, a higher current and voltage must be used to sustain the arc. Secondly, the arc efficiency is lowered due to heat loss to the environment.

Tsai and Eagar [22] did extensive work in measuring the heat and current fluxes for GTAW. They were able to correlate their data for arc lengths, currents, tip angles, and different shielding gas mixtures by means of a heat and a current distribution function. Their model relied on the premise that the heat and current sources are Gaussian in nature. However, studies by Lu and Kou [23] indicated that although the sources have the same trends as the Gaussian function, they are not strictly Gaussian. They were unable to conclude as to under what condition a Gaussian distribution holds except that they reported that these deviations from the Gaussian shape can be significant. This observation reflects the limitation of the Gaussian model and the advantage of calculating the arc behavior fundamentally.
<table>
<thead>
<tr>
<th>Arc Length</th>
<th>3.2 mm</th>
<th>6.3 mm</th>
<th>10.0 mm</th>
<th>12.2 mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q_{a,\text{max}}$ (W/mm²)</td>
<td>123.2</td>
<td>63.1</td>
<td>38.3</td>
<td>29.9</td>
</tr>
<tr>
<td>$J_{a,\text{max}}$ (A/mm²)</td>
<td>11.7</td>
<td>5.4</td>
<td>3.3</td>
<td>2.6</td>
</tr>
<tr>
<td>$u_{\text{max}}$ (m/s)</td>
<td>274</td>
<td>278</td>
<td>274</td>
<td>285</td>
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<tr>
<td>$T_{\text{max}}$ (K)</td>
<td>22,500</td>
<td>22,680</td>
<td>22,590</td>
<td>22,300</td>
</tr>
<tr>
<td>$P_{a,\text{max}}$ (Pa)</td>
<td>656</td>
<td>519</td>
<td>435</td>
<td>369</td>
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<tr>
<td>$V_{\text{arc}}$ (V)</td>
<td>11.9</td>
<td>14.8</td>
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</tr>
<tr>
<td>$\eta$ (%)</td>
<td>76</td>
<td>64</td>
<td>59</td>
<td>58</td>
</tr>
<tr>
<td>Electrode radius (mm)</td>
<td>1.6</td>
<td>1.5</td>
<td>1.5</td>
<td>1.45</td>
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</tbody>
</table>

Table 5. Calculated arc parameters at various arc lengths with 200 A arc and $J_{c} = 6.5 \times 10^{7}$ A/m².
2.4.2.C High Current Arcs With Surface Depression (Case C)

The effect of surface depression on arc behavior is shown in Figs. 22-25. The maximum velocity increases in respond to the applied current (Fig. 22) while the plasma plume shape is basically the same (Fig. 23). The corresponding current and body force plots (Figs. 24-25) are shown for completeness. The maximum current density reported in Fig. 24 represents the magnitude at one grid below the electrode. This difference with respect to the cathode spot current density of $6.5 \times 10^7$ A/m$^2$ is due to the summation of the axial and radial components. In addition, the body force does not reflect the same trend as the current density (with increasing surface depression) because the individual component of $J_x$ and $J_z$, which contribute to the effective body force are strongly dependant upon the current path as given by the weld pool surface shape. Clearly, a simple relationship of the effect of current density on body force is not that obvious. This observation indicates the complex interactive forces occurring within the welding arc.

The most visible change is seen in the heat and current flux distributions (Figs. 26 (a-b)). The single peak distribution commonly seen in Figs. 16 (a-b) and Figs. 21 (a-b) has now assumed a bi-modal off-center peak. The peak heat and current fluxes are substantially less than the flat weld pools (Table 6 versus Table 4). Here, the relative ratio of the maximum to the minimum is more critical since it defines the extent of the heat flow to the specific regions of the weld pool. This ratio is given in Table 7.

As the depression increases, this ratio can be quite significant. The current ratio shows a rather large divergence due to the nature of the current path. As the depression increases, the arc length from the electrode to the hump is much shorter than that to the bottom of the depression; thus, the bulk of the electrons travel to the hump. The heat ratio does not show as large a divergence with increasing current as there are other contributions to the heat source. The convective contribution increases corresponding to the increase in current due to the higher plasma velocities. Nevertheless, this heat ratio is important for it dictates the surface temperature and thus the flow field in the weld pool as governed by the surface tension driven flows.
Figure 22  Velocity profile at various surface depressions with arc lengths at 6.3 mm. The maximum velocity vector (m/s) is shown at right of figure.
Symbols
1 = 10,000 K
2 = 12,000 K
3 = 14,000 K
4 = 16,000 K
5 = 18,000 K
6 = 20,000 K
7 = 22,000 K

Figure 23 Temperature contours at various surface depression with arc length at 6.3 mm.
Figure 24 Current density at various surface depressions with arc length at 6.3 mm. The maximum current density vector (A/m²) is shown at right of figure.
Figure 25 Body force at various surface depressions with arc length at 6.3 mm. The maximum body force vector (N/m²) is shown at right of figure.
Figure 26 Plot of (a) heat flux and (b) current flux distributions as a function of radial position at the anode at 6.3 mm arc length with various surface depressions (1.0-4.0 mm).
Figure 26 Plot of (c) arc pressure distribution as a function of radial position at the anode at 6.3 mm arc length with various surface depressions (1.0-4.0 mm).
<table>
<thead>
<tr>
<th>Arc Current (Pool Depression)</th>
<th>$Q_{a,\text{max}}$ (W/mm²)</th>
<th>$J_{a,\text{max}}$ (A/mm²)</th>
<th>$V_{\text{max}}$ (m/s)</th>
<th>$T_{\text{max}}$ (K)</th>
<th>$P_{a,\text{max}}$ (Pa)</th>
<th>$V_{\text{arc}}$ (V)</th>
<th>$\eta$ (%)</th>
<th>$R_c$ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>200 A (1.0 mm)</td>
<td>32.9</td>
<td>3.67</td>
<td>282</td>
<td>22,250</td>
<td>827</td>
<td>14.2</td>
<td>66.9</td>
<td>1.0</td>
</tr>
<tr>
<td>300 A (4.0 mm)</td>
<td>28.3</td>
<td>3.34</td>
<td>390</td>
<td>23,900</td>
<td>1,156</td>
<td>15.2</td>
<td>66.4</td>
<td>1.13</td>
</tr>
<tr>
<td>260 A (1.8 mm)</td>
<td>36.9</td>
<td>3.96</td>
<td>373</td>
<td>23,590</td>
<td>1,069</td>
<td>15.9</td>
<td>65.9</td>
<td>1.22</td>
</tr>
</tbody>
</table>

Electrode radius is 1.35 mm.

Table 6. Arc parameters at various pool depressions with 6.3 mm arc length and $I_e = 6.5 \times 10^7$ A/m².
<table>
<thead>
<tr>
<th>Current (A)</th>
<th>Anode Heat (Q_{a,\text{max}}/Q_{a,\text{min}})</th>
<th>Anode Current (I_{a,\text{max}}/I_{a,\text{min}})</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>1.6</td>
<td>2.6</td>
</tr>
<tr>
<td>260</td>
<td>1.6</td>
<td>3.1</td>
</tr>
<tr>
<td>280</td>
<td>1.6</td>
<td>3.5</td>
</tr>
<tr>
<td>300</td>
<td>2.4</td>
<td>10.3</td>
</tr>
</tbody>
</table>

Table 7. Ratio of the maximum to the minimum heat and current fluxes at the anode for various currents.

The maximum arc temperature also increase with increasing current but not very significantly (Table 6). The arc efficiency remains quite stable between 64.5-66.9%.

The primary observation of case C is that the free surface shape controls the nature of the heat and current distributions. Sorenson and Eagar [16] reported oscillatory surface fluctuations of the order of 50-60 Hz for spot welds. This translates to about 0.02 second period. The question lies in the sensitivity of the weld pool to such periodic surface fluctuations, and thus heat source fluctuations. The more important question is how will these fluctuations affect weld pool circulation and melting.

If the fluctuations are not important, then on average, one may employ a time-averaged heat and current source. If the fluctuations are important, that is, weld pool circulation and melting characteristics are affected, then the heat and current fluxes must be modified to reflect such changes. This can result in a rather complicated problem in that not only multiple flow loops result but oscillatory flows are possible too.

These analyses indicate the complexity of the flow phenomena in the weld pool. It indicates the importance of modelling the arc and the influence of the weld pool surface on the arc behavior.
2.4.3 Comparison of the Calculated Arc Parameters

The calculated arc parameters in Tables 4 and 5 can be compared with those of Hsu et al. [20] (Table 8). For the case of constant arc length, all the arc parameters (except arc efficiency) increase with increasing current. This observation is similar to that observed by Hsu et al. [20] although they did not report the arc efficiencies. In the case of constant current and increasing arc length, the changes in arc parameters are less obvious. They claimed that as the arc length increases, peak current density, anode over-pressure, temperature, and velocity all decrease while the arc voltage increases. The decrease in peak current density and anode over-pressure were obvious but those for temperature and velocity were not significant; a 100% increase in arc length produced a maximum change of only 2.8% at most in peak temperature and velocity. Hsu et al. [20] reported these less obvious changes as due to the complex fluid dynamics interactions in the cathode region but did not elaborate on them any further.

Direct comparison can be made between the values reported by Hsu et al. [20] (Table 8) and those found in this study (Table 5). For the 200 A - 10 mm arc, the maximum deviation in reported values is about 9.4%. This is reasonable in light of the fact that both calculated results are only in general agreement with experimental results. In addition, Hsu et al. [20] did not take into account of the anode and cathode fall regions, thus the 9.4% deviation seems acceptable as computational accuracy in model description. The general agreement between our computational results with experimental results and other numerical results reported in the literature provide confidence to our calculations.

2.5 Summary of Results

We now have the capability of providing the boundary conditions for the weld pool on the basis of the solution of the conservation equations for the arc. The following observations are noted:

1. For a constant arc length, all the arc parameters except the arc efficiency increase on increasing current.
<table>
<thead>
<tr>
<th>Conditions (arc length)</th>
<th>Max Temp (K)</th>
<th>Max Vel (m/s)</th>
<th>Max J atode (A/mm²)</th>
<th>Max Anode (Pa)</th>
<th>Arc Voltage (V)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100A (10 mm)</td>
<td>18,200</td>
<td>173</td>
<td>1.96</td>
<td>71.9</td>
<td>11.2</td>
</tr>
<tr>
<td>100A (20 mm)</td>
<td>18,400</td>
<td>171</td>
<td>0.973</td>
<td>38.1</td>
<td>14.1</td>
</tr>
<tr>
<td>200A (10 mm)</td>
<td>21,200</td>
<td>294</td>
<td>3.10</td>
<td>394</td>
<td>13.3</td>
</tr>
<tr>
<td>200A (20 mm)</td>
<td>20,600</td>
<td>290</td>
<td>1.73</td>
<td>188</td>
<td>17.7</td>
</tr>
<tr>
<td>300A (10 mm)</td>
<td>23,100</td>
<td>395</td>
<td>4.71</td>
<td>869</td>
<td>15.2</td>
</tr>
<tr>
<td>300A (20 mm)</td>
<td>22,500</td>
<td>388</td>
<td>2.38</td>
<td>475</td>
<td>19.8</td>
</tr>
</tbody>
</table>

Table 8. Arc parameters obtained from Hsu et al [20].
2. The arc behavior changes more dramatically at shorter arcs than longer arcs; thus indicating its sensitivity in this regime of operation. Empirical Gaussian formulations of the heat and current sources are unable to incorporate the effect of the arc length variations directly in their formulations.

3. The free surface weld pool shape has significant effect on arc behavior in terms of heat and current flux distributions. The normal Gaussian distribution can change to a bi-modal distribution even with small surface fluctuations of 1 mm.

4. The weld pool is dependant upon the heat and current sources it receives. The critical and sensitive variations of the arc characteristics necessitates its modelling to ensure proper boundary conditions are transmitted to the weld pool.
3. WELD POOL MODELLING

This chapter develops the mathematical formulation for the weld pool and compares the model with published results to permit a consistency check. It emphasizes the basic modelling scheme that is employed and which is common to the subsequent chapters.

The primary purpose of this chapter is to test the reliability and accuracy of the present model. In the first instance, the model is tested with just pure conduction mode where analytical solutions are available; the results, however, are not reproduced here. Convection is examined by reproducing the calculated results for weld pools found in the literature. This will provide confidence to the model.

3.1 Weld Pool Model Development

The GTAW process is shown schematically in Fig. 27. An arc is struck between the electrode (cathode) and the workpiece (anode). Some of the heat which strike the surface are absorbed while the rest are reflected. The heat absorbed will raise the temperature of the surface and a molten pool develops. This pool will grow until the heat input equals the heat loss by radiation, convection, conduction, and vaporization. Flows in the pool are driven by a combination of forces described earlier in chapter 1.2 and are shown schematically in Fig. 27.

The important macroscopic transport processes are:

i) heat and current flux distributions due to the arc

ii) interaction of the arc with the free surface

iii) convective heat transfer due to fluid flow in the weld pool

iv) thermal conduction into the solid workpiece

v) convective and radiative heat losses from the surface

vi) heat and mass losses due to vaporization

In addition, two other processes that are of concern include (i) the transient solidification and melting of the pool, and (ii) the Lorentz forces due to the divergent current path. There is a third process, the free surface deformation, but this is not considered in this thesis.
Figure 27. Schematic representation of gas tungsten welding arc with weld pool. The left portion indicates the various physical phenomena occurring within the workpiece while the right portion shows the computational domain. The computational origin for the weld pool is located at point E.
In order to simplify the mathematical treatment, the following assumptions for the model are employed:

i) Laminar flow is assumed.

ii) The surface is assumed to be a grey body ($\varepsilon=0.4$) [29].

iii) All transport, physical, and electrical properties of the liquid and solid are assumed constant, independent of temperature with the exception of surface tension. This permits the simplification of the model but can be relaxed if their temperature dependence are known.

iv) The model is solved in 2D assuming cylindrical geometry.

v) Joule heating and viscous dissipation in the weld pool are assumed to be negligible.

vi) The efflux of latent heat in the energy equation is neglected.

On the basis of the above assumptions, the physical processes occurring in the weld pool are cast into mathematical forms analogous to the arc model in Chapter 2. Figure 27 together with the governing transport equations, described below, and its associated boundary conditions constitute the mathematical model. The solution of these simultaneous equations of mass, momentum, energy, and Maxwell's electromagnetic equations will provide detailed information of the workpiece from which properties of the weldment are predicted. In this chapter, the effect of gas shear stress on the weld pool and vaporization heat loss will be neglected since the early publications of weld pool modeling did not consider these additional boundary conditions. These, however, will be covered in greater detail in the next chapter.

3.2 Governing Transport Equations

The relevant governing transport equations are:

**Conservation of mass**

\[
\frac{\partial u}{\partial t} + \frac{u}{r} \frac{\partial u}{\partial r} + \frac{\partial w}{\partial z} = 0
\]  \hspace{1cm} (3)

**Conservation of radial momentum**

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial r} + w \frac{\partial u}{\partial z} = -\frac{1}{\rho} \frac{\partial P}{\partial r} + \nu \left[ \frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} \frac{\partial u}{\partial z} + \frac{\partial^2 u}{\partial z^2} \right] - \frac{1}{\rho} (J_B) - \frac{1}{\rho} Ku
\]  \hspace{1cm} (4)
Conservation of axial momentum

\[
\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial r} + w \frac{\partial w}{\partial z} = -\frac{1}{\rho \partial z} \frac{\partial p}{\partial z} + \nu \left[ \frac{\partial^2 w}{\partial r^2} + \frac{1}{r} \frac{\partial w}{\partial r} + \frac{\partial^2 w}{\partial z^2} \right] + \frac{1}{\rho} \left[ J_r B_0 \right] - \frac{1}{\rho} K_w + g \beta (T - T_r)
\]  

(5)

Conservation of differential thermal energy

\[
\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial r} + w \frac{\partial T}{\partial z} = \alpha \left[ \frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2} \right] + \frac{\Delta H}{\rho C_p} \frac{\partial h}{\partial t}
\]  

(6)

In eqns. (4) and (5), the expressions, from left to right, are the transient term, the two convective terms, the pressure gradient term, the diffusive term, the Lorentz force term, and the drag term due to the mushy zone. The last term in eqn. (5) is the buoyancy force term. The drag term serves to simulate the reduction of velocity in the mushy zone. In eqn. (6), the expressions, from left to right, are the transient term, the two convective terms, the diffusive term, and the term due to the latent heat on phase change.

3.3 Workpiece Boundary Conditions

The case study is taken from Oreper and Szekely [44,56] in which a constant \( \partial \gamma / \partial T \) is used.

The boundary conditions are summarized in Table 9.

3.3.1 Momentum Boundary Conditions

The momentum boundary conditions (b.c.'s) are given by the second and third column in Table 9. The b.c.'s at region ABCD and region EFA (refer to Fig. 27 for region description) are self-explanatory. At the free surface (region DE), Marangoni or surface tension driven flow is described by:

\[
\tau_{ss} = \mu_{liq} \left( \frac{\partial u}{\partial z} \right)_{liq} = \left( \frac{\partial \gamma}{\partial T} \right) \left( \frac{\partial T}{\partial r} \right)
\]  

(7)

3.3.2 Thermal Boundary Conditions

The thermal boundary conditions are shown in column four of Table 9. The assumption of zero flux at the bottom plate (region AB), \( z = L_z \), implies that the surface is insulated. This is based on the premise that the surrounding air is a poor conductor of heat which is quite reasonable. The
<table>
<thead>
<tr>
<th>Region</th>
<th>$u$</th>
<th>$w$</th>
<th>$\frac{\partial T}{\partial z}$</th>
<th>$\frac{\partial \phi}{\partial z}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>AB</td>
<td>0</td>
<td>0</td>
<td>$\frac{\partial T}{\partial z} = 0$</td>
<td>$\frac{\partial \phi}{\partial z} = 0$</td>
</tr>
<tr>
<td>BC</td>
<td>0</td>
<td>0</td>
<td>$\frac{\partial T}{\partial r} = 0$</td>
<td>0</td>
</tr>
<tr>
<td>CD</td>
<td>0</td>
<td>0</td>
<td>$-k_s \frac{\partial T}{\partial z} = -q_a$</td>
<td>$J_a = -\sigma_v \frac{\partial \phi}{\partial z}$</td>
</tr>
<tr>
<td>DE</td>
<td>$\frac{\partial u}{\partial z}_{</td>
<td>_{\text{ukq}}} = \left( \frac{\partial y}{\partial T} \right) \left( \frac{\partial T}{\partial r} \right)$</td>
<td>0</td>
<td>$-k_i \frac{\partial T}{\partial z} = -q_a$</td>
</tr>
<tr>
<td>EF</td>
<td>0</td>
<td>$\frac{\partial w}{\partial r} = 0$</td>
<td>$\frac{\partial T}{\partial r} = 0$</td>
<td>$\frac{\partial \phi}{\partial r} = 0$</td>
</tr>
<tr>
<td>FA</td>
<td>0</td>
<td>0</td>
<td>$\frac{\partial T}{\partial r} = 0$</td>
<td>$\frac{\partial \phi}{\partial r} = 0$</td>
</tr>
</tbody>
</table>

Table 9: Boundary conditions of workpiece for confirmation of Oreper and Szekely's model [36].
zero flux at the side wall (region BC), \( r = L_r \), assumes similar argument as the above for a finite plate or that the temperature gradient approaches zero for a semi-infinite plate. The latter assumption is based on the premise that far away from the heat source, \( \partial T / \partial r \approx 0 \).

At the free surface (region CDE), the heat flux is given by [56]:

\[
q_a = q_o \exp (-\alpha_q r^2) = 6.135 \times 10^7 \exp (-10^2 r^2)
\]

which is for a cathode spot mode of operation. Radiation losses from the workpiece were omitted in the original study [56] and the peak surface temperature is assumed to be 2,500 K. This assumption is based on the experimental evidence that the peak surface temperature is about 500 K below the melting point of the workpiece [101,102]. The justification is that at this temperature, the heat loss by vaporization equals the heat input from the arc. The critical implication of this peak surface temperature assignment is that Marangoni shear is negated whenever the peak temperature is reached as \( \partial T / \partial r \approx 0 \).

Finally, symmetry conditions are assumed at regions EF and FA. The location of region DF is calculated from the energy equation using a latent heat source term for the phase change. This front is transient and needs to be evaluated at each time step. The source terms will now be considered.

3.4 Source Terms and Auxiliary Phenomenological Equations

3.4.1 Melting and Solidification Modelling

The enthalpy method is used in this analysis to take advantage of the fixed grid system. Here, a drag term, analogous to the Darcy-type flow, is included into the momentum equation to inhibit flow when the temperature falls below the liquidus point. A latent heat term is added to the energy equation for phase change. In particular, the method proposed by Hirt [114] is chosen for its simplicity.

The temperature-dependent drag terms are incorporated into the momentum equations via \(-K_u\) and \(-K_w\) where:
\[ K = \begin{cases} 
K_{max} \left( T_{liq} - T \right) / \left( T_{liq} - T_{sol} \right) & T > T_{liq} \\
0 & T_{sol} \leq T \leq T_{liq} \\
\infty & T < T_{sol} 
\end{cases} \quad (9) \]

The K-coefficient can be combined with the transient term in eqns. (4) and (5) to obtain the drag coefficient, DRG, defined as:

\[ DRG = \frac{1}{1.0 + \Delta t \cdot K} \quad (10) \]

Thus, DRG = 1.0 for pure liquid and 0.0 for solid state. The DRG term is also a function of the time step; for \( \Delta t \approx 10^{-3} \) s, \( K_{max} \) is chosen as \( 10^4 \). The effect of DRG as a function of temperature for two different values of \( K_{max} \) are shown in Fig. 28. Figure 28 (a) represents drag in the mushy zone better than Fig. 28 (b).

The latent heat term is added to the energy equation via \( -\frac{\Delta H_L}{C_p} \frac{df_L}{dt} \) where

\[ f_L = \begin{cases} 
1 & T > T_{liq} \\
\left( T - T_{sol} \right) / \left( T_{liq} - T_{sol} \right) & T_{sol} \leq T \leq T_{liq} \\
0 & T < T_{sol} 
\end{cases} \quad (11) \]

\( f_L \), defined as the fraction of liquid, has been linearized for simplicity. It can be used to simulate true volume fraction liquid if the phase diagram of the alloy is known. This model is being used in the commercial fluid flow and heat transfer package FLOW-3D [95] and has also been used to model a mold-filling problem [115].

### 3.4.2 Electromagnetic Source Terms

The continuity equation for electric charge and current is given by Gauss law as:

\[ \nabla \cdot J + \frac{\partial \rho_c}{\partial t} = 0 \quad (12) \]

where \( \rho_c \) is the charge density. If the electric field is assumed to be in quasi-steady state, or that it achieve equilibrium potential fields instantaneously, then the continuity equation becomes:

\[ \nabla \cdot J = 0 \quad (13) \]

From Ohm's law (assuming that the magnetic Reynolds number is much less than unity*):

\[ J = \sigma_e E \quad (14) \]

* By assuming the magnetic Reynolds number to be much less than unity, the \( u \times B \) term in Ohm's law can be neglected. The magnetic Reynolds number is calculated from \( \sigma_e \mu_0 U_0 L \) [116] and is indeed less than unity for the characteristic values of the weld pool.
Figure 28. Drag coefficient as a function of temperature.
(a) $K_{\text{max}} = 10^4$ kg/m$^3$-s (b) $K_{\text{max}} = 10^3$ kg/m$^3$-s
The drag coefficient represents the conductance to fluid flow where 1.0 is for liquid (maximum conductance) and 0.0 is for solid (no conductance).
and since the scalar electric potential, \( \phi \), is defined as \( \mathbf{E} = -\nabla \phi \), thus eqns. (13) and (14) can be combined to give:

\[
\nabla^2 \phi = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \phi}{\partial r} \right) + \frac{\partial^2 \phi}{\partial z^2} = 0
\]

(15)

assuming that the electrical conductivity is constant for steel. This is the standard Laplace equation for electrical charge continuity.

The current density is calculated from:

\[
J_r = -\sigma_e \frac{\partial \phi}{\partial r} \tag{16}
\]

\[
J_z = -\sigma_e \frac{\partial \phi}{\partial z} \tag{17}
\]

while the self-induced azimuthal magnetic field is derived from Ampere's law as:

\[
B_\theta = \frac{\mu_0}{r} \int_0^r J_z r \, dr \tag{18}
\]

The integration constant in eqn. (18) is assumed zero for \( B_\theta \rightarrow 0 \) as \( r \rightarrow 0 \) since the integrand approaches zero as \( r \rightarrow 0 \). Equations (15-18) complete the information required to determine the electromagnetic body force. The Lorentz force, \( \mathbf{J} \times \mathbf{B} \), is then given by:

\[
\mathbf{J} \times \mathbf{B} \bigg|_r = -J_z B_\theta \tag{19}
\]

\[
\mathbf{J} \times \mathbf{B} \bigg|_z = J_r B_\theta \tag{20}
\]

The above scheme of calculating \( \mathbf{J} \times \mathbf{B} \) takes advantage of the symmetry of the system concerned.

The electric potential b.c.'s, shown in column 5 of Table 9, are quite straightforward. The selection of an isopotential line (\( \phi = 0 \)) at region BC is such that the right wall is far away from the weld pool and \( J_z \sim 0 \) in this region. This Dirichlet boundary condition is meant to assist in the computational process. The current flux at the free surface for the cathode spot operation (CE) is given by [56]:

\[
J_s = J_0 \exp(-\alpha r) = 5.11 \times 10^6 \exp(-230 r) \tag{21}
\]

A brief note of some of the techniques for solving the Lorentz force with a distributed current source is helpful at this time. There are currently three methods known to this author for solving the Lorentz force for the direct current GTAW process. Kou et al [4,47] and Zacharia et al [57,58] both employed an analytical solution derived by Atthey [43] for cylindrical coordinates. The
solution is given as a Hankel transformation and is only valid if the current flux has the following Gaussian form:

\[ J_0 = \frac{1}{\pi b^2} \exp(-r^2/b^2) \]  

(22)

However, experimental studies by Kou and Lu [23] indicated that the current distribution did not necessarily follow a Gaussian behavior. The second method employed by Oreper and Szekely [44,56] used an electromagnetic stream function relation to derive the current density. This scheme is quite different from the traditional method of solving JxB. The third method employed by Correa and Sundell [51] is identical to the one used here. In fact, the technique proposed in this dissertation has been derived independently of Correa and Sundell's studies [51].

3.5 Material Properties for the Workpiece

Table 10 lists the material properties and workpiece information employed for the test case. They are taken from Oreper and Szekely [44,56]. \( \partial \gamma / \partial T \) is assumed constant but the value employed (10^5 N/m-K) is an order of magnitude smaller than those typically found in steels [117].

In general, it is quite tedious to obtain accurate material properties, especially for stainless steels since these properties are not only temperature dependant but also composition dependant [118]. As a result, the values reported here reflect order of magnitude approximation. In the liquid phase where forced convection is important due to the high Peclet number, the role of the physical properties is not that critical. However, in the solid phase, the isotherm fronts movements have a square root dependance*. Thus, some variations in the predicted and experimental pool size can be expected if constant physical properties are used.

3.6 Solution Technique and Implementation

The PHOENICS [93,119] numerical code is employed to model the workpiece. This is a commercial finite volume 3D code based on the "SIMPLE" algorithm [120]. The detailed

* The rate of advance of an isotherm in the solid phase for a semi-infinite plate can be approximated from the Fourier number as \( d \sim \sqrt{\alpha t} \).
description of PHOENICS is given elsewhere [93] and not discussed here. This section describes some of the numerical settings imposed for this and subsequent chapters. The computations are done on a series of computers ranging from engineering workstations (VAX Stations II, 2000, 3100/30, 3100/38) to desk-top supercomputer (APOLLO DN 10000). The time step in all runs is set at 10^{-3} \text{s}.

<table>
<thead>
<tr>
<th>Nomenclature</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>coefficient of thermal expansion</td>
<td>$\beta$</td>
<td>$10^{-4}$ K^{-1}</td>
</tr>
<tr>
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</tr>
<tr>
<td>drag coefficient (max)</td>
<td>$K_{\text{max}}$</td>
<td>$10^{4}$ kg/m^{3}s</td>
</tr>
<tr>
<td>electrical conductivity</td>
<td>$\sigma_{e}$</td>
<td>$7.14 \times 10^{5}$ $\Omega^{-1}$ m^{-1}</td>
</tr>
<tr>
<td>heat capacity</td>
<td>$C_p$</td>
<td>$753$ J/kg-K</td>
</tr>
<tr>
<td>latent heat of fusion</td>
<td>$\Delta H$</td>
<td>$2.47 \times 10^{3}$ J/kg</td>
</tr>
<tr>
<td>liquidus temperature</td>
<td>$T_{\text{liq}}$</td>
<td>$1523$ K</td>
</tr>
<tr>
<td>maximum surface temperature</td>
<td>$T_{\text{s, max}}$</td>
<td>$2,500$ K</td>
</tr>
<tr>
<td>permeability of free space</td>
<td>$\mu_0$</td>
<td>$1.26 \times 10^{8}$ H/m</td>
</tr>
<tr>
<td>plate radius</td>
<td>$L_r$</td>
<td>$20.0$ mm</td>
</tr>
<tr>
<td>plate thickness</td>
<td>$L_z$</td>
<td>$12.7$ mm</td>
</tr>
<tr>
<td>solidus temperature (steel)</td>
<td>$T_{\text{sol}}$</td>
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</tr>
<tr>
<td>surface tension coefficient</td>
<td>$\partial \sigma / \partial T$</td>
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</tr>
<tr>
<td>thermal conductivity (liquid steel)</td>
<td>$k_l$</td>
<td>$15.48$ W/m-K</td>
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<tr>
<td>thermal conductivity (solid steel)</td>
<td>$k_s$</td>
<td>$31.39$ W/m-K</td>
</tr>
<tr>
<td>viscosity</td>
<td>$\mu$</td>
<td>$0.006$ kg/m-s</td>
</tr>
</tbody>
</table>

Heat Flux : \[ q_x = 6.135 \times 10^7 \exp(-10^5 r^2) \] W/m^{2}

Current flux : \[ j_x = 5.11 \times 10^6 \exp(-23C_r) \] A/m^{2}

Initial condition : $300$ K

Grid configuration : Uniform grids of $0.5$ mm radial and $0.4$ mm axial

Table 10 Material properties and workpiece information for confirmation of\cref{44,56}. [44,56].

\section{a) Grid Configuration}

The grid configuration is identical to that employed by the original authors [56] so as to provide a consistent check. This is given in Table 10. It must be stressed that the original authors did not explicitly describe their grid configurations and those shown here were deduced from their published figures. In subsequent chapters, the grid configuration, in general, contains at least 20 by
20 grids in the molten zone during steady state conditions so as to ensure that there are sufficient grids to represent the flow circulations. Grid independence is achieved by examining various grid configurations; the details of which are given later in this chapter.

**b) Initial Condition**

In modelling the transient behavior of the workpiece, there is a fundamental problem with the numerical simulation particularly during the initial stages of melting. During this time, there are only a few grids in the molten zone and as a result, the convective flow loops that develop are unlikely to be converged. Furthermore, the greatest errors during the calculations probably occur during this stage. To circumvent this numerical difficulty, the initial condition is prescribed as a "small" molten pool (3 mm radius and 0.3 mm deep) of uniform temperature (1,800 K) while the rest of the domain is at 300 K. This pool size corresponds to at least 20 by 4 grid nodes. Naturally, this initial condition for the pool size is smaller than the steady state pool size. The purpose of this prescription are two-fold:

i) **It overcomes the problem of initial melting when there are few grids in the pool.**

ii) **A uniform molten weld pool temperature resembles more closely to the workpiece of uniform initial temperature of 300 K.**

In order to ensure that this initial condition did not produce different solutions at later times, further runs were carried out in which the pool was assumed to be at 2,000 K and after a 1-s real time simulation, the field values for all the dependant variables were essentially identical (< 0.01 % variation). In a separate test case where the initial condition was assumed to be 300 K for the entire workpiece, it was discovered that the residuals* at the initial heating stages prior to melting were decreasing monotonously. However, with the onset of melting of the first grid node directly below the arc, the residuals increased by 3 orders of magnitude. This inaccuracy should be minimized if not avoided. Using the initial condition described above, this sudden change in

* The residual is defined as the value that results when the field values (say temperature) are substituted into the governing equation. A perfect solution of the field values will produce zero residual. In practice, the residual is non-zero due to the finite resolution of the machine.
residuals was indeed avoided. Incidentally, the field values when the initial condition was 300 K for the entire domain were at most 0.2 % different from that of the 1,800 K case. Thus, this indicates the order of magnitude as well as the accuracy of the initial conditions imposed. For practical purpose, it can be said that the results for the 1,800 K and 300 K initial conditions are comparable.

The disadvantage of this artificial prescription is that the model will not simulate the weld pool in real time, that is a 5-second simulation may not correspond to 5-second real time in the actual experiment. This prescription is not a serious drawback if we are interested in steady state situations in which most of the experimental work are carried out. However, should real time simulation be desired, there are two options: a) acknowledge that there is a 0.2 % error in the calculated values which seems acceptable, or b) modify the code to accurately model the initial melting stage.

An alternate scheme to the above methodology is to initially assume pure conduction and heat the workpiece to just above the melting point for a short time (say 50 ms). Convection can then be activated thereafter. The disadvantage of this method is that some initial surface temperature distribution will be given to the weld pool and since Marangoni flows completely dominate pool circulation, this may introduce errors to the computations due to different initial conditions. Preliminary trials indicated that by assuming pure conduction for 50 ms, 100 ms, and 200 ms, and activating convection thereafter all produced different surface temperatures distributions (sometimes varying by as much as 200 K) after a 1-second simulation. Thus, this method needs to be implemented with caution.

c) Convergence Criterion

Convergence is achieved when the spot values of temperature, electric potential, pressure, and velocities at the “worst” grid location remain unchanged while the residuals of all the governing equations continue to decrease. In general, the residuals must decrease by at least 2 orders
of magnitude with respect to the first sweep before the run is terminated. The "worst" location is
determined to be the second node under the free surface adjacent to the z-axis.

d) Reference Residuals

The reference residual is assumed to be $10^{-6}$ for $u, w, T,$ and $P$. The reference residual is used
as a stopping criterion to determine when the calculations should advance to the next time step.
Although the actual stopping criterion is grid-dependent**, it is found that consistent field and spot
values are obtained when various grid configurations are tested with a reference residual of $10^{-6}$.
Furthermore, as the weld pool problem does not have inflow or outflow boundary conditions, the
critical monitoring values are the not the residuals but the spot values.

Frequently, the residuals of the momentum (velocity) and continuity (pressure) equations
tend to oscillate even though the spot values of temperature, velocity, and electric potential have
remained constant. This is due to the machine resolution of the numbers which in single precision is
seven significant figures. In this problem, the main driving forces are $J \times B$ and surface temperature.
$J \times B$ is governed by the charge continuity equation which has a monotonously decreasing absolute
residual down to $10^{-7}$. This is probably the precision of the electric potential field values. Since
the $J \times B$ forces are only spatially dependent, they are not affected by the pressure fields. The second
driving force is the temperature which remains essentially unchanged during the later iterations
and sweeps. The spot values that oscillate are the pressure fields which respond to the
fluctuations in the velocity fields. When the machine resolution is reached, the fluctuations are
due to the uncertainties in the last few digits of the field values. In general, it is observed that the
fourth significant digit of the velocity fields fluctuates in response to these uncertainties. To
overcome this problem, one may under-relax the iterative process, employ more sweeps and
iterations, or even employ a smaller time-step. However, it is found that the actual field values

---

* Since the charge continuity equation is time-independent, the reference residual is $10^{-7}$ for the
electric potential to assist in the stopping criterion.
** This is because more grids entail more calculations and the residuals are expected to increase due
to the additional computations in the finite volume approximations.
vary by < 0.1% even with the additional sweeps and thus these calculated values are considered to be accurate to 0.1%.

e) Under-Relaxation Factors

The majority of the runs are conducted without the need of relaxation factors. However, in certain instances, relaxation factors are needed to assist convergence. In these cases, the solutions or field values fluctuate by one or two orders of magnitude during subsequent sweeps. This is the scenario regardless of the choice of initial condition described in part (a) above. Such situations occur, for instance, when the heat flux is too large such that the iterative scheme is unable to produce convergence due to large “swings” or changes in the field values during each iteration and sweep. Other possible explanations can be due to the existence of multiple flow loops and the mesh employed is too coarse to resolve these loops. Thus, the iterative step is unable to march towards the converged solution. The net effect are that the field values, spot values, and residuals fluctuate by orders of magnitude with each sweep; the solution is said to be unconverged.

There are several remedies to these large fluctuations and they are 1) increase the number of sweeps to assist in the convergence, 2) decrease the time step so that the large changes in values are reduced, 3) increase the number of nodes at the problem area to resolve the flow field, and 4) under-relax the iterative scheme so as to permit only small changes during each cycle. Usually, several combination of these remedies are needed to obtain a converged solution and trial and errors are required to achieve this combination.

3.7 Results and Discussion

Since much of the interesting phenomena in the workpiece occur within a 5 mm radius, even though the computations have to simulate up to 20 mm, the graphic outputs are plotted at most up to 10 mm radial distance. The same scaling factor is used for all figures to allow for direct comparison.
3.7.1 Oreper and Szekely's Model [44,56]

Figures 29 (a) and (b) show a plot of the heat and current flux distributions, respectively, employed (unfilled box) in this section. For comparison, the heat and current fluxes calculated in Chapter 2 - Fig. 10 (filled triangle) and that used by Kou and Wang (circle) [4] are also shown. It appears that the arc current used is about 200 A. The current distribution used by Oreper and Szekely [56] tends to be exponential rather than Gaussian*. The heat and current fluxes described by Kou and Wang [4] is obtained by adjusting the parameters a and b to get the approximate distribution. The arc efficiency employed for Kou's model is assumed to be identical to that calculated in the arc model.

The Gaussian heat flux distribution due to Oreper et al [56] and Kou et al [4] matches identically. However, the current flux distribution differs somewhat. This is because Oreper et al [56] assumed an exponential function rather than a Gaussian function which suggests a slightly different driving force for JxB in the weld pool when compared to the traditional Gaussian sources.

The calculated weld pool shape and surface temperature are shown in Figs. 30 (a) and (c) while the result of Oreper and Szekely [56] is shown in Fig. 30 (b). The weld pool (Fig. 30 (a)) has a width of 4.5 mm and a penetration depth of 3.5 mm. The maximum characteristic weld pool velocity is about 3.1 cm/s at r=0.25 mm. Oreper and Szekely [56] reported a width of 4.5 mm, a penetration of 3.1 mm, and a characteristic velocity of 2.7 cm/s at r = 0.5 mm (Fig. 30 (b)). The results are comparable for the pool dimensions. The maximum characteristic velocity in Fig. 30 (a) is slightly larger than that in Fig. 30 (b) since the first grid in (a) is located closer to the z-axis and thus the volume element is smaller. Consequently, the velocity in (a) is slightly larger.

Figure 30 (c) shows the calculated surface temperature plot of the workpiece at t= 8.0 s. The peak temperature is set at 2,500 K [56] which results in a profile that is not very realistic. This has an important implication in that it suggests that surface tension driven flow is negated near the pool center. Thus, most of the Marangoni flows are driven by the temperature gradient between

* Private communication with Dr. G.M. Oreper indicated that he approximated his current function from Nestor's data [24] for a 200 A arc at 6.3 mm.
Figure 29. Plot of (a) heat flux and (b) current flux distributions as a function of radial position at the anode from various sources. The filled triangles are from Figs. 16 (a-b).
Figure 30. Computed weld pool results at t=8.0s due to Oreper and Szekely's sources [56].
(a) Calculated weld pool shape ($T_{liq}$=1723 K and $T_{sol}$=1523 K).
(b) Calculated weld pool shape by Oreper and Szekely [56].
(c) Calculated surface temperature profile.
r=2.75 mm and r=4.25 mm. Furthermore, as the ργ/ρT employed is 10⁻⁵ N/m-K, which is an order of magnitude less than those typically found for steels [117], the role of Marangoni shear may not be dominant in this particular case. It is suspected that JxB is the more dominant driving force. The figure also suggests the importance of addressing the issue of vaporization at the free surface in order to provide a better model for the surface temperature distribution.

The calculated current density and electromagnetic body force are shown in Figs. 31 (a) and (b), respectively. In Fig. 31 (a), at r = 20 mm, Jₓ ~ 0 and only the Jᵧ component is present. In this region, the JxB force is vertically downwards near the top of the plate (z~0) and zero near the bottom of the plate (z~12 mm). The reason for this unbalance JxB force at r~20 mm is due to the nature of the induced magnetic fields, B₀, at r~0. At r~0, Jₓ ≠ 0 for z~0 but Jᵧ ~ 0 for z~10 mm, and this Jᵧ in the vicinity of r ~ 0 is responsible for the resultant JxB forces at r~20 mm. At the free surface (z~0), Jₓ varies from a maximum at r~0 to negligible at r~20 mm. Thus, at r=10 mm, Jₓ is no longer zero and the body force “bends” in response to the current path. Notice that the maximum body force occurs at the region where the current path is about 45° to the horizontal. At this orientation, both Jₓ and Jᵧ contributions to JxB will be the greatest. Figures 31 (a-b) are shown primarily to indicate the nature of the current density and the JxB forces. It appears that the strongest JxB component occurs a few mm from the center of the pool near the free surface.

In analyzing the manner Oreper et al [44,56] derived their JxB forces, they solved the current density by defining the electromagnetic stream function as:

\[ J = \nabla \times \left[ \frac{\psi_e}{rT₀} \right] \]  \hspace{1cm} (23)

In the deriving the anode current flux, they stated that “close to the free surface” (presumably one node below the free surface), the electromagnetic stream function is calculated to have the following form:

\[ \psi_e = \psi_e(z=0) \left( 1 - \frac{Cz}{L} \right) \]  \hspace{1cm} (24)

and

\[ \psi_s(z=0) = \frac{1}{2\pi} \frac{Iα_x r^2}{\alpha_x} \] \hspace{1cm} for r ≤ 1/αₓ \hspace{1cm} (25)

where C = 10 for cathode spot mode. On the basis of eqn. (23), at z = 0:
Figure 31. Plot of (a) current density and (b) JxB body force due to Oreper and Szekely [56]. The maximum vector is shown at the top of each figure.
\[ J_z = \frac{1}{r} \frac{\partial \psi_z}{\partial r} = -\frac{1}{\pi} \frac{\alpha_i}{L} (1 - \frac{C_z}{L}) \]  

which essentially states that \( J_z \) is a constant “close” to the free surface. If this is the case, then a less divergent \( J \times B \) will result which helps explain the slightly shallower depression and lower velocity they obtained. It noted from Fig. 31 (a) that \( J_z \) is not a constant between \( r = 0 \) and \( r = 1/\alpha_i \approx 4.3 \) mm.

Detailed analyses of the original work of Oreper and Szekely [44] for the calculations of the \( J \times B \) forces indicate that certain assumptions, such as the approximation of the \( J_z \) distribution near the free surface, were made in the computation of the body force. Since it has been proposed that the \( J \times B \) forces predominates relative to the smaller \( \partial \gamma / \partial T \) value, such assumption of the \( J_z \) distribution may reduce its \( J \times B \) intensity. In current model, the \( J \times B \) forces have been calculated rigorously and thus a slightly higher pool penetration and velocity are obtained. Having explained this small discrepancy, our calculated results can be said, for practical purposes, to be comparable and consistent with those findings of Oreper and Szekely’s [56] and it can be concluded that the proposed mathematical model is sound.

### 3.7.2 Grid Independence Test

A second test of the current model is to ensure that the computed solution is grid-independent. This exercise involves using various grid configurations with the same initial condition. The arc characteristics have been calculated from the governing equations given in Chapter 2 and Appendix A for a 100 A argon arc at 1.5 mm arc length. Mixed control vaporization is employed for the workpiece; the details of which are given in the next chapter. The arc characteristics, workpiece b.c.’s, workpiece composition, thermodynamic and physical properties for this test are given in Chapter 4.1. In order not to detract from the focus of this exercise, the discussion of the b.c.’s and material properties are postponed till the next chapter.

In all cases, variable grids are used due the nature of the problem where an intense arc exists within a small weld pool but the workpiece is large relative to the pool dimensions. The
following grid structure is utilized: uniform grids are deployed within the liquid phase \((r \leq 4 \text{ mm})\) and \((z \leq 4 \text{ mm})\) while variable grids are deployed in the solid phase. The variable grids increase by 10-15\% geometrically in the solid phase.

The grid configurations are shown in Table 11. This test exercise involves comparing the surface temperature and field values at \(t=2\) s and \(t=3\) s. It is understood that numerically, the greatest errors in the computations occur during the initial stages of the calculations \((t \sim 1\) s). Thus, if the results are comparable at intermediate times \((t \sim 2-3\) s), then they should be comparable at later times \((t > 5\) s).

<table>
<thead>
<tr>
<th>CASE</th>
<th>GRIDS</th>
<th>Min r-grid (mm)</th>
<th>Max r-grid (mm)</th>
<th>Min z-grid (mm)</th>
<th>Max z-grid (mm)</th>
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<tbody>
<tr>
<td>I</td>
<td>40 x 37</td>
<td>0.15</td>
<td>3.48</td>
<td>0.15</td>
<td>1.82</td>
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<td>II</td>
<td>68 x 37</td>
<td>0.075</td>
<td>4.00</td>
<td>0.15</td>
<td>1.82</td>
</tr>
<tr>
<td>III</td>
<td>88 x 37</td>
<td>0.05</td>
<td>3.50</td>
<td>0.15</td>
<td>1.82</td>
</tr>
<tr>
<td>IV</td>
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<td>0.15</td>
<td>3.48</td>
<td>0.075</td>
<td>1.90</td>
</tr>
<tr>
<td>V</td>
<td>40 x 86</td>
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<td>3.48</td>
<td>0.05</td>
<td>2.23</td>
</tr>
<tr>
<td>VI</td>
<td>88 x 86</td>
<td>0.05</td>
<td>3.50</td>
<td>0.05</td>
<td>2.23</td>
</tr>
</tbody>
</table>

Table 11. Grid configurations for grid-independence tests.

Since the most dominant driving force is the Marangoni shear, the nature of the surface temperature distribution must be determined as accurately as possible. Several general observations can be drawn regarding the nature of the grid configurations:

1) The effect of the radial grid size is not so critical is affecting the surface temperature distribution if \(\Delta r_{\text{min}}\) is less than 0.15 mm. If \(\Delta r_{\text{min}}\) is larger than 0.15 mm, the calculated results are significantly different from those of smaller grid size. However, if \(\Delta r_{\text{min}}\) is less than 0.15 mm, the surface temperature distribution are comparable for different grid configurations (~1% variation).

2) The effect of the axial grid size is more critical in affecting the surface temperature distribution. This is because PHOENICS does not have any grid at the free surface, rather, the
first axial node is located within the computational domain. The surface temperature must be back-calculated from the heat flux.

3) The effect of the axial grids in affecting surface temperature distribution is reduced if the minimum grid size is less than 0.075 mm. The difference in computed results between 0.075 mm and 0.050 mm is about 2% which is acceptable. The primary reason in choosing the 0.075 mm grid is that the smaller grids (0.050 mm) requires excessive computational time.

4) Thus, the minimum grid sizes employed in all subsequent chapters are 0.15 mm radial and 0.075 mm axial with at least 200 grids in the molten zone.

Figure 32 shows the results of the calculations due to a 100 A arc for two different grid configurations. The velocity vectors are not shown in Fig. 32 (c-d) as they are too closely spaced to be resolved visually. Figures 32 (a) and (b) are for 2- and 3-s simulations and they are comparable to the results in (c) and (d), respectively, in terms of pool size. It can be safely concluded that grid-independence has been achieved and that the minimum 0.15 mm radial and 0.075 axial grids* will be employed in later chapters.

Incidentally, the maximum temperature and maximum velocity reported for the 40x64 grids are smaller than that for the 88x86 grids because the first axial and radial nodes of the 88x86 grids are located closer to the origin. The first node in the 40x64 grid configuration is located at (0.075 mm, 0.0375 mm) while the first node in the 88x86 grid configuration is located at (0.025 mm, 0.025 mm). This explains the higher maximum temperature in the 88x86 grid configuration. The higher maximum velocity in the 88x86 grid configuration is due to the first radial node being closer to the z-axis and since flow is directed inward towards the center, the fluid velocity increases as the volume element becomes smaller as $r \to 0$ for cylindrical coordinate system.

3.8 Summary of Results

The mathematical model employed in this study showed good agreement with published numerical results. Furthermore, grid-independence have been tested and achieved. This exercise provides confidence to the mathematical model proposed and the numerical scheme employed.

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* Actually, the minimum grid criterion is always satisfied but in subsequent chapters, the grid configuration has been optimized to 40x41 grids in order to reduce the computational times.
Figure 32. Weld pool shape due to different grid configurations. (a) and (b) have minimum grid size of 0.15 mm radial and 0.075 mm axial. (c) and (d) have minimum grid size of 0.050 mm radial and 0.050 mm axial. (c) and (d) are drawn on a slightly reduced scale due to the large number of grids.
4. COUPLING OF THE WELDING ARC WITH THE WELD POOL

This chapter explores the effect of a one-way coupling between the welding arc and the weld pool. The arc behavior is assumed to be in quasi-steady state in that it will not change once the weld pool surface geometry is established. Among the issues addressed include vaporization and plasma shear stress on the free surface. The purpose of this chapter is to investigate the sensitivity of the weld pool shape and surface temperature to surface tension and arc power distribution; primarily to develop an understanding of how the various phenomena interact. The importance of the free surface temperature has been discussed in Section 1.7.1 and not re-iterated here.

4.1 Material Properties and Input Conditions

Figure 33 shows the combined welding arc and weld pool phenomena. The b.c.'s for the welding arc are given in Table 12 while the b.c.'s for the workpiece are given in Table 13. The arc characteristics are calculated on the basis of the governing equations given in Appendix A and the results are shown in Fig. 34 (a-b) which serve as b.c.'s for the region cde in Fig. 33. These results are for a tungsten electrode (2 mm diameter) with 1.5 mm arc gap and argon shielding gas. The cathode spot current density is assumed to be 45 A/mm² with an arc current of 100 A. The workpiece size is 40 mm by 40 mm by 12.5 mm.

The material properties for the workpiece are taken from various references [29,30,56,63,69,121-123]. The composition of the workpiece material (AISI 304) is given in Table 14. The physical and thermodynamic properties for the workpiece are given in Tables 15 and 16. In general, all the physical properties, except for the surface tension, are assumed constant.

4.2 Vaporization Kinetics in Arc Welding

The vaporization of gaseous species from the molten surface consists of four steps (Fig. 35):

i) The molten species M must be transported to the free surface.

ii) The molten species must vaporize into the anode solute boundary layer.
Figure 33. Schematic representation of combined gas tungsten arc and weld pool phenomena. The left portion indicates the various physical phenomena occurring within the workpiece while the right portion shows the computational domain. The origin for the weld pool is at point e while the origin for the welding arc is at point A.
Figure 34. Plot of (a) heat flux and surface temperature, and (b) current flux and surface velocity as a function of radial position for a 100 A arc at 1.5 mm arc length.
Figure 35. Vaporization stages of gaseous species from the weld pool.

The diagram on the left shows the mechanisms by which high vapor pressure species escape from the weld pool while the diagram on the right shows the concentration profile of that vapor species as a function of distance from the free surface.

Stage 1: Convected to the free surface by fluid flow circulation
Stage 2: Vaporized from the free surface
Stage 3: Diffused across the solute boundary layer
Stage 4: Transported away by the carrier gas
<table>
<thead>
<tr>
<th>Region</th>
<th>$u$</th>
<th>$w$</th>
<th>$h$</th>
<th>$\phi$</th>
</tr>
</thead>
<tbody>
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<td>0</td>
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<td>$J_c = \frac{1}{\pi R_c^2}$</td>
</tr>
<tr>
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<td>0</td>
<td>$T = 3,000\ K$</td>
<td>$\frac{\partial \phi}{\partial z} = 0$</td>
</tr>
<tr>
<td>CD</td>
<td>0</td>
<td>0</td>
<td>$T = 3,000\ K$</td>
<td>$\frac{\partial \phi}{\partial r} = 0$</td>
</tr>
<tr>
<td>DE</td>
<td>0</td>
<td>$\frac{\partial p w}{\partial z} = 0$</td>
<td>$T = 1,000\ K$</td>
<td>$\frac{\partial \phi}{\partial z} = 0$</td>
</tr>
<tr>
<td>EF</td>
<td>$\frac{\partial p u}{\partial r} = 0$</td>
<td>$\frac{\partial w}{\partial r} = 0$</td>
<td>$T = 1,000\ K$</td>
<td>$\frac{\partial \phi}{\partial r} = 0$ (inflow)</td>
</tr>
<tr>
<td>FG</td>
<td>$\frac{\partial p u}{\partial r} = 0$</td>
<td>$\frac{\partial w}{\partial r} = 0$</td>
<td>$\frac{\partial h}{\partial r} = 0$</td>
<td>$\frac{\partial \phi}{\partial r} = 0$ (outflow)</td>
</tr>
<tr>
<td>GH</td>
<td>0</td>
<td>0</td>
<td>$T = 1,000\ K$</td>
<td>$\phi = \text{const}$</td>
</tr>
<tr>
<td>HA</td>
<td>0</td>
<td>$\frac{\partial w}{\partial r} = 0$</td>
<td>$\frac{\partial h}{\partial r} = 0$</td>
<td>$\frac{\partial \phi}{\partial r} = 0$</td>
</tr>
</tbody>
</table>

Table 12. Boundary conditions for the welding arc model.

(iii) The vapor species must diffuse across the anode solute boundary layer.

(iv) The vapor species is then transported away by the carrier gas or plasma.

Any one of these four steps can be rate limiting. In general, step (i) is not considered rate-limiting in that the molten species are transported to the free surface as rapidly as they are vaporized from the surface. This assumption appears reasonable in light of the fact that the weld pool is rigorously stirred. Also, step (iv) is not rate-limiting as the plasma is moving at a high velocity.

The second step is frequently referred to as Langmuir vaporization if the gaseous species escape into a vacuum. In the case of welding, the plasma arc is not under a vacuum environment and so the rate of mass loss will be over-predicted if this is the sole mechanism for mass loss. However,
<table>
<thead>
<tr>
<th>Region</th>
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<th>$T$</th>
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<tr>
<td>$ab$</td>
<td>0</td>
<td>0</td>
<td>$T = 288$ K</td>
<td>$\frac{\partial \phi}{\partial z} = 0$</td>
</tr>
<tr>
<td>$bc$</td>
<td>0</td>
<td>0</td>
<td>$T = 288$ K</td>
<td>0</td>
</tr>
<tr>
<td>$cd$</td>
<td>0</td>
<td>0</td>
<td>$-k \frac{\partial T}{\partial z} = -q_a$</td>
<td>$J_a = -\sigma_e \frac{\partial \phi}{\partial z}$</td>
</tr>
<tr>
<td>$de$</td>
<td>$\left. \frac{\partial u}{\partial z} = \left( \frac{\partial T}{\partial r} \right) \left( \frac{\partial r}{\partial z} \right) \right</td>
<td>_{liq}$</td>
<td>0</td>
<td>$-k \frac{\partial T}{\partial z} = -q_a + q_{vap}$</td>
</tr>
<tr>
<td>$ef$</td>
<td>0</td>
<td>$\frac{\partial w}{\partial r} = 0$</td>
<td>$\frac{\partial T}{\partial r} = 0$</td>
<td>$\frac{\partial \phi}{\partial r} = 0$</td>
</tr>
<tr>
<td>$fa$</td>
<td>0</td>
<td>0</td>
<td>$\frac{\partial T}{\partial r} = 0$</td>
<td>$\frac{\partial \phi}{\partial r} = 0$</td>
</tr>
</tbody>
</table>

Table 13. Boundary conditions for the workpiece.
AISI 304 Stainless steel (Composition in wt-%)

<table>
<thead>
<tr>
<th>Element</th>
<th>Content</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.1</td>
</tr>
<tr>
<td>Cr</td>
<td>18.1</td>
</tr>
<tr>
<td>Cu</td>
<td>0.33</td>
</tr>
<tr>
<td>Mn</td>
<td>0.31</td>
</tr>
<tr>
<td>Mo</td>
<td>0.31</td>
</tr>
<tr>
<td>Fe</td>
<td>69.928</td>
</tr>
<tr>
<td>Ni</td>
<td>8.4</td>
</tr>
<tr>
<td>P</td>
<td>0.040</td>
</tr>
<tr>
<td>S</td>
<td>0.022</td>
</tr>
<tr>
<td>Si</td>
<td>0.69</td>
</tr>
<tr>
<td>V</td>
<td>0.48</td>
</tr>
</tbody>
</table>

Table 14. Composition of AISI 304 [30].

<table>
<thead>
<tr>
<th>Nomenclature</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>activity of sulphur</td>
<td>( a_s = [S] )</td>
<td>0.022 wt %</td>
</tr>
<tr>
<td>atomic weight (Ar)</td>
<td>( M_{Ar} )</td>
<td>39.948 g/mole</td>
</tr>
<tr>
<td>atomic weight (Fe)</td>
<td>( M_{Fe} )</td>
<td>55.847 g/mole</td>
</tr>
<tr>
<td>atomic weight (Mn)</td>
<td>( M_{Mn} )</td>
<td>54.938 g/mole</td>
</tr>
<tr>
<td>coefficient of thermal expansion</td>
<td>( \beta )</td>
<td>( 10^{-4} ) K(^{-1} )</td>
</tr>
<tr>
<td>constant in surface tension coefficient</td>
<td>( A )</td>
<td>( 4.3 \times 10^{-4} ) N/m-K</td>
</tr>
<tr>
<td>density (steel)</td>
<td>( \rho )</td>
<td>7.200 kg/m(^3)</td>
</tr>
<tr>
<td>density (Ar)</td>
<td>( \rho_{Ar} )</td>
<td>1.400 kg/m(^3)</td>
</tr>
<tr>
<td>density (Fe)</td>
<td>( \rho_{Fe} )</td>
<td>7.020 kg/m(^3)</td>
</tr>
<tr>
<td>density (Mn)</td>
<td>( \rho_{Mn} )</td>
<td>6.430 kg/m(^3)</td>
</tr>
<tr>
<td>electrical conductivity (steel)</td>
<td>( \sigma_e )</td>
<td>( 7.14 \times 10^5 ) (\Omega) m(^{-1})</td>
</tr>
<tr>
<td>emissivity</td>
<td>( \varepsilon )</td>
<td>0.4</td>
</tr>
<tr>
<td>function of entropy of segregation</td>
<td>( k_1 )</td>
<td>( 3.18 \times 10^3 )</td>
</tr>
<tr>
<td>gas constant</td>
<td>( R )</td>
<td>8314.3 J/kg-mole</td>
</tr>
<tr>
<td>heat capacity (steel)</td>
<td>( C_p )</td>
<td>753 J/kg-K</td>
</tr>
<tr>
<td>latent heat of fusion (steel)</td>
<td>( \Delta H )</td>
<td>( 2.47 \times 10^3 ) J/kg</td>
</tr>
<tr>
<td>latent heat of vaporization (Fe)</td>
<td>( \Delta H_{Fe} )</td>
<td>( 6.091 \times 10^3 ) J/kg</td>
</tr>
<tr>
<td>latent heat of vaporization (Mn)</td>
<td>( \Delta H_{Mn} )</td>
<td>( 4.0135 \times 10^3 ) J/kg</td>
</tr>
<tr>
<td>liquidus temperature (steel)</td>
<td>( T_{liq} )</td>
<td>1523 K</td>
</tr>
<tr>
<td>melting point (Ar)</td>
<td>( T_{mp}(\Delta r) )</td>
<td>87.2 K</td>
</tr>
<tr>
<td>melting point (Fe)</td>
<td>( T_{mp}(Fe) )</td>
<td>1809 K</td>
</tr>
<tr>
<td>melting point (Mn)</td>
<td>( T_{mp}(Mn) )</td>
<td>1518 K</td>
</tr>
<tr>
<td>permeability of free space</td>
<td>( \mu_o )</td>
<td>( 1.26 \times 10^{-6} ) H/m</td>
</tr>
<tr>
<td>plate thickness</td>
<td>( L_z )</td>
<td>12.5 mm</td>
</tr>
<tr>
<td>plate radius</td>
<td>( L_r )</td>
<td>20 mm</td>
</tr>
<tr>
<td>reference temperature for Table 16</td>
<td>( T_{ref} )</td>
<td>1863 K</td>
</tr>
<tr>
<td>solidus temperature (steel)</td>
<td>( T_{sol} )</td>
<td>1723 K</td>
</tr>
<tr>
<td>standard heat of adsorption</td>
<td>( \Delta H^s )</td>
<td>( -1.88 \times 10^8 ) J/kg-mole</td>
</tr>
<tr>
<td>Stefan-Boltzmann constant</td>
<td>( \sigma_b )</td>
<td>( 5.67 \times 10^8 ) W/m(^2)K(^{-1})</td>
</tr>
<tr>
<td>surface excess at saturation</td>
<td>( \Gamma_s )</td>
<td>( 1.3 \times 10^8 ) J/(kg-mole) m(^2)</td>
</tr>
<tr>
<td>thermal conductivity (liquid steel)</td>
<td>( k_{liq} )</td>
<td>20 W/m-K</td>
</tr>
<tr>
<td>thermal conductivity (solid steel)</td>
<td>( k_{sol} )</td>
<td>20 W/m-K</td>
</tr>
<tr>
<td>viscosity</td>
<td>( \mu )</td>
<td>0.006 kg/m-s</td>
</tr>
</tbody>
</table>

Table 15. Material properties and workpiece information of AISI 304 [29,30,56,63,69,121-123].
<table>
<thead>
<tr>
<th>Mole Fraction $X_{Mn}$</th>
<th>Activity $a_{Mn}$</th>
<th>Partial Excess Free Energy $\frac{\Delta G^{xs}}{Mn} \text{ (cal/mole)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>1050</td>
</tr>
<tr>
<td>0.1</td>
<td>0.126</td>
<td>851</td>
</tr>
<tr>
<td>0.2</td>
<td>0.240</td>
<td>672</td>
</tr>
</tbody>
</table>

\[ \log_{10} P_{Mn}^o \text{ (mm Hg)} = \frac{-14520}{T} - 3.02 \log_{10} T + 19.24 \]

<table>
<thead>
<tr>
<th>Mole Fraction $X_{Fe}$</th>
<th>Activity $a_{Fe}$</th>
<th>Partial Excess Free Energy $\frac{\Delta G^{xs}}{Fe} \text{ (cal/mole)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>1050</td>
</tr>
<tr>
<td>0.1</td>
<td>0.126</td>
<td>851</td>
</tr>
<tr>
<td>0.2</td>
<td>0.240</td>
<td>672</td>
</tr>
<tr>
<td>0.3</td>
<td>0.345</td>
<td>515</td>
</tr>
<tr>
<td>0.4</td>
<td>0.443</td>
<td>378</td>
</tr>
<tr>
<td>0.5</td>
<td>0.537</td>
<td>263</td>
</tr>
<tr>
<td>0.6</td>
<td>0.628</td>
<td>168</td>
</tr>
<tr>
<td>0.7</td>
<td>0.718</td>
<td>95</td>
</tr>
<tr>
<td>0.8</td>
<td>0.809</td>
<td>42</td>
</tr>
<tr>
<td>0.9</td>
<td>0.902</td>
<td>11</td>
</tr>
<tr>
<td>1.0</td>
<td>1.000</td>
<td>0</td>
</tr>
</tbody>
</table>

\[ \log_{10} P_{Fe}^o \text{ (mm Hg)} = \frac{-19710}{T} - 1.27 \log_{10} T + 13.27 \]

Table 16. Thermodynamic properties of Mn and Fe used in calculating surface temperature [121,122].

The advantage of this method is that the treatment is very simple; requiring a simple analytical expression for the rate of mass loss. One assumption that is frequently invoked in this step is that the partial pressure of the gaseous species is in equilibrium with the free surface temperature. This assumption is routinely employed in surface kinetics.

After vaporizing from the anode surface, the gaseous species must diffuse through the anode solute boundary layer. The concentration profile of this gaseous species is shown in Fig. 35 which indicates that as we move away from the free surface, the concentration gradient decreases and thus the mass flux decreases. In order to obtain a rigorous account of the mass flux, the concentration profile in this boundary layer must be solved. Instead, a simpler approach is taken.
whereby the mass flux is approximated by a mass transfer coefficient analogous to the heat transfer coefficient in convective heat transfer from a solid surface. This treatment should provide a second* order estimate of the mass diffusion rates and thus heat losses from the free surface.

It can be deduced that step (iii) is most rate-limiting. In order to account for both Langmuir vaporization and mass diffusion across the solute boundary layer, a mixed control vaporization model similar to a parallel circuit is employed:

$$\frac{1}{h_{\text{m(ef)}}} = \frac{1}{h_{\text{vap}}} + \frac{1}{h_{\text{mass}}} \quad (27)$$

such that $h_{\text{m(ef)}}$ is the effective mass transfer coefficient. The rate of mass loss from the surface due to the species $i$ is then given as:

$$m_{i} = h_{\text{m(ef)},i} \Delta C_{i} = h_{\text{m(ef)},i} [C_{i}^{s} - C_{i}^{\infty}] \quad (28)$$

and the corresponding rate of heat loss due to vaporization is:

$$q_{\text{vap},i} = m_{i} L_{\text{vap},i} \quad (29)$$

In eqn. (28), the concentration of species $i$ in the bulk is assumed zero such that $C_{i}^{\infty} \to 0$. In addition, since it is previously assumed that the partial pressure of the vapor species is in equilibrium with the surface temperature, the concentration of species $i$ at the free surface, $C_{i}^{s}$, can be related to its partial pressure by the ideal gas law such that $P_{i} = C_{i}^{s} RT_{s}$. Therefore, eqn. (29) is re-written as:

$$q_{\text{vap},i} = \frac{h_{\text{m(ef)},i} L_{\text{vap},i} P_{i}}{R T_{s}} \quad (30)$$

The two unknowns in eqn. (30) are the effective mass transfer coefficient, $h_{\text{m(ef)},i}$, and the partial pressure of the vapor species $i$, $P_{i}$. These will be derived below in Sections 4.2.1-4.2.3.

Experimental studies by Block-Bolten and Eagar [101,102] indicated that the two dominant vapor species in the gas tungsten arc welding of steel are Fe and Mn. Only these two elements will be considered in the vaporization analysis. Fe and Mn are dominant because of their high vapor pressures. The discussion that follows will consider Mn as the vapor species although it is implicit that similar treatment is given to Fe. Thus, the net heat loss due to vaporization is given as:

$$q_{\text{vap,tot}} = q_{\text{vap,Fe}} + q_{\text{vap,Mn}} \quad (31)$$

* Zero order - assume a "cut-off" peak surface temperature. First order - assume Langmuir kinetics.
4.2.1 Derivation of the Mass Transfer Coefficient Due to Langmuir Vaporization

Langmuir vaporization [124] is given by:

\[ m_{\text{L,Mn}} = \frac{\alpha_s M_{\text{Mn}} P_{\text{Mn}}}{\sqrt{2 \pi M_{\text{Mn}} R T_s}} \text{ kg/m}^2\text{s} \tag{32} \]

When vaporizing into a vacuum, \( h_{\text{mass}} \) is very large because the gaseous species will travel very fast when they escape from the surface; thus \( h_{\text{m(eff)}} \) equals \( h_{\text{vap}} \) from eqn. (27). \( h_{\text{vap}} \) is obtained from eqn. (32) by assuming \( P_{\text{Mn}} = C_{\text{Mn}}^s R T_s \) at the pool surface and \( C_{\text{Mn}}^s = 0 \) in the bulk of the shielding gas:

\[ h_{\text{vap}} = h_{\text{L,vap}} = \frac{\alpha_s R T_s}{\sqrt{2 \pi M_{\text{Mn}} R T_s}} \tag{33} \]

In this study, the sticking coefficient, \( \alpha_s \), is assumed to be unity. If \( \alpha_s \neq 1 \), then we have Knudsen effusion [124].

A similar treatment for vaporizing a gaseous species into a vacuum environment using the kinetic theory of gases is given by [101,102,125]:

\[ m_{\text{k,Mn}} = 443.31 P_{\text{Mn}} \sqrt{M_{\text{(Mn)}} / T_s} \text{ kg/m}^2\text{s} \tag{34} \]

where \( P_{\text{Mn}} \) is the partial pressure in atmosphere and \( M_{\text{(Mn)}} \) is the atomic weight in g/mole. Both eqns. (32) and (34) give identical results.

4.2.2 Derivation of the Mass Transfer Coefficient Due to Mass Diffusion

In the normal case of welding in an argon environment, the mass transfer coefficient, \( h_{\text{mass}} \), must be calculated from the Sherwood number or from an analogous empirical correlation derived for the system concerned. McKelliget and Szekely [80] employed a convection correlation for stagnation point flow over a flat surface as given by:

\[ \frac{N_{\text{uw}}}{{\sqrt{Re_w}}} = 0.515 \left( \frac{h_{\text{ef}}}{\mu_{\text{w}} \rho_{\text{w}}} \right)^{0.11} \tag{35} \]

\[ Q_{a,\text{conv}} = \left( \frac{N_{\text{uw}}}{{\sqrt{Re_w}}} \right) \left( h_{\text{e}} - h_{\text{w}} \right) \frac{\rho_{\text{w}}}{Pr_{\text{w}}} \sqrt{ \mu_{\text{w}} \rho_{\text{w}} \frac{\partial u_e}{\partial r} } \tag{36} \]

\( u_e \) is the plasma velocity taken at the edge of the anode boundary layer. Numerically, this correspond to the first node (~ 0.1 mm) above the anode surface for the welding arc model. Equations (35) and (36) were originally obtained from a heat transfer correlation for jet flow from a rocket.
nozzle impinging onto a flat surface [126]. There is a 16% error associated with these correlations. Re-writing eqns. (35) and (36) and modifying \( \partial u_e / \partial r \) [84]:

\[
q_{\text{conv}} = 0.515 \left( \frac{\mu_e \rho_e}{\mu_w \rho_w} \right)^{0.11} \sqrt{\mu_w \rho_w} u_e \left[ \frac{C_p}{Pr_w} \right] [T_e - T_w] \tag{37}
\]

where \( \overline{C_p} \) is the integral mean heat capacity given by:

\[
\overline{C_p} = \frac{1}{T_e - T_w} \int_{T_w}^{T_e} C_p \, dT \tag{38}
\]

The integral mean quantity is employed due to the large variations in the physical properties, such as thermal conductivity, in the plasma for the temperature concern. In addition, previous studies [127,128] have indicated that this method of obtaining the physical property is a better approximation than just taking the property value at that temperature.

Equation (37) can be written as \( q = h_{\text{heat}} \Delta T \), thus:

\[
h_{\text{heat}} = 0.515 \left( \frac{\mu_e \rho_e}{\mu_w \rho_w} \right)^{0.11} \sqrt{\mu_w \rho_w} u_e \left[ \frac{C_p}{Pr_w} \right] \tag{39}
\]

where \( h_{\text{heat}} \) is the heat transfer coefficient. Using a mass transfer-heat transfer analogy, the mass transfer coefficient can be related to the heat transfer coefficient by:

\[
\frac{h_{\text{heat}}}{h_{\text{mass}}} = \left[ \rho C_p \frac{Sc}{Pr} \right]^{n_{Le}} \tag{40}
\]

where

\[
Pr, \text{ Prandtl Number} \quad = \quad \frac{C_p \mu}{k} \tag{41}
\]

\[
Pr_w, \text{ Prandtl Number at anode wall} \quad = \quad \left[ \frac{C_p \mu \Delta T}{k} \right]_{\text{wall}} \tag{42}
\]

\[
Sc, \text{ Schmidt Number} \quad = \quad \frac{v}{D_{\text{Mn-Ar}}} \tag{43}
\]

and \( n_{Le} \) is between 0 and 1. For a flat surface, \( n_{Le} \approx 0.6 \) [129]. In any case, the term in brackets in eqn. (40), also known as the Lewis number, is very close to unity for argon gas and the effect of the exponent is less than 5% for \( n_{Le}=0.5 \) and \( n_{Le}=0.6 \). The terms at the right side of eqn. (40) with the overstrike symbol are evaluated at the mean integral quantities similar to the expression given in eqn. (38). The subscript "w" indicates properties evaluated at the wall temperature while the rest (both subscript "e" and unsubscript) are evaluated at the edge of the anode boundary layer.
The diffusivity in the Schmidt number is calculated from the Chapman-Enskog relationship [130]:

\[
D_{Mn-Ar} = 1.8583 \times 10^{-3} \left[ T_s^3 \left( \frac{1}{M_{(Mn)}} + \frac{1}{M_{(Ar)}} \right) \right] \frac{P_{atm}^2}{\sigma_{Mn-Ar} \Omega_{Mn-Ar}} \text{ cm}^2/\text{s} \tag{44}
\]

where

\[
\varepsilon_{Mn-Ar} = \sqrt{\varepsilon_{Mn} \varepsilon_{Ar}} \tag{45a}
\]
\[
\sigma_{Mn-Ar} = 0.5(\sigma_{Mn} + \sigma_{Ar}) \tag{45b}
\]

\(P_{atm}\) is assumed to be 1 atmosphere since the anode plasma over-pressure as calculated in Chapter 2 (Fig. 16(c)) is of the order of 0.01 atm. The \(\varepsilon\)'s and \(\sigma\)'s in eqns. 45 (a-b) are estimated at their melting points for the metallic species:

\[
\frac{\varepsilon_{Mn}}{k_b} = 1.92 \frac{T_{mp(Mn)}}{k_b} \tag{45c}
\]
\[
\sigma_{Mn} = 1.222 V_{Mn,soln}^{1/3} \tag{45d}
\]
\[
V_{Mn,soln} = \frac{M_{(Mn)}}{\rho_{(Mn)}} \tag{45e}
\]
\[
\Omega_{Mn-Ar} = \Omega \left( \frac{T}{\varepsilon_{Mn-Ar}/k_b} \right) \tag{45f}
\]

while the values for argon gas are estimated at the boiling point by:

\[
\frac{\varepsilon_{Ar}}{k_b} = 1.15 \frac{T_{bp(Ar)}}{k_b} \tag{45g}
\]
\[
\sigma_{Ar} = 1.166 V_{Ar,liq}^{1/3} \tag{45h}
\]
\[
V_{Ar,liq} = \frac{M_{(Ar)}}{\rho_{bp(Ar)}} \tag{45i}
\]

The values for the \(\Omega\) function in eqn. (44) are obtained from Bird et al [131]. This completes the information for calculating \(h_{m(\text{eff}),l}\) via eqns. (27), (33), and (38-45).

### 4.2.3 Derivation of the Partial Pressure of the Vapor Species

The equilibrium partial pressure of a pure gaseous species can be obtained from published literature [132]. However, because most workpiece are generally alloys such as steel, the treatment is slightly modified. We assume the molten pool to be a binary solution. This is because a) the treatment is substantially easier for binary solutions, and b) thermodynamic data for binary
solutions are more readily available [122]. Using the method similar to that developed by Block-Bolten and Eagar [101,102], the partial pressure of Mn is given by:

\[ P_{Mn} = a_{Mn} P^o_{Mn} \]  \hspace{1cm} (46)

\[ \Rightarrow \log P_{Mn(T_s)} = \log a_{Mn(T_s)} + \log P^o_{Mn} \]  \hspace{1cm} (47)

The vapor pressure of pure Mn is obtained from published data [132] as:

\[ \log_{10} P^o_{Mn} \text{ (mm Hg)} = \frac{-14.520}{T_s} - 3.02 \log T_s + 19.24 \]  \hspace{1cm} (48)

Similarly for pure Fe:

\[ \log_{10} P^o_{Fe} \text{ (mm Hg)} = \frac{-19.710}{T_s} - 1.27 \log T_s + 13.27 \]  \hspace{1cm} (49)

In order to obtain \( P_{Mn} \) at any temperature \( T_s \), the activity at that temperature must be known. In general, the tabulated results [122] normally provide the activity of the binary alloy at some reference temperature, \( T_{ref} \). The activity of Mn at temperature \( T_s \) can then be calculated using the Gibbs-Helmholtz relationship [133] where:

\[ \log a_{Mn(T_s)} = \log a_{Mn(T_{ref})} + \frac{\overline{G^s}_{Mn}}{4.575} \left( \frac{1}{T_s} - \frac{1}{T_{ref}} \right) \]  \hspace{1cm} (50)

The thermodynamic data for \( a_{Mn(T_{ref})} \) and \( \overline{G^s}_{Mn} \) are given by Hultgren et al [122]. Incidentally, the binary solution is assumed to be regular such that \( \overline{G^s}_{Mn} = \overline{\Delta H}_{mix,Mn} \) and is independent of temperature. This assumption is generally valid for steel. This completes the information for calculating \( P_i \) via eqns. (47), (48), and (50).

4.3 Trends in Vaporization Rates

It is useful to develop some trends on the vaporization rates on the basis of the principles established above. This will provide some guiding principles in predicting the type of weld pool behavior one may obtain.

4.3.1 Effect of Langmuir Vaporization

A plot of the mass transfer coefficient due to the Langmuir vaporization model (or Langmuir transfer coefficient) is shown in Fig. 36 (a) while the corresponding heat loss is given in Fig. 36 (b).
Figure 36. Plot of (a) mass transfer coefficient and (b) heat loss from the free surface as a function of surface temperature due to Langmuir vaporization. The heat loss, $q_{LJ}$ is calculated via eqns. (30–47) while $q_{LJtot}$ is given by eqn. (31).
In this instance, $h_{L,i}$ is calculated from eqn. (33). The plot of Langmuir transfer coefficient for Fe, $h_{L,Fe}$, is almost identical to Mn since the atomic mass of Fe is very close to that of Mn. Also, note that at $T \leq 2,800$ K, the heat loss due to Langmuir vaporization for Fe, $q_{L,Fe}$, is less than $q_{L,Mn}$ but at $T \geq 2,800$ K, $q_{L,Fe}$, tends to be larger because of the higher Fe vapor pressure. Incidentally, pure Fe boils at 3,273 K while pure Mn boils at 2,423 K; thus the mass transfer coefficient and heat loss rates shown are extrapolated. It is can be seen that $h_{L,i}$ is of the order of 250 m/s.

To provide proper perspective of the nature of the weld pool surface temperature, a 100 A arc generally produce a peak heat flux of the order of 100 W/mm$^2$. Thus, on the basis of Langmuir vaporization in the absence of weld pool convection, the peak surface temperature will be of the order of 3,000 K. Naturally, with weld pool convection, the peak surface temperature is much lower since convection can remove part of the thermal energy from the free surface.

4.3.2 Effect of Mixed Control Vaporization

In order to illustrate the effect of mixed control vaporization, the temperature and velocity of the plasma gas at the anode boundary layer must be known. These are obtained from Figs. 34 (a-b). Furthermore, since the effective mass transfer coefficient is also spatially dependant due to the spatial dependance of plasma temperature and velocity at the anode boundary layer, only the peak values of $h_{m(ef)}$ versus surface temperature will be plotted. Figures 37 (a-b) show the effective peak mass transfer coefficient and the corresponding heat loss from the anode as a function of surface temperature. $h_{m(ef),Mn}$ is not shown since it virtually superimpose on $h_{m(ef),Fe}$. The reason for this is due to the close proximity of their atomic weights.

It is observed that $h_{m(ef)}$ is of the order of 16 m/s which is about 1/16 that due to Langmuir vaporization (Fig. 36 (a)). This is also reflected in the rate of heat loss (Fig. 37 (b)) where mixed control vaporization is predicting a much lower heat loss rate than Langmuir vaporization. This suggests that the weld pool surface will have an even higher peak temperature than that due to Langmuir alone since less heat will be vaporized by the mixed control model. Certainly, this is not realistic as it has been shown above that Langmuir vaporization alone already predicts a peak
Figure 37. Plot of (a) effective mass transfer coefficient and (b) heat loss from the free surface as a function of surface temperature due to mixed control vaporization. The slight “kink” in $h_{m(\text{eff})}$ around 3,000 K is due to the evaluation of the physical properties in the plasma using the integral mean method, in particular $\rho_{\text{Ar}}$ which changes slope at 3,000 K. $q_{\text{vap},i}$ is calculated via eqns. (27,30,40,47). $h_{m(\text{eff}),\text{Mn}}$ essentially superimpose onto $h_{m(\text{eff}),\text{Fe}}$ and thus is not shown.
surface temperature of 3,000 K which is very close to the boiling point of steel, in general. Thus, there must be another mechanism that controls the surface temperature.

This mechanism is the convective heat flow in the weld pool as governed by Marangoni shear. It can be deduced that the higher the surface velocity, the lower will be the surface temperature since the fluid is convecting thermal energy away from the surface at a faster rate. In this sense, the phenomenon becomes highly coupled as the surface temperature distribution governs Marangoni flow and this in turn governs the surface temperature by the strength of the surface velocity. It is thus a logical extension to examine the nature of the surface tension driven flows in greater detail.

4.4 Effect of Surface Tension Coefficient

Surface tension can be loosely defined as a measure of the strength of the bond between 2 atoms at the free surface. For most pure species, surface tension decreases as temperature increases since at a higher temperature, the bonds are weaken due to the higher thermal and kinetic energies. At the boiling point, the surface tension essentially goes to zero since these bonds are broken. Thus, the surface tension coefficient, $\gamma/\partial T$, is seen to be negative.

The presence of surface active elements such as oxygen and sulphur can produce the opposite effect for the surface tension dependance on temperature. In this instance, these elements strengthen the surface bonds between the atoms as the temperature increases. It is believed that this strengthening of bonds is due to segregation effect [7]. The net effect is that $\gamma/\partial T$ will have a positive value due to these surface active elements.

Physically, the surface tension cannot increase indefinitely since at the boiling point, the surface tension must be zero. Thus, there exists a temperature range where the surface tension must decrease with increasing temperature. This implies that there is also a temperature where $\gamma/\partial T$ is zero. For discussion purposes, the temperature where $\gamma/\partial T=0$ is referred to as the surface tension turning point temperature. The main observation is that $\gamma/\partial T$ can change from a positive value to
a negative value, that is, the weld pool fluid flow changes direction depending upon the surface temperature.

Marangoni shear has been identified as the most dominant driving force in the weld pool and so the effect of this flow reversal has a profound effect on the pool shape [63,64]. Although this surface tension phenomenon is well understood, it is quite difficult to quantify. Thus, the early mathematical models of weld pool modelling assumed a constant $\gamma \frac{\partial T}{\partial T}$ of the order of $10^4$ N/m-K. Sahoo et al. [69] were the first to develop a semi-empirical relationship between surface tension, temperature, and concentration of the surface active elements. Most of their analyses were for binary alloys and the calculated values compare very well with experimental results. Their expression for sulphur as the surface active element is given as [69]:

$$\frac{\partial \gamma}{\partial T} = -A - R_g \Gamma_s \ln(1 + K_{seg} a_s) - \frac{K_{seg} a_s}{(1 + K_{seg} a_s)} \frac{\Gamma_s \Delta H^o}{T}$$

(51)

where $K_{seg} = k_1 \exp\left(-\frac{\Delta H^o}{R_g T}\right)$

(52)

and

- $A$ = constant in surface tension coefficient $4.3 \times 10^4$ N/m-K
- $R_g$ = gas constant $8314.3$ J/kg-mole-K
- $\Gamma_s$ = surface excess at saturation $1.3 \times 10^{-8}$ kg/(kg-mole)-m²
- $K_{seg}$ = equilibrium constant for segregation (eqn. 52)
- $a_s$ = activity of sulphur (~ wt-% S) 0.022
- $\Delta H^o$ = standard heat of adsorption $-1.88 \times 10^8$ J/kg-mole
- $k_1$ = function of entropy of segregation $3.18 \times 10^3$
- $\gamma$ = surface tension (N/m)
- $T$ = temperature (K)

This formula is derived from a combination of Gibbs and Langmuir adsorption isotherms. Sahoo et al [69] concluded that $\partial \gamma / \partial T$ is strongly influenced by the heat of adsorption, $\Delta H^o$. It is clear from eqn. (52) that $\partial \gamma / \partial T$ is most sensitive to $\Delta H^o$ particularly because it has an exponential dependence. $\Delta H^o$ is estimated from an empirical function of the difference in electronegativity between the solute and solvent ions. For an Fe-S binary alloy, $\Delta H^o$ is estimated to be $-1.66 \times 10^8$ J/kg-mole. $\Delta H^o$ for AISI 304 is not so easily estimated since there are multiple surface active components
(P and S) present as evident by Table 14. Zacharia et al [63] employed a value of $-1.88\times10^8$ J/kg-mole for AISI 304 and it seemed to work quite well.

4.5 Trends in Surface Tension Coefficient

The effect of $\partial \gamma / \partial T$ changing from a positive value to a negative value on increasing temperature in weld pool modelling was first examined by Zacharia et al [63,94]. They obtained very good agreement between calculated* and experimental results. Figure 38 (a) shows a plot of the sensitivity of $\partial \gamma / \partial T$ vs T due to different heats of adsorption, $\Delta H^*$, for 0.022 wt-% S in AISI 304. The reference $\Delta H^*$ value for stainless steel is taken as $-1.88\times10^8$ J/kg-mole [63]. It is clear that a 10% change in $\Delta H^*$ can result in a rather large change in the temperature where $\partial \gamma / \partial T=0$. The fact of the matter is $\Delta H^*$ which is estimated from the difference in the electronegativities between the solute and solvent atoms has a certain uncertainty associated with it. From the analyses of Sahoo et al [69], this uncertainty is estimated to be about 10% for the FeS binary alloy. $\Delta H^*$ for FeS† is $-1.66\times10^8 \pm 0.21\times10^8$ J/kg-mole. Zacharia et al [63] selected $-1.88\times10^8$ J/kg-mole for stainless steel which is within the range of the experimental error for FeS. Presumably, there are other surface active elements present, such as phosphorus and perhaps oxygen from the gas entrainment, that can alter the $\Delta H^*$ value; the effect of these multiple elements are unclear. Despite the uncertainty associated with $\Delta H^*$, this semi-empirical relationship is perhaps the best description available for predicting $\partial \gamma / \partial T$ as a function of surface active element composition and temperature.

The effect of sulphur concentration on $\partial \gamma / \partial T$ is shown in Fig. 38 (b). It is noted that a 20% variation in the sulphur content using 0.022 wt-% S as the reference produce only a small change (~1%) in the surface tension turning point temperature. Clearly, small changes in the workpiece

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* One of the problems with their calculations is their choice of the effective thermal conductivity and effective viscosity which are both 10 times the laminar values. This is physically incorrect since it will result in the laminar Prandtl number being equal to the turbulent Prandtl number. Their laminar Prandtl number is estimated to be about 0.24.
† FeS is the stable compound in the temperature range examined [7].
Figure 38. Surface tension coefficient dependance on temperature using Sahoo et al's [69] expression. 
a) \( \frac{\partial \gamma}{\partial T} \) due to different heats of adsorption, \( \Delta H^* \)  
b) \( \frac{\partial \gamma}{\partial T} \) due to different sulphur contents  
+10\% refers to 1.1 times the reference value while -10\% refers to 0.9 times the reference value.
composition due to different batches or samples play a relatively minor role in affecting the $\partial \gamma / \partial T$ distribution.

Although small changes in sulphur concentration results in small changes in $\partial \gamma / \partial T$, however, the variation is much larger in practice due to different heats†. In the production of stainless steels, one of the main goal is to keep the Cr content at the specified level since Cr tends to oxidize with respect to Fe. However, the sulphur content can vary considerably with a maximum of about 0.03 wt-% S depending on the specification. In one study of SS 316L steels by Kraus [30], the sulphur content changed by an order of magnitude from 0.001 wt-% to 0.013 wt-% due to different heats. From Fig. 38 (b), the variation from 0.022 wt-% to 0.002 wt-% results in a 400 K drop in the temperature where $\partial \gamma / \partial T$ is zero. This can result in a substantial change in the weld pool shape since it is very easy to heat the pool to above 2,000 K. The main observation is that it seems that the precise workpiece composition is critical in determining the Marangoni shear although small variations in composition are not critical. The effect of 0.200 wt-% S is also shown in Fig. 38 (b) primarily to indicate the trend for $\partial \gamma / \partial T$ although it is understood that such high sulphur content does not exist for stainless steels.

Thus, it can be summarized that the precise concentration of the surface active element plays a rather large role in affecting the weld pool shape. Its main influence is through the temperature where $\partial \gamma / \partial T=0$; the effect of which will be discussed later in this chapter (Section 4.7.5). Although this is well known in the welding community, the ability to quantify it more precisely has generally been a more complex task until the studies of Sahoo et al [69].

† In metallurgical terminology, heats refer to the different batches of steel produced during the smelting process due to different furnace conditions. In general, no two heats are completely identical.
4.6 Role of Gas Shear Stress

4.6.1 Background Information

From Fig. 33 given in Section 4.1, the various driving forces for the weld pool have been identified as buoyancy, electromagnetic, surface tension, and gas shear stress. Of the four forces, the first three have been treated very extensively in the literature [13,4,46,47,56-58,63,64]. The reason is that these three forces can be calculated quite independently of the welding arc. In order to consider the fourth driving force, the welding arc must be simulated to obtain the gas shear. In addition, the coupling of the welding arc with the weld pool has only been carried out recently [19]. Virtually all previous modelling efforts model the weld pool independently of the arc.

The role gas shear stress plays at the free surface is actually quite complex. Most models assume that the momentum transferred by the plasma jet to the weld pool is negligible due to the small value of the argon gas viscosity relative to the liquid metal. However, if magnitude of the gas shear stress approaches that of the Marangoni shear in the weld pool, then the effect of the gas shear can be important. This section examines the role of gas shear on Marangoni flows for planar weld pool surfaces.

There is a more subtle role that the gas shear plays and that is the gas shear may be responsible for surface instabilities such as waves and ripples. It is well known that when two fluids of different viscosities flow parallel to each other in the same direction, Kelvin-Helmholtz instabilities can form due to the mismatch in velocities at the interface [86,134]. In this instance, perturbations in the free surface can result in waves that either grow and produce spray formation or damp out and oscillate. In the extreme situation, these phenomena are suspected to be responsible for the onset of deep penetrations found in high arc currents [5]. At low currents, surface oscillations are common [16].

In this thesis, we shall be primarily concerned with low current welding operations. The free surface is assumed planar in order to examine the effect of the gas shear on the surface velocity and surface temperature of the weld pool. It is felt that by first addressing a planar surface, this will provide insights into the more complex problem of deformable free surfaces. Although it is
known that at high current (> 260 A), the free surface deforms, the effect of high arc currents is examined in a theoretical manner using a planar surface in the light of whether its role is important in affecting weld pool flow profile. The dynamic coupling of the welding arc and the weld pool with a deformable free surface for representing surface fluctuations is a complex moving boundary problem that is beyond the scope of this thesis. Nevertheless, it represents a challenging problem that needs to be addressed.

Some studies of the effect of gas shear on the weld pool have been carried out by Matsunawa and Yokoya [135] who defined it as aerodynamic drag. Their analyses involved the modelling of an isothermal arc with a uniform heat and current fluxes at the weld pool surface. The arc is uncoupled from the weld pool. They concluded that the electromagnetic force is the more dominant driving force for short arcs (~ 2 mm) while aerodynamic drag is more dominant for long arcs (~ 8 mm). These results seemed to be in disagreement with the findings of other investigators which identified surface tension as the most dominant driving force [3,4,63,64]. In addition, at longer arc lengths, the actual drag should be reduced relative to a short arc since the arc is now less intense (Fig. 21 (c)).

The importance of the gas shear stress in affecting the weld pool surface temperature and penetration profile is emphasized. The primary objective is to determine whether is it valid to neglect the gas shear stress from the weld pool model.

4.6.2 Mathematical Formulation of the Shear Stress Boundary Condition

In the welding arc domain, the plasma shear stress at the anode is defined as:

\[ \tau_{\text{gas}} = -\mu_{\text{gas}} \left( \frac{\partial u}{\partial z} \right)_{\text{gas}} \] (53)

In the weld pool domain, the surface tension shear stress or Marangoni shear is defined as:

\[
* \text{In the analysis of the trends of the gas shear stress with arc length, it was found that the peak gas shear stress first increases as the arc length increases from a short arc length (~1.5mm) and then it decreases as the arc length continues to increase to 13.2 mm. The turning point appears to be in the vicinity of 2-3 mm.}
\[ \tau_{s.t.} = \left( \frac{\partial \gamma}{\partial T} \right) \left( \frac{\partial T}{\partial r} \right) \]  

(54)

while the liquid shear stress is defined as:

\[ \tau_{\text{liq}} = -\mu_{\text{liq}} \left( \frac{\partial u}{\partial z} \right)_{\text{liq}} \]  

(55)

For isothermal systems, the momentum transferred by the gas jet to the free surface is given as:

\[ \tau_{\text{gas}} = \tau_{\text{liq}} \]  

(56)

\[ -\mu_{\text{gas}} \left( \frac{\partial u}{\partial z} \right)_{\text{gas}} = -\mu_{\text{liq}} \left( \frac{\partial u}{\partial z} \right)_{\text{liq}} \]  

(57)

Usually, \( \mu_{\text{gas}} \ll \mu_{\text{liq}} \) and so free slip is assumed at the surface:

\[ \left( \frac{\partial u}{\partial z} \right)_{\text{liq}} = 0 \]  

(58)

If thermal gradients exist in the weld pool, then:

\[ \tau_{\text{gas}} = \tau_{\text{s.t.}} + \tau_{\text{liq}} \]  

(59)

In most modelling studies of the weld pool, \( \tau_{\text{gas}} \) is ignored on the assumption that \( \tau_{\text{gas}} \) is negligible compared to the surface tension shear stress. Thus:

\[ \mu_{\text{liq}} \left( \frac{\partial u}{\partial z} \right)_{\text{liq}} = -\tau_{\text{s.t.}} \]  

(60)

\[ \mu_{\text{liq}} \left( \frac{\partial u}{\partial z} \right)_{\text{liq}} = \left( \frac{\partial \gamma}{\partial T} \right) \left( \frac{\partial T}{\partial r} \right) \]  

(61)

Equation (61) is the surface tension shear stress boundary condition that is employed in previous and in this study. However, if \( \tau_{\text{gas}} \) is of the same order of magnitude as \( \tau_{\text{s.t.}} \), then the assumption of \( \tau_{\text{gas}} \ll \tau_{\text{s.t.}} \) is invalid. Thus, eqn. (59) should be used where:

\[ \left[ \tau_{\text{liq}} \right] = <\text{sign}> \left[ \tau_{\text{s.t.}} \right] - <\text{sign}> \left[ \tau_{\text{gas}} \right] \]  

(62)

\[ \mu_{\text{liq}} \left( \frac{\partial u}{\partial z} \right)_{\text{liq}} = <\text{sign}> \left[ \left( \frac{\partial \gamma}{\partial T} \right) \left( \frac{\partial T}{\partial r} \right) \right] + <\text{sign}> \left[ \mu_{\text{gas}} \left( \frac{\partial u}{\partial z} \right)_{\text{gas}} \right] \]  

(63)

The nature of eqn. (63) is straightforward. However, the sign of each of the terms in eqn. (63) depends on the location of the origin in each of the computational domain. In this case, where the weld pool origin is at the center of the free surface and the welding arc origin is at the cathode tip, both signs on the right of eqn. (63) are positive.

The additional input condition required is the gas shear stress as calculated from eqn. (53).

Note that \( \mu_{\text{gas}} \) is the viscosity of the argon gas which is strongly temperature dependant as seen in
Appendix A. The viscosity is taken for the temperature at the edge of the anode boundary layer. The $\tau_{gss}$ input conditions will be given later in this chapter (Section 4.7.7) along with the computed results.

4.7 Computed Results and Discussion

4.7.1 Preliminaries

All results are for 5.0 s simulation. In general, the pool shape, peak temperature, peak velocity, and weld pool circulation are established very early during the heating cycle; usually within 1.0 s. Beyond 1 second, the weld pool continue to grow in size while the peak temperature and velocity remain unchanged to within 1%. In the results presented below, the maximum velocity refers to the largest vector in the weld pool which need not necessarily be at the free surface. In some instances, the largest velocity vector is located adjacent to the z-axis particularly when the flow is inward towards the pool center such as that due to a positive $\partial \gamma / \partial T$.

Due to the nature of the computational grids employed by PHOENICS, there are no surface nodes. Thus, the surface velocity reported here is located at the first node below the free surface or the computational wall which is 0.0375 mm. In this sense, the experimentally observed surface velocity should be slightly higher. Similarly, the first temperature node below the free surface is located at 0.0375 mm. In order to obtain the actual surface temperature, this value is back-calculated from the first node via the heat flux. In most of the plots for the flow field, only the solidus and liquidus isotherms are shown to indicate the size of the weld bead.

The results presented below represent a parametric study of the various factors that affect and govern the convective flows in the weld pool. In particular, valuable insights can be gained from the trends that develop.

4.7.2 Effect of The Individual Driving Forces on Langmuir Vaporization

In this section, the effect of the individual forces of buoyancy, electromagnetic, and surface tension responsible for fluid flow in the weld pool are examined primarily to compare the nature of
Langmuir versus mixed control vaporization. The surface temperature is allowed to achieve its dynamic state on the basis of the balance of energy between the input heat flux, vaporization losses, and convective heat transfer at the free surface due to Marangoni flows. In this sense, no "cut-off" temperature is invoked and the calculated surface temperature may exceed the boiling point of the workpiece. Although this is physically unrealistic, the prescription of a limiting surface temperature (or static state) is equally unsatisfactory since this may overshadow the strength of Marangoni shear with \( \partial T/\partial r=0 \). By allowing the surface temperature to achieve its dynamic state, the characteristics of the weld pool flow behavior may be better evaluated.

Figures 39 (a-b) show the surface temperature and surface velocity, respectively, due to the three main driving forces found in the weld pool. The positive velocity is for radially outward flow while the negative value is for radially inward flow. The corresponding weld pool shapes and their flow fields are shown in Fig. 40.

From Fig. 34 (a), the peak input heat flux for the 100 A arc is about 105 W/mm\(^2\). Referring to Fig. 36 (b) for Langmuir vaporization, assuming that all the input heat flux goes to vaporizing the pool, then this peak flux will correspond to about 3,000 K peak surface temperature. It can be seen from Fig. 39 (a) that the peak temperature for buoyancy and electromagnetically driven flows is about 2,900 K. The maximum surface velocity for these two forces are 4 mm/s and 7 cm/s, respectively. However, with surface tension driven flow, the peak surface temperature is reduced to about 2,400 K and the maximum surface velocity is about 60 cm/s. It appears that the weld pool must achieve a certain threshold velocity before convective heat transfer due to Marangoni flow is able to significantly reduce the surface temperature below the boiling point. In the case of buoyancy and JxB driven flows, even though the velocity due to JxB is an order of magnitude larger than that due to buoyancy, the convective heat transfer is unable to limit surface temperature. Here, the surface temperature is limited by vaporization.

For the purpose of discussion, the threshold velocity discussed here is defined as the minimum velocity by which the peak surface temperature falls below the boiling point (assumed at 3,000 K) of the workpiece. The reason for this definition is that the surface temperature cannot
Figure 39. Plot of (a) surface temperature and (b) surface velocity using Langmuir vaporization model for the individual driving forces in the weld pool.
Figure 40. Weld pool profile using Langmuir vaporization model for the individual driving forces corresponding to Fig. 39.

a) buoyancy: $u_{\text{max}}=4.1 \text{ mm/s} \ ; T_{\text{max}}=2,891 \text{ K}$

b) electromagnetic: $u_{\text{max}}=6.9 \text{ cm/s} \ ; T_{\text{max}}=2,943 \text{ K}$

c) surface tension: $u_{\text{max}}=69.1 \text{ cm/s} \ ; T_{\text{max}}=2,400 \text{ K}$

The inner line is the liquidus isotherm (1723 K) while the outer line is the solidus isotherm (1523 K) for each plot.
exceed its boiling point. Furthermore, the rate of heat loss increases exponentially as it approaches the boiling point.

As the surface velocity increases beyond the threshold velocity, the convective heat transfer will be the limiting mechanism to surface temperature. In this case, a velocity of the order of 60 cm/s is able to reduce the peak temperature from 2,900 K to 2,400 K (Fig. 39 (a)). This indicates the importance of convective heat transfer due to Marangoni shear. The higher the velocity above this threshold velocity, which will be examined in greater detail in Section 4.7.4, the more critical is convection in controlling peak surface temperature. It can be deduced that if the surface velocity is below this threshold velocity, the surface temperature is limited by vaporization effect. Above this velocity, the surface temperature is limited by convective heat transfer in the weld pool.

The critical implication of this threshold velocity is that by controlling the peak surface temperature, it also controls the nature of the weld pool shape. It has been shown earlier in Fig. 38 that in the presence of $S$, $\partial \gamma / \partial T$ can change from a positive value to a negative value. Thus, if the surface velocity is able to limit the peak surface temperature below the $\gamma$ turning point temperature, then a single flow loop will be produced. Otherwise, two flow loops will be obtained due to both the positive and negative $\partial \gamma / \partial T$'s and the weld pool shape that results is significantly different as will be seen in Section 4.7.5.

4.7.3 Effect of The Individual Driving Forces on Mixed Control Vaporization

Figures 41 and 42 show the computed results using mixed control as the vaporization model. Since the rate of heat loss due to mixed control is less than that due to Langmuir, a higher surface temperature would be predicted. This is indeed observed for buoyancy and electromagnetically driven flows (Fig. 41 (a)) where both peak temperatures are not only greater than the Langmuir model but also greater than the boiling point. Because of the higher surface temperature, and thus more heat input, the weld pools are larger and have higher maximum velocities (Fig. 42 (a-b)) than that due to the Langmuir model (Fig. 40 (a-b)). In both buoyancy and JxB driven flows, it can
Figure 41. Plot of (a) surface temperature and (b) surface velocity using mixed control vaporization model for the individual driving forces in the weld pool.
Figure 42. Weld pool profile using mixed control vaporization model for the individual driving forces corresponding to Fig. 41.

a) buoyancy: \( u_{\text{max}} = 13.1 \text{ mm/s} \); \( T_{\text{max}} = 3,663 \text{ K} \)  
b) electromagnetic: \( u_{\text{max}} = 7.9 \text{ cm/s} \); \( T_{\text{max}} = 3,752 \text{ K} \)  
c) surface tension: \( u_{\text{max}} = 69.2 \text{ cm/s} \); \( T_{\text{max}} = 2,419 \text{ K} \)

The inner line is the liquidus isotherm (1723 K) while the outer line is the solidus isotherm (1523 K) for each plot.
be said that the surface temperature is vaporization limited and that the weld pool velocity is inadequate in convecting away the surface heat.

In contrast, the results of the surface tension driven flow for the two models are identical (Figs. 39 (a-b) and 40 (c) vs Fig. 41 (a-b) and 42 (c)). In this respect, the surface temperature is not limited by vaporization but by convective heat transfer due to Marangoni shears which are identical for the two cases with the same heat input. Thus, the same results are obtained.

This observation has important repercussion in that vaporization models that predict the surface temperature of molten surfaces but do not take into account of the convective flows within the weld pool are liable to over-predict this temperature. In this sense, this is a disadvantage. However, the advantage of this finding is that previous mathematical models which simulate the weld pool but did not account for heat loss due to vaporization is probably not too critically affected. Previous finding (Fig. 37 (b)) showed that the peak heat loss by mixed control vaporization is $\sim 8 \text{ W/mm}^2$ which is only about 8% of the maximum for the 100 A arc. However, a certain threshold surface velocity must be achieved before convection can begin to limit the surface temperature. Thus, the role of surface tension as the most dominant driving force must be examined in greater detail in order to gain insights and understanding of its influences.

Although the above observation seems relatively trivial, its conclusion is only possible when the vaporization kinetics at the weld pool surface are established. Prior models which did not have this capability were not able to arrive at this conclusion.

4.7.4 Effect of Surface Tension Coefficient

In order to examine the nature of the surface velocity in affecting surface temperature, a parametric study using constant $\partial \gamma / \partial T$ rather than the variable $\partial \gamma / \partial T$ given by eqn. (51) is implemented. Figures 43 and 44 show the nature of these positive and negative $\partial \gamma / \partial T$ driven flows. The value of $\partial \gamma / \partial T$ used is $\pm 10^{-5}$, which is an order of magnitude lower than that commonly found in steels [117]. The primary emphasis here is on the nature of the surface temperature distribution due to the reversal in flow direction.
Figure 43. Plot of (a) surface temperature and (b) surface velocity using mixed control vaporization model for $\partial \gamma / \partial T = +10^{-5}$ N/m-K and $\partial \gamma / \partial T = -10^{-5}$ N/m-K.
Figure 44. Weld pool profile and temperature contours due to mixed control vaporization model for $\frac{\partial y}{\partial T} = +10^{-5}$ N/m-K and $\frac{\partial y}{\partial T} = -10^{-5}$ N/m-K corresponding to Fig. 43.

a) $\frac{\partial y}{\partial T} = +10^{-5}$: $u_{max}=18.2$ cm/s  
b) $\frac{\partial y}{\partial T} = +10^{-5}$: $T_{max}=3,331$ K  
c) $\frac{\partial y}{\partial T} = +10^{-5}$: $u_{max}=7.2$ cm/s  
d) $\frac{\partial y}{\partial T} = +10^{-5}$: $T_{max}=3,603$ K
Positive $\partial \gamma / \partial T$ results in an inward flow field (Fig. 44 (a)). When $\partial \gamma / \partial T > 0$, $\gamma$ increase as $T$ increases. Thus, the bond strength increases as $T$ increases. As the weld pool surface is hotter in the center than the edge, there is a spatial variation in bond strength; with the strongest in the middle of the pool. The stronger bonds will cause the fluid to flow towards the center of the pool and thus an inward flow loop results. Naturally, the flow direction reverses if $\partial \gamma / \partial T < 0$.

The surface temperature profile is generally steeper for positive $\partial \gamma / \partial T$ when compared to the negative $\partial \gamma / \partial T$ driven flow (Fig. 43 (a)). This is due to the manner in which the heat is being distributed by the convective loop. In a positive $\partial \gamma / \partial T$ flow, heat is being brought to the center of the workpiece from the surface resulting in a sharper temperature gradient at the free surface. The steeper temperature gradient will result in a stronger Marangoni shear as evident from the higher surface velocities in Fig. 43 (b) for the positive $\partial \gamma / \partial T$. This will cause more thermal energy to be transported away from the free surface into the bulk of the workpiece; as a result, a lower surface temperature distribution is obtained when compared to the negative $\partial \gamma / \partial T$ (Fig. 43 (a)).

In surface tension shear, there are two components in the shear equation (eqn. (54)), namely $\partial \gamma / \partial r$ and $\partial T / \partial r$. In $\partial T / \partial r$, $\partial T$ is more sensitive to variations as there are large temperature changes in the small weld puddle although the relative change in $\partial T / \partial r$ is not as large. In Figs. 43 (a) and (b), the main driving force is $\partial T / \partial r$ as $\partial \gamma / \partial T$ is identical in magnitude. The temperature gradient is sufficient to alter the fluid velocity* such that the positive $\partial \gamma / \partial T$ has a peak surface velocity that is two times greater than that due to a negative $\partial \gamma / \partial T$ (Fig. 43 (b)). However, the surface velocity has probably not reach the threshold velocity yet since the peak temperatures shown in Fig. 43 (a) are greater than 3,000 K. Thus, it is can be said that the heat loss from the free surface where $\partial \gamma / \partial T = \pm 10^{-5}$ N/m-K is vaporization limited.

The weld pool velocity and temperature profiles shown in Figs. 44 (a) and (c), respectively, are quite typical of the flow produced by a positive $\partial \gamma / \partial T$. However, Figs. 44 (b) and (d) are atypical of the negative $\partial \gamma / \partial T$ effect. The two loops are obtained due to a combination of negative

* Actually this is a coupled phenomena as $\partial T / \partial r$ controls the strength of the velocity field which in turn controls the thermal energy transport, and thus the temperature contours.
\[ \partial \gamma / \partial T \] and the Lorentz force. The negative \[ \partial \gamma / \partial T \] produces a counter-clockwise surface loop while the Lorentz force produces clockwise loop in the bulk. This flow profile is captured as a result of the finer grids employed (0.15 mm radial and 0.075 mm axial) since in an earlier study with a rather coarse mesh, the second (Lorentz) loop is not observed. Furthermore, the characteristic velocity in the weld pool in Fig. 44 (b) is about \(7 \text{ cm/s}\). The characteristic velocity due solely to Lorentz forces is also of the same order of magnitude (Fig. 42 (b)). As a result, the Lorentz forces compete with the surface tension forces to drive the flow. In later studies, to be shown immediately below, where \[ \partial \gamma / \partial T \] is of the order of \(10^{-4} \text{ N/m-K}\), the flow due to negative \[ \partial \gamma / \partial T \] overwhelms that due to the Lorentz force resulting in a shallower penetration. However, this second loop is still visible but of much lower velocity (10 times lower).

Extending the analyses to more realistic \[ \partial \gamma / \partial T \]'s, Figs. 45 and 46 represent a parametric study of different but constant \[ \partial \gamma / \partial T \]'s on peak surface temperature, peak surface velocity, and pool size. The nature of the surface temperature distribution, surface velocity distribution, and pool shape are very similar to those shown in Figs. 43-44.

As \( | \partial \gamma / \partial T |^* \) increases, it is seen that the peak surface velocity also increases (Fig. 45 (b)). Correspondingly, the peak surface temperature (Fig. 45 (a)) falls. It appears that Marangoni shear plays a stronger role in limiting surface temperature than that due to vaporization. Furthermore, the threshold velocity when the surface temperature is below 3,000 K is about \(-25 \text{ cm/s}\) for positive \[ \partial \gamma / \partial T \] and \(+20 \text{ cm/s}\) for negative \[ \partial \gamma / \partial T \] (Fig. 45 (a)). The reason for the higher velocity in positive \[ \partial \gamma / \partial T \] is due to the steeper \[ \partial T / \partial r \] in positive \[ \partial \gamma / \partial T \]. In other words, if the surface velocity falls below these quoted values, then the surface temperature will be limited by vaporization as the boiling point will be reached. It is well known that the weld pool never reaches the boiling temperature [136] and so, the controlling mechanism must be surface tension. Besides, \[ \partial \gamma / \partial T \] is generally of the order of \(10^{-4} \) for steel [117], whereas Fig. 45 (a) indicates that \( | \partial \gamma / \partial T |^* \) must be less than \(0.5x10^{-4} \) for the boiling point to be reached. Thus, there are sound qualitative and

---

* Refers to the magnitude of \[ \partial \gamma / \partial T \].
Figure 45. Plot of (a) peak surface temperature and (b) peak surface velocity due to constant $\frac{\partial \gamma}{\partial T}$'s. The filled symbols are for positive $\frac{\partial \gamma}{\partial T}$ while the unfilled ones are for negative $\frac{\partial \gamma}{\partial T}$. 
Figure 46. Plot of (a) weld pool radius and (b) weld pool depth due to constant $\partial \gamma / \partial T$'s. The filled symbols are for positive $\partial \gamma / \partial T$ while the unfilled ones are for negative $\partial \gamma / \partial T$. 
quantitative agreements for the calculated values of surface temperature employing mixed control vaporization.

Figures 46 (a-b) show the resultant pool size due to various values of $\partial y/\partial T$. The trends are well known in that positive $\partial y/\partial T$ will produce a deeper but narrower pool. The reason for this behavior has been explained previously and can be seen directly and qualitatively from the flow fields in Figs. 44 (a-b). Negative $\partial y/\partial T$ shows the opposite behavior in that a shallower but wider pool is observed. The interesting feature in Fig. 46 is that at $\partial y/\partial T = -10^{-5}$, a deeper but narrower pool is obtained relative to those of higher $|\partial y/\partial T|$. The deeper penetration is due to the Lorentz forces which begin to compete with Marangoni forces to drive the fluid into the bulk at that velocity range. This phenomenon has been previously discussed (Fig. 44 (b)).

It appears that at $|\partial y/\partial T|$ larger than $10^{-4}$, the weld pool size (not the shape) is independent of the magnitude of $\partial y/\partial T$. This observation should be qualified by the nature of the boundary conditions imposed. Firstly, the pool can only extend to a certain width from the center since this is dependant upon the nature of the heat source and convective flows in the weld pool. The pool cannot grow beyond this width as the heat from the arc is insufficient to melt it; although the nature of the convective flow can extend the width somewhat. The latter effect is clearly seen in Fig. 44 (b) where the radius of the pool due to a negative $\partial y/\partial T$ is slightly larger than that due to a positive $\partial y/\partial T$ because of the manner the negative $\partial y/\partial T$ distributes its thermal energy. Secondly, the depth can only extend to a finite limit in this case because the sample is assumed to be sitting on a water-cooled plate and a constant boundary condition (15 °C) is imposed at the bottom surface. Naturally, this boundary condition can be modified by means of a heat transfer coefficient for plates exposed to air to investigate the depths of the penetration due to different $\partial y/\partial T$'s.

In order to examine the relative magnitude of $\partial y/\partial T$ and $\partial T/\partial r$, Figs. 47 (a-b) show a plot of the surface temperature as a function of radial position for the various constant $\partial y/\partial T$'s. The general trend is that as $\partial y/\partial T$ increases in magnitude, the temperature distribution decreases. This phenomenon is best explained by the surface tension shear stress which is defined by $\tau_{s} = (\partial y/\partial T) \cdot \partial T/\partial r$. Figure 48 shows a plot of the Marangoni shear corresponding to the temperature
Figure 47. Plot of surface temperature of weld pool as a function of radial position for (a) positive $\partial\gamma/\partial T$ and (b) negative $\partial\gamma/\partial T$ corresponding to those cases examined in Figs. 45 and 46. The data below the liquidus temperature have been truncated.
Figure 48. Plot of surface tension shear stress across the weld pool corresponding to the cases shown in Fig. 47.

$\tau_{sl}$ in the mushy zone ($T_{sol} < T < T_{liq}$), shown by the dashed lines, should be taken as order of magnitude indication as the temperature is strongly dependant upon drag in this zone.
distributions in Fig. 47. It is clear that as the magnitude of $\partial \gamma / \partial T$ increases, $\tau_{s.l.}$ also increases even though $\partial T / \partial r$ appears to be decreasing in Fig. 47. The higher shear stress helps explain the higher surface velocities obtained in Fig. 45 (b). This in turns explain the lower surface temperature distribution in Fig. 47 (a-b) since the higher velocities will convect more thermal energy away from the free surface.

The temperature gradient, $\partial T / \partial r$, alone is not a good measure of $\tau_{s.l.}$ although this information is more readily accessible. Firstly, the cases examined in Fig. 47 all have the same heat input which means that the pool width will be constant. Thus, the peak surface temperature is a direct measure of $\partial T / \partial r$ as it can be seen that the lines in Figs. 47 (a-b) are generally straight. Although as $|\partial \gamma / \partial T|$ increases, $\partial T / \partial r$ decreases, the initial guess is that $\tau_{s.l.}$ will decrease accordingly. However, as Figs. 48 (a-b) clearly shows, this is not the case. The main reason is due to the relative changes in $\partial \gamma / \partial T$ and $\partial T / \partial r$. From $\partial \gamma / \partial T = +1 \times 10^{-4}$ to $\partial \gamma / \partial T = +2 \times 10^{-4}$, the change is a 100% but the corresponding change in $\partial T / \partial r$ are (2678-1700)/2 K/mm and (2519-1700)/2 K/mm. Although the actual temperature drop between $+1 \times 10^{-4}$ N/m-K and $+2 \times 10^{-4}$ N/m-K is almost 160 K, the relative $\partial T / \partial r$ change is only 6%. Thus, temperature gradients should not be used as a direct measure of the strength of Marangoni shear; rather $\tau_{s.l.}$ should be used. This observation is directed at the first order estimates made on the strengths of Marangoni shear.

4.7.5 Effect of Heats of Adsorption

The effect of small variations in the heats of adsorption as it appeared in the $\partial \gamma / \partial T$ relationship in eqn. (51) was first examined in Fig. 38 and Section 4.5. It was noted that a 10% variation in $\Delta H^*$ resulted in a rather large change in $\partial \gamma / \partial T$ values and particularly to the temperature where $\partial \gamma / \partial T$ is zero.

Figures 49 (a-b) show the surface temperature and surface velocity, respectively, due to the various $\Delta H^*$ values. The corresponding weld pool shapes are shown in Fig. 50. The reference $\Delta H^*$ is defined as the value taken by Zacharia et al [63] for AISI 304, that is $-1.88 \times 10^8$ J/kg-mole. +10% $\Delta H^*$ indicates that $\Delta H^*$ is 1.1 times the reference case while -10% $\Delta H^*$ for 0.9 times the reference
Figure 49. Plot of (a) surface temperature and (b) surface velocity 
due to different heats of adsorption, $\Delta H'$ as derived in Fig. 38. 
$\Delta H' = -1.88 \times 10^5$ J/kg-mole is taken as the reference value. +10% $\Delta H'$ indicates that $\Delta H'$ is 1.1 
times the reference value while -10% $\Delta H'$ indicates that $\Delta H'$ is 0.9 times the reference value.
Figure 50. Weld pool profile due to different heats of adsorption, $\Delta H^*$, corresponding to Fig. 49.

a) $\Delta H^* = -1.692 \times 10^9$ J/kg-mole (+10%): $u_{\text{max}} = 85.3$ cm/s; $T_{\text{max}} = 2,349$ K

b) $\Delta H^* = -2.068 \times 10^9$ J/kg-mole (-10%): $u_{\text{max}} = 44.3$ cm/s; $T_{\text{max}} = 2,580$ K

c) $\Delta H^* = -1.88 \times 10^9$ J/kg-mole (ref): $u_{\text{max}} = 69.8$ cm/s; $T_{\text{max}} = 2,417$ K
case. The change is most pronounced with -10% ΔH* where the pool changes shape completely. This can be explained from Fig. 38 (a) where the temperature at which \(\partial y/\partial T = 0\) for -10% ΔH* occurs at about 2,100 K. Since it is relatively easy for the pool to achieve a temperature of 2,100 K, which is only 400 K beyond its liquidus temperature, two flow loops are expected. An outward anti-clockwise loop occurs for \(T > 2,100\) K while the inward clockwise loop occurs for \(T < 2,100\) K. The outward anti-clockwise loop generates a flatter temperature profile (Fig. 49 (a)), which is more typical of negative \(\partial y/\partial T\) driven flows, and the surface velocity in this region is likewise reduced (Fig. 49 (b)).

In the case of the +10% ΔH*, the pool shape does not differ much from the reference case since the temperature where \(\partial y/\partial T = 0\) is now at 2,600 K (Fig. 38 (a)). This indicates that a large portion of the weld pool surface will have positive \(\partial y/\partial T\). Furthermore, Fig. 38 (a) also indicates that a larger \(\partial y/\partial T\) value will be observed for the same surface temperature when compared to the reference case.

In Section 4.7.4, on the examination of the role of surface tension, it is concluded that the higher \(|\partial y/\partial T|\) is, the higher will be the surface velocity, and the lower will be the surface temperature distribution since the stronger convective flow is able to convect more heat away from the free surface. This phenomenon is also observed in Figs. 49 (a-b) for the reference case and the +10% ΔH* case. As the +10% ΔH* case has higher \(|\partial y/\partial T|\) values, and thus higher surface velocity (Fig. 49 (b)), its surface temperature distribution will be slightly lower than the reference case (Fig. 49 (a)).

The weld pool flow fields and shapes corresponding to the 3 cases examined in Fig. 49 are shown in Figs. 50 (a-c). Figures 50 (a) and (c) with their single flow loops are the result of a predominantly positive \(\partial y/\partial T\) driven flow as described above. However, Fig. 50 (b) with two flow loops are due to both positive and negative \(\partial y/\partial T\)'s. The penetration is not as deep and the weld puddle is somewhat larger. This is the primary difference between the single-flow loop and the double-flow loop weld pool shape.
The purpose of this exercise is to examine the sensitivity of $\Delta H^\circ$. Since small variations in $\Delta H^\circ$ can lead to large variations in calculated pool shape (Fig. 50), the value of $\Delta H^\circ$ chosen seems critical. Thus, the conclusions drawn should reflect these assumptions.

4.7.6 Effect of Arc Power Distribution

So far the various factors affecting the weld pool have been examined from the workpiece perspective. In this section, the nature of the welding arc in affecting pool shape will be examined.

The welding arc can influence the weld pool primarily in two ways, namely, the intensity of the heat source and the nature (slope) of the heat flux distribution. The former tends to control the peak surface temperature of the weld pool while the latter controls $\partial T/\partial r$ at the weld pool surface which in turn affect $\tau_{at}$. These 2 factors will be systematically examined in this section.

The reference power distribution is the 100 A arc as given in Fig. 34. In analyzing the effect of the power distribution on the weld pool, the velocity and temperature of the welding arc at the anode boundary layer is assumed to be that of the 100 A arc (Figs. 34 (a-b)). This information is needed to compute the rate of heat loss by mixed control vaporization. Although it is understood that the arc velocity and temperature will change when the power distribution changes, it is felt that this change is not substantial if the power distribution changes only slightly, say 10-20 %. Furthermore, by maintaining these input conditions of velocity and temperature constant, thereby reducing the amount of parametric variations of the boundary conditions, a more definitive study of the weld pool behavior can be achieved.

4.7.6 (a) Arc Power Intensity

A parametric analysis of the heat source intensity is straight-forward in that the heat and current distributions can be raised by, say, 10 % increments. In practice, this is similar to increasing the arc current. There are 2 ways in which the heat intensity can be raised.
(i) Adding a constant or to the heat source

In this case, a constant heat flux independent of radial position is added to the original heat flux distribution. This method allows the same heat flux slope, \( \frac{dq}{dr} \), to be maintained. The reason for this technique of heat increment is to ensure that the change in the heat flux does not alter \( \frac{dq}{dr} \) as it is suspected that \( \frac{dq}{dr} \) may influence \( \frac{dT}{dr} \) on the weld pool.

Let us define the reference heat flux distribution given in Fig. 34 as \( q_{\text{arc}}(r) \) and the revised flux, \( q'_{\text{arc}}(r) \) as:

\[
q'_{\text{arc}}(r) = q_{\text{arc}}(r) + q_{\text{const}} \tag{64}
\]

Now the total power received by the workpiece for the reference heat flux is then given by:

\[
Q_{\text{total}} = 2\pi \int_{r}^{\infty} q_{\text{arc}}(r) \, dr \tag{65}
\]

Let the revised power, \( Q'_{\text{total}} \) due to the revised heat flux \( q' \) be a percentage factor of the reference power, that is \( Q'_{\text{total}} = (1+x) Q_{\text{total}} \). Thus, expressing eqn. (64) in terms of total power received by the workpiece:

\[
(1+x) Q_{\text{total}} = 2\pi \int_{r}^{\infty} q_{\text{arc}}(r) \, dr + 2\pi \int_{0}^{r} q_{\text{const}} \, dr \tag{66}
\]

where \( x \) is the fraction of power increment and \( r' \) is the size of the anode spot. Equation (66) can be reduced to:

\[
x Q_{\text{total}} = 2\pi \int_{0}^{r} q_{\text{const}}(r) \, dr \tag{67}
\]

\[
\Rightarrow q_{\text{const}} = \frac{x Q_{\text{total}}}{\pi r'^{2}} \tag{68}
\]

In this study, \( x = 0.1, 0.2, \) and \( 0.3 \) while the size of the anode spot is assumed to be 3 mm. From Fig. 34, the heat flux at this distance corresponds to about 6% of the maximum. The primary purpose of imposing this form of heat flux as described by eqn. (64) is to ensure that:

\[
\frac{dq'_{\text{arc}}(r)}{dr} = \frac{dq_{\text{arc}}(r)}{dr} \tag{69}
\]

By this token, the slope of the heat flux distribution remains unchanged but the curve has been raised by a constant factor, \( q_{\text{const}} \). In this manner, the effect of \( \frac{dq'_{\text{arc}}(r)}{dr} \) will be held constant in order to examine the effect of small power increments on weld pool behavior.
Incidentally, the total power received by the workpiece for the 100 A arc with 1.5 mm arc gap is 753.35 W. Thus, \( q_{\text{cons}} \) corresponds to 2.6644 W/mm\(^2\) for \( x=0.1 \), 5.3287 W/mm\(^2\) for \( x=0.2 \), and 7.9933 W/mm\(^2\) for \( x=0.3 \). Naturally, the same treatment is given for the current flux distribution since the bulk of the heat is carried by the electrons. The heat and current flux distribution for eqn. (64) is shown in Fig. 51. The reference case (100 A) is also shown. Notice that the slope of each curve is unchanged.

**(ii) Multiplying by a constant factor to the heat source**

\( q_{\text{arc}}(r) \) can be multiplied by a constant factor indicative of the increments such that the revised heat flux \( q''_{\text{arc}}(r) \) is given by:

\[
q''_{\text{arc}}(r) = (1+x) \, q_{\text{arc}}(r)
\]  

(70)

This causes the local heat flux to increase by a common factor but the more important implication is that:

\[
\frac{dq''_{\text{arc}}(r)}{dr} = (1+x) \frac{dq_{\text{arc}}(r)}{dr} \neq \frac{dq_{\text{arc}}(r)}{dr}
\]  

(71)

Here, the heat flux distribution not only increases but the slope of the distribution also changes. Thus, Gaussian function such as that employed in eqn. (72) below where the arc efficiency is part of the function, the change in efficiency is more subtle in that both \( q_{\text{arc}} \) and \( dq_{\text{arc}}/dr \) change. Figure 52 shows a plot of the increments for eqn. (70). Notice that the slope of each curve increases slightly as \( x \) increases.

The purpose of these changes in the power distribution is to examine the sensitivity of the weld pool to small changes in power distribution particularly to both \( q_{\text{arc}} \) and \( dq_{\text{arc}}/dr \). Practically, this refers to small fluctuations in arc efficiency or even arc current.

**(iii) Computed results and discussion**

The total power received by the workpiece for the two power distributions described above are actually the same although the form of the distributions differs slightly. Figures 53 and 54
Figure 51. Plot of (a) heat flux and (b) current flux distributions for constant increments of power source. The curves are drawn via eqn. (64) where +10% refers to a 10% increase of the total power source. The reference case is the 100 A arc shown in Figs. 34 (a-b).
Figure 52. Plot of (a) heat flux and (b) current flux distributions for a relative increment of power source. The curves are drawn via eqn. (70) where +10% refers to a 10% increase of the local power flux. The reference case is the 100 A arc shown in Figs. 34 (a-b).
Figure 53. Plot of (a) surface temperature and (b) surface velocity for constant power increments as given by the power distributions in Fig. 51. The data are plotted for the molten pool surface only.
Figure 54. Plot of (a) surface temperature and (b) surface velocity for relative power increments as given by the power distributions in Fig. 52. The data are plotted for the molten pool surface only.
show the surface temperature and surface velocity, respectively, corresponding to the power distributions examined above. The expected trend of increasing temperature corresponding to the additional heat source is obvious. The trend for the surface velocity is less obvious at first but can be explained directly from \( \partial T / \partial t \) and \( \partial y / \partial T \) as has been done in the previous sections and will not be dealt with here. The more important observation is that the small increases (10-30\%) in power distribution result in correspondingly small changes in the surface temperature and surface velocity distributions. A 10\% change in the heat source evoke a 2-4 \% (50-100 K) change in the local temperatures and about 4-5 \% change (4 cm/s) in the local velocities. The shape of the weld pool is strongly related to the surface temperature distribution and in all these cases, the general shape of the pool and the flow fields are similar to those in Fig. 50 (a). The pool size also increases in response to the increasing heat sources (Table 17) but the changes are small.

Recapping the analyses from surface tension coefficient (Section 4.7.4), the \( \gamma \) turning point temperature is 2,400 K. Below this temperature, and which most of the regions at the free surface of all the cases studied above are, \( \partial y / \partial T \) is positive and a deep penetration results. In Figs. 53 and 54, the region close to the origin is above 2,400 K because the arc contains sufficient local power to achieve that temperature. Although the slope of the temperature distribution increases suddenly, \( \partial y / \partial T \) is small around this temperature and thus a lower velocity is obtained. Consequently, the fluid gets heated up much faster.

<table>
<thead>
<tr>
<th>Heat Source</th>
<th>Increments (%)</th>
<th>Pool Radius (mm)</th>
<th>Pool Dept'h (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Figure 51</td>
<td>+ 10</td>
<td>2.8</td>
<td>6.3</td>
</tr>
<tr>
<td></td>
<td>+ 20</td>
<td>2.9</td>
<td>6.4</td>
</tr>
<tr>
<td></td>
<td>+ 30</td>
<td>3.0</td>
<td>7.0</td>
</tr>
<tr>
<td>Figure 52</td>
<td>x 10</td>
<td>2.7</td>
<td>6.3</td>
</tr>
<tr>
<td></td>
<td>x 20</td>
<td>2.8</td>
<td>6.4</td>
</tr>
<tr>
<td></td>
<td>x 30</td>
<td>2.9</td>
<td>7.0</td>
</tr>
</tbody>
</table>

Table 17. Weld pool size corresponding to the heat sources in Figs. 51 and 52. The sizes quoted here are taken at the solidus temperature (1523 K).
4.7.6 (b) Arc Power Distribution Parameters

The second aspect of altering the heat source involves maintaining the same current but varying the power distribution, in particular the slope of the heat and current fluxes. In practice, this corresponds to altering the shielding gas composition or changing the electrode tip angle. Mathematically, it has the same effect as altering the heat and current distribution parameters \( a \) and \( b \) in the following equations:

\[
q = \frac{3\eta VI}{\pi a^2} \exp\left[\frac{-3r^2}{a^2}\right] \tag{72}
\]

\[
J = \frac{3I}{\pi b^2} \exp\left[\frac{-3r^2}{b^2}\right] \tag{73}
\]

Figure 55 shows the heat and current flux distributions for a 100 A arc (80% efficiency at 13.2 V with a pre-weld gap of 2.0 mm) but for three different distribution parameters. Although the total power input is the same for each curve, the nature of the power distribution is very different. It should be expected that the weld bead is similarly affected by the power distribution.

A brief examination of the behavior of the variations in distribution parameters is helpful in providing proper perspective of the nature of these parameters with respect to actual welding conditions. In particular, the analysis focus on the studies of Tsai and Eagar [22] where extensive investigations have been made on relating distribution parameters to cathode tip angle, arc length, shielding gas composition, and arc current. The key finding in their study is that the power distribution is strongly dependent on the arc current and arc length, and less so on shielding gas composition and cathode tip angle. Furthermore, they found that the heat flux distribution is not truly Gaussian. They fitted their power distributions in accordance to the following functions:

\[
q = \frac{Q_{\text{total}}}{2\pi \sigma_H^2} \exp\left[\frac{-r^2}{2\sigma_H^2}\right] \tag{74}
\]

\[
J = \frac{I}{2\pi \sigma_I^2} \exp\left[\frac{-r^2}{2\sigma_I^2}\right] \tag{75}
\]

A selection of Tsai and Eagar’s results [22] are shown in Figs. 56 (a-d). In general, most of these figures show positive and direct relationship between the independent and dependent variables. The effect of the shielding gas is less certain and shows much scatter.
Figure 55. Plot of (a) heat flux and (b) current flux distributions for the various distribution parameters. The case examined is a 100 A arc with 80% arc efficiency and an applied voltage of 13.2 V [30]. The pre-weld arc gap was 2.0 mm. The functions are calculated via eqns. (72) and (73). The reference case is a=b=3 mm.
Figure 56. Plot of experimental heat and current distribution parameters due to the various welding conditions as examined by Tsai and Eager [22].

a) arc length  b) arc current  c) cathode tip angle  d) shielding gas composition and arc length
Finally, in order to determine $\sigma_{11}$ and $\sigma_1$ from eqns. (74-75), the total power of the arc and the arc current must be known. Although the arc current can be determined immediately, $Q_{\text{total}}$ must be measured which severely handicaps the numerical treatment. The alternate way to getting $Q_{\text{total}}$ is to assume some functions of arc efficiency, voltage, and current as given in eqn. (72).

Kou et al [4,52,47] and Zacharia et al [63] have frequently used a value of $a=b=3$ mm for their Gaussian heat and current functions as shown in eqns. (72-73). However, Tsai and Eagar [22] employing the Gaussian functions of eqns. (74-75) give a much lower value for both distribution parameters (Figs. 56 (a-d)). The question then arises as to which of these power approximations most accurately represent the arc behavior and if so, how does the weld pool respond to these variations in distribution parameters? These represent some of the difficulties inherent in assigning the power source distributions a priori and also in experimentally determining the power source functions. Fortunately, on the basis of the analyses in the previous section (Section 4.7.6 (a)), the weld pool does not respond greatly to minor variations in the heat and current sources.

(i) Computed results and discussion

The computed weld pool surface temperature and surface velocity for the power distribution given in Fig. 55 are shown in Fig. 57. The immediate observation is the $a=2.5$ mm case where there is not only a flat temperature profile near the pool center (Fig. 57 (a)) but also there are 2 flow loops as evident by the positive and negative velocities in Fig. 57 (b). The surface temperature and surface velocity are strong functions of the peak power distribution. Although it is clear from the previous section that small power changes result in correspondingly small changes in weld pool characteristics, the effect of the power changes in Fig. 55 is more drastic in order to reflect the changes in welding conditions as shown in Fig. 56.

Ultimately, it seems that the material property is that which determines the pool shape. The arc has the ability to provide a certain heat intensity which can raise the pool surface to some temperature. However, it is the surface tension of the surface active element which determines the final pool shape. The understanding here is that in practice, the minimum current will be used to
Figure 57. Plot of (a) surface temperature and (b) surface velocity for the various distribution parameters as given in Fig. 55.
achieve the optimum weld. If the sulphur content of the workpiece have been different, then the \( \gamma \) turning point temperature would also be different and the weld pool shape changes correspondingly.

Extending the power distribution to the bi-modal type power fluxes (2 peaks) found in high arc currents such as those examined in Chapter 2 (Fig. 26) may not be as straight-forward in that there are other factors that come into play such as pool depression, curvature effects, gas shear stress, and arc pressure which may play significant roles in determining pool shape.

The major implications of this section are:

1) Small fluctuations in arc power intensity does not alter pool behavior significantly. This may help explain why minor variations in arc efficiencies employed in the empirical Gaussian functions of heat and current or even an estimate of the arc efficiency generally will not affect the weld pool shape substantially. This observation is noted bearing in mind of the experimental errors and physical data uncertainties.

2) The larger changes in the nature and shape of the arc power distribution, such as that due to changes in the distribution parameters, are more dominant in affecting pool shape. This also includes the effect of weld pool depression where the power distribution changes from a uni-modal to a bi-modal distribution.

3) Ultimately, the pool shape seems dependent on the \( \gamma \) turning point temperature (a material property) since this temperature dictates the direction of fluid flow and thus pool shape. The surface tension driven flow per se does not control the gross pool shape as much as the ability of the arc, through its intensity, of raising the pool above this temperature. Thus, the ability to predict the \( \partial \gamma / \partial T \) relationship is all the more critical.

### 4.7.7 Effects of Gas Shear Stress

The primary test here is for the 100 A and 200 A cases where a planar weld pool surface exists. The 300 A case is also tested in a theoretical manner since at such a high current, the surface will deform. Deformable free surface is not investigated in this thesis. Despite the handicap,
useful insights can still be obtained from these analyses. Figures 58 (a-e) show the input b.c.'s for the weld pool for I=100-300 A.

The key information particular to the analyses are $\tau_{gas}$ and $\tau_{s,l}$. $\tau_{gas}$ is given in Fig. 58 (e). $\tau_{s,l}$, as derived from eqn. (54) can best be analyzed from the surface temperature distribution. Inherently linked to the surface temperature is the surface velocity. Figures 59, 60, and 61 show the plot of surface temperature, surface velocity, and surface tension shear stress, respectively, for the b.c.'s given in Fig. 58.

The sharp surface temperature drop in Figs. 59 (a-b) is due to the change in $\partial \gamma / \partial T$ from a positive value to a negative value. This can be explained by the nature of the convective loop in Figs. 62 (a-b). For discussion purposes, the 200 A case will be elaborated in greater detail because the data are better differentiated. Similar behavior is also seen in the 300 A case. The 100 A case, however, is slightly different in that there is only single flow loop (Fig. 62 (c)) due to the lower applied current.

As stated earlier, negative $\partial \gamma / \partial T$ driven flows bring heat from the center of the pool outwards and generally produce a flatter surface temperature profile. Correspondingly, as $\partial T / \partial r$ is flatter, $\tau_{s,l}$ is also smaller and the resultant surface velocity in this region is reduced (Fig. 60 (b)). With positive $\partial \gamma / \partial T$ driven flows, a sharper temperature gradient arises. The region where $\partial \gamma / \partial T \approx 0$ or where the opposing shears meet such as that around $r \approx 1.5$ mm for the 200 A arc (Fig. 59 (b)), the temperature changes drastically. The reason is due to the thermal energy being brought directly into the bulk of the weld pool. This sudden change in the slope of the temperature is reflected as a large shift in $\tau_{s,l}$ as shown in Fig. 61 (b), which is out of the scale of the plot. Naturally the exact value of $\tau_{s,l}$ is not meaningful here but the order of magnitude is; which for the 200 A case the maximum $\tau_{s,l}$ is +520 Pa and the minimum $\tau_{s,l}$ is -430 Pa. This sharp temperature drop is unavoidable regardless of the number of grids employed. Furthermore, this location moves as the pool grows. It is apparent that this sharp temperature drop is an inherent property of high current simulations where the arc is able to provide a local heat intensity which heats the surface above the surface tension turning point temperature.
Figure 58. Plot of (a) heat flux and (b) current flux of a 1.5 mm arc for 100-300 A with $J_c=4.5$ A/mm$^2$. 
Figure 58. Plot of (c) anode boundary layer surface temperature and (d) anode boundary layer surface velocity of a 1.5 mm arc for 100-300 A with $J_e=4.5$ A/mm$^2$. 
Figure 58. Plot of (e) anode gas shear stress distributions of a 1.5 mm arc for 100-300 A with $J_c=4.5$ A/mm$^2$. 
Figure 59. Plot of surface temperature as a function of radial position for (a) 300 A and (b) 200 A arc due to the power source distributions given in Fig. 58.
Figure 59. Plot of surface temperature as a function of radial position for (c) 100 A arc due to the power source distributions given in Fig. 58.
Figure 60. Plot of surface velocity as a function of radial position for (a) 300 A and (b) 200 A arc due to the power source distributions given in Fig. 58.
Figure 6j. Plot of surface velocity as a function of radial position for (c) 100 A arc due to the power source distributions given in Fig. 58.
Figure 61. Plot of surface tension shear stress as a function of radial position for (a) 300 A and (b) 200 A arc due to the power source distributions given in Fig. 58.
Figure 61. Plot of surface tension shear stress as a function of radial position for (c) 100 A arc due to the power source distributions given in Fig. 58.
Figure 62. Weld pool profile with gas shear stress for (a) 300 A (b) 200 A (c) 100 A arc corresponding to the power source distributions given in Fig. 58.
The more interesting region is the region adjacent to this stagnation point flow where a plot of $\tau_{s.t}$ is given in Fig. 61 (b). This should be compared with the $\tau_{gas}$ in Fig. 59 (e). It is evident that $\tau_{s.t}$ is usually much larger than $\tau_{gas}$ even for the 100 A case (Fig. 61(c)). For the 100 A case, $\tau_{gas}<<\tau_{s.t}$ such that both results are essentially identical whether $\tau_{gas}$ is applied or not. Thus, in general, for a planar weld pool surface, $\tau_{gas}$ does not play a crucial role in affecting pool shape.

As a final note, the arc behavior in all these figures are consistent. For instance, $\tau_{gas}$ shears in a direction away from the pool center as the gas is flowing outwards and thus should drive the the surface fluid outwards. This means that it could strengthen the velocity when $\partial\gamma/\partial T<0$ but weakens it when $\partial\gamma/\partial T>0$. As evident from Fig. 60 (b) for the 200 A case, with $\tau_{gas}$, the surface velocity is increased and the increased velocity results in a decrease in the surface temperature as seen in Fig. 59 (b). On the other hand for the 100 A case (Fig. 60 (c)), the reverse occurs where the surface velocity is reduced by the gas shear as $\partial\gamma/\partial T$ is predominantly positive here. The shear stress in Fig. 61 (b) also shows consistent behavior where $\tau_{s.t}$ is enhanced when $\tau_{gas}$ is included at $r<1.5$ mm. However, at $r>1.5$ mm, $\tau_{s.t}$ is about the same with or without $\tau_{gas}$ since $\tau_{gas}$ is much smaller here. The pool sizes for the cases studied are summarized in Table 18 for completeness. The pool radius remains unchanged with or without $\tau_{gas}$ as the heat intensity is identical for each current. The pool depth is generally reduced when $\tau_{gas}$ is included as $\tau_{gas}$ is opposite in direction to the positive $\partial\gamma/\partial T$ driven flows.

<table>
<thead>
<tr>
<th>Condition</th>
<th>Arc Current (A)</th>
<th>Pool Radius (mm)</th>
<th>Pool Depth (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>With Gas Shear</td>
<td>100</td>
<td>2.6</td>
<td>5.8</td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>3.5</td>
<td>8.5</td>
</tr>
<tr>
<td></td>
<td>300</td>
<td>4.3</td>
<td>9.6</td>
</tr>
<tr>
<td>Without Gas Shear</td>
<td>100</td>
<td>2.6</td>
<td>5.9</td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>3.5</td>
<td>8.6</td>
</tr>
<tr>
<td></td>
<td>300</td>
<td>4.2</td>
<td>10.1</td>
</tr>
</tbody>
</table>

Table 18. Weld pool size due to the additional boundary condition of gas shear stress on weld pool surface as given in Fig. 58 (e). The sizes quoted here are taken at the solidus temperature (1523 K).
A brief comparison must be made of this study with that of Matsunawa and Yokoya [135] where they concluded that $\tau_{gas}$ played a very important role in affecting pool shape. In their calculations of $\tau_{gas}$, they showed that $\tau_{gas}$ is of the order of 400 Pa for an isothermal welding arc (2 mm arc gap). Assuming their plasma viscosity of $2.9 \times 10^{-4}$ kg/m-s, this indicates that the velocity gradient at the anode boundary layer is of the order of $1.4 \times 10^{6}$ m/s$^2$. If the boundary layer is assumed to be 0.1 mm thick, then $\partial u_\ast \partial x$ will be of the order of 140 m/s since $u_{wall}$ is zero. This value is unrealistically large. Nevertheless, their conclusion based on $\tau_{gas} \sim$ 400 Pa is consistent with our results since the $\tau_{s,t}$ calculated here is of the order of 100 Pa but it is questionable if the actual $\tau_{gas}$ is 400 Pa.

4.8 General Observations

4.8.1 Vaporization Kinetics

Surface tension driven flows due to the temperature gradient at the free surface plays a major role in limiting the surface temperature. Some modelling efforts which assumed Langmuir-type vaporization rates gave reasonable results because of the vapor pressure dependance of the gaseous species with temperature where they increase exponentially as the boiling point is approached. However, with mixed control vaporization, the mass transfer coefficient is an order of magnitude less and thus the heat loss by vaporization cannot be the limiting factor to peak surface temperature. It was shown that the nature of $\partial \gamma / \partial T$ exhibits a stronger influence on the peak surface temperature than vaporization.

4.8.2 Surface Tension

Most stainless steels exhibit $\partial \gamma / \partial T$ of the order of $10^{-4}$ N/m-K. However, most stainless steels also contain S which is one of the surface active elements. Sulphur influences the surface tension by enhancing it, resulting in $\partial \gamma / \partial T$ being positive. In this sense, the absolute value of $\partial \gamma / \partial T$ per se is not so critical as the pool shape is generally established once the sign of $\partial \gamma / \partial T$ is determined. The temperature where $\partial \gamma / \partial T = 0$ is more critical since dual-loop flow fields can form.
This results in a pool shape (Figs. 62 (a-b)) that differs from that of a single loop (Fig. 62 (c)). Thus, the primary focus is on the accuracy of the $\gamma/\partial T$ relationship as function of the surface active element composition and temperature. In this analysis, the emphasis is on sulphur as the primary surface active species primarily because the role of the other surface active species is either unknown or difficult to quantify. In particular, how does the presence of other elements affect the calculations? For instance, even though there is negligible oxygen content in the workpiece, some oxygen entrainment from the atmosphere is inevitable, despite the argon shielding, and oxides inclusions are indeed seen on the surface of the weld pool. The manner by which these oxide are incorporated into the $\gamma/\partial T$ relationship is probably through thermodynamic and kinetic considerations which are unexplored at this time. There is an added complication in that studies by Collur et al [137] using laser beam welding showed that in Fe-S-O systems, the oxygen will be the dominant surface active species relative to sulphur.

The effect of the interactions between surface active species has been ignored in this and previous studies [69]. The extent of this omission is unclear. Although as a first approximation, one may include the effects of all the surface active elements by super-positioning of all the binary components that are surface active with Fe, it is unclear how these element will interact in reality. For instance, Walsh and Savage [7] reported that Group IV elements (O,Se,S,Te) are surface active in Fe-based alloys while Group V elements (N,P,As,Sb) are generally not surface active in Fe. However, there is an interaction between these surface active elements when present in combination but they did not elaborate on the nature of these interactions. Thus, the extent of phosphorus, which is present in AISI 304, interaction with sulphur in almost unknown mathematically.

The above represent some of the problems that are encountered in determining the effects of surface tension. If the role of surface tension is as crucial as indicated above, and the mathematical model can only be as accurate as the precision of the surface tension coefficient, then major thrusts

* There should be a qualification with this observation in that the weld pool surface temperature in laser beam welding is much higher.
should be directed at the fundamental studies of the determination of surface tension applicable to welding systems.

Knowing the nature of the behavior of the surface tension as examined above, there are now several ways by which the penetration of the weld can be controlled. If the workpiece composition cannot be changed, then the nature of the welding arc must be altered. The analysis above suggests that increasing the arc current and thus the heat flux may not necessarily increase penetration. In fact, a pool that is shallow in the middle and deep around the edges may be obtained due to the surface temperature exceeding the surface tension turning point temperature. Although the precise description of the weld pool shape is possible, more important, the development of the trends in the weld pool behavior are equally important for it allows valuable insights and understanding to be gained.

The role of sulphur in stainless steels deserves special attention. Sulphur is considered an impurity in steel and its presence is generally detrimental as it decreases the notch hardness. Thus, there is a strong tendency to produce clean steels with very low sulphur content*. However, the net effect, as observed from Fig. 38, is that a substantial portion of the weld pool surface will have negative $\gamma/\partial T$. This will produce a very shallow but wide weld pool which is undesirable in welding. In this sense, very low sulphur content in steels is undesirable for welding applications.

4.8.3 Arc Power Distribution

The weld pool shape is more strongly affected by material property and composition than by the arc behavior. For normal GTAW with planar weld pool surface, small variations in the single peak heat source is not critical in affecting weld pool features. Again, the main issue here is not so much the nature (slope) of the power distribution but more so on the intensity of the arc in raising the weld pool temperature above the surface tension turning point temperature.

* Sulphur content of the order of 0.0001 to 0.001 wt-% is now possible.
It is conceivable that there exists a relationship between the arc intensity, weld pool peak surface temperature, and thus penetration depth for a specific material. This data base can be established empirically and by numerical simulation. However, the key unknown here is still the temperature where $\gamma/\partial T = 0$ for this determines the flow direction and pool shape. Thus, the $\gamma/\partial T$ relationship must be refined particularly with respect to the presence of other surface active species besides sulphur.

4.8.4 Gas Shear Stress

For planar weld pool surfaces, the gas shear stress does not influence weld pool behavior significantly. This is because it is shown that $\tau_{gas} \ll \tau_{s1}$. However, the effect on non-planar surface such as that occurring in high arc current when surface depression occurs or even those with oscillating surface is unclear from this investigation. No parallels can be drawn from the planar surface analyses since the deformable surface exhibits quite different behavior: a) the surface temperature will no longer be a simple single peak and thus $\tau_{s1}$ can be significantly modified, b) surface curvature of the pool and arc pressure may begin to play more important roles, and c) fluctuations in the surface can significantly affect the temperature distribution as the heat source and surface temperature can change continuously. For all practical purpose, at low currents, the role of $\tau_{gas}$ is unimportant and the early modelling analysis which did not take into account of this is not critically affected.

4.8.5 Overview of the Problem

After extensive evaluations of the weld pool shape and flow profile in this chapter and after preliminary investigation of the experimentally obtained weld pool shape data* (more will be said of this in Chapter 5), it is found that the calculated results do not really resemble the experimental results in virtually all cases!! The calculated results generally predict too deep a

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* The experimental data are taken at face value although they can be challenged.
penetration. It is well known that GTAW is mainly for welding thin sheets less than 6.35 mm (1/4-in). Furthermore, most of the experimental data show rather flat welds with penetration no more than 4 mm for a 150 A arc. A possible explanation is perhaps the $\partial \gamma / \partial T$ relationship is incorrect but variations of the $\partial \gamma / \partial T$ relationship examined in this chapter show otherwise; in that a deep penetration is still observed despite the second loop for cases with both positive and negative $\partial \gamma / \partial T$ driven flows. Another explanation may be that the mathematical model is incorrect but this is unlikely as the model has been tested with published results and has also given consistent results with the many variations in power distribution and weld pool conditions.

All the analyses in this chapter were carried out assuming laminar flow. The Prandtl number is between 0.2 to 0.3, thus the fluid is better at transmitting thermal energy than momentum which helps explain why the heat from the surface is quickly brought into the workpiece. It is suspected that this may not provide the correct rate of heat transfer in the weld pool and that the flow may in fact be turbulent! An initial indication of this proposal was found from Zacharia et al [63] where they assumed an effective viscosity and thermal conductivity and produce more realistic computed results. A second indication was that when a 50 A arc was used, it produced a pool of 3 mm diameter but only 0.66 mm deep. This is in total conflict with the model proposed above in that with a low current arc, the surface temperature will be correspondingly low. With the $\gamma$ turning point temperature at 2,400 K, we should expect a predominantly positive $\partial \gamma / \partial T$ driven flow which implies deep penetration ($>> 0.66$ mm). The experimental result shows that the weld puddle is shallow and wide which is more typical of negative $\partial \gamma / \partial T$ driven flows. It is with this contention that the rate of heat transfer in the weld pool may be under-predicted. The nature of turbulent flows will be examined further in Chapter 5.

4.9 Summary

The various phenomena, vaporization and shear stress, at the free surface have been investigated. These are translated into boundary conditions which have been previously ignored by other modellers. From the analyses of the results, the following summaries are noted:
1) **Mixed control vaporization** which consists of Langmuir vaporization and mass transfer across the anode solute boundary layer is not the limiting factor to weld pool surface temperature.

2) **Surface tension driven flow** is responsible for limiting the surface temperature.

3) **Weld pool shape** is a strong function of $\partial \gamma / \partial T$, particularly where the temperature when $\partial \gamma / \partial T=0$ is since flow reversal can occur and the pool shape can change correspondingly.

4) **Minor fluctuations in arc power distributions** are not crucial in affecting weld pool shape for low currents. The more crucial factor is still the surface tension turning point temperature and the ability of the arc intensity to raise the pool above this temperature.

5) The **gas shear stress** does not play a significant role in affecting weld pool characteristics since $\tau_{gas} \ll \tau_{st}$. This is the case for planar weld pool surface.
5. EXPERIMENTAL VERIFICATION OF MATHEMATICAL MODEL

This chapter compares the computed results with experimental results and attempts to identify critical parameters that control weld pool characteristics. Section 5.1 describes the experimental procedure highlighting the results. This is deemed necessarily in order to realize the limitations and sensitivities of the experimental technique. Section 5.2 compares the computed arc results with experimental studies focusing on the issue of short arcs typically found in GTAW. Section 5.3 compares the computed weld pool results with experimental data.

5.1 Description of Experimental Studies

The experimental studies of Kraus [30] of Idaho National Engineering Laboratory (INEL) will be featured extensively in this chapter primarily because he has developed quite an accurate method of determining weld pool surface temperature and bead diameter. Complementing his study are the weld pool data of the same workpiece material from David and Zacharia [138] of Oak Ridge National Engineering Laboratory (ORNL). David and Zacharia have close links with Kraus such that the discrepancies between the input process parameters for the experimental work can be minimized. There, there is a high level of confidence and consistency in the reported data.

The details of the experimental set-up had been given elsewhere [30]. However, the basic features of that set-up will be highlighted here. Single heats of 50-200 A autogeneous stationary gas tungsten arc welds were performed on 40 mm by 40 mm by 12.5 mm horizontal AISI 304 plates. The composition of AISI 304 had been given in Table 14. The cathode consists of a 1/8-th inch (3.2 mm) diameter, 30° tip angle, 2 % thoriated-tungsten. The pre-weld arc gap was 2.0 mm and argon shielding at 8.5 l/min was used. The specimen sat on a water-cooled copper plate that was initially at 15 °C. An Astro-Arc Astromatic E-300-PC welding unit was used for all the welds.

The workpiece was heated for 25 s and then the arc was extinguished. The resulting arc decay times were about 3 to 11 ms as shown in Fig. 63 for the various arc currents. The decay time represents the time required for the current to drop to zero after the arc was extinguished. The maximum temperature was recorded on the first frame of the film when arc emission was not present
Figure 63. Arc extinguish times for GTA welds as a function of current for 2 mm gap, 15 V, 8.5 lpm argon shielding, 1.25-cm thick AISI 304 using Astro-Arc Astromatic E-300-P welding unit [30].
on the film image. The time between frames was about 3.6 ms. The error in the temperature readings was reported to be about ± 2.5 %. Thus, the maximum temperature reported was taken a few ms after the arc had been extinguished within the constraints of the frame speed.

In addition, during the welding operation, the surface topology of the weld pool was also determined. This surface profile was reported to oscillate continuously during the arc decay and “long” (no time frame was given but it was suspected that the oscillations could be seen on film) after the arc was extinguished, particularly for some of the 150 and 200 A cases. The amplitude of oscillation could vary up to a few tenths of a mm. The error of the profile measurements was estimated to be ± 0.025 mm. A summary of the experimental conditions is given in Table 19.

5.1.1 Surface Temperature Data

Figures 64-66 (b)'s show the surface temperature contour plots as reported by Kraus [30] while the surface temperature as a function of radial position is shown in Figs. 64-66 (a)'s. Due to the asymmetrical nature of the contour plots, Figs. 64-66 (a)'s are drawn from the center point (between the electrode and electrode reflection) horizontally to the left until the solid-liquid interface. This is meant to be representative of the surface temperature. Temperatures below the 1,700 K melting temperature are not shown. It is not known whether this is a limitation of the technique or just for easy representation of the contour plots. The latter is a more reasonable answer.

5.1.2 Arc Decay Times

Figure 67 shows the maximum pool surface temperature as a function of time for the 150 A arc. The experimental technique is only able to determine the surface temperature after the arc emission is not present which in this case is about 7.2 ms after arc shutdown. The main point is that during the arc decay, the arc is still adding energy to the weld. A linear rate of decay in time was employed by Kraus [30] to estimate the maximum surface temperature just prior to arc extinction. The experimentally observed maximum temperatures were reported as 1.5, 3.0, and 4.5 % decrease from the actual maximum just prior to arc extinction for the 50 A, 100 A, and 150 A, respectively.
<table>
<thead>
<tr>
<th>Case No</th>
<th>Voltage (V)</th>
<th>Current (A)</th>
<th>Time after beginning of emissions decay (ms)</th>
<th>Maximum Observed Temperature (K)</th>
<th>Predicted Maximum Temperature (K)</th>
<th>Weld Pool Diameter (mm)</th>
<th>Weld Pool Dome Height (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>10.1</td>
<td>50</td>
<td>&lt; 3.6</td>
<td>2,220</td>
<td>2,253</td>
<td>3.0</td>
<td>0.16</td>
</tr>
<tr>
<td>2</td>
<td>13.2</td>
<td>100</td>
<td>3.6-7.2</td>
<td>2,433</td>
<td>2,506</td>
<td>5.8</td>
<td>0.41</td>
</tr>
<tr>
<td>3</td>
<td>15.1</td>
<td>150</td>
<td>7.2-10.8</td>
<td>2,699</td>
<td>2,820</td>
<td>8.8</td>
<td>0.51</td>
</tr>
</tbody>
</table>

Table 19. Conditions summary for AISI 304 stationary GTAW [30].
The predicted maximum temperature (column 6) is estimated on the basis of linear rate of decay in time. The data in column 4 can be seen from Fig. 67 for the first part of the curve.
Figure 64. Experimental surface temperature plot at 50 A [30].
(a) radial function of surface temperature  (b) contour plot of surface temperature.
Part (a) has been interpolated from part (b)
Figure 65. Experimental surface temperature plot at 100 A [30].
(a) radial function of surface temperature (b) contour plot of surface temperature.
Part (a) has been interpolated from part (b)
Figure 66. Experimental surface temperature plot at 150 A [30].
(a) radial function of surface temperature (b) contour plot of surface temperature.
Point (a) has been interpolated from part (b)
Figure 67. Maximum pool surface temperature as a function of time for AISI 304, 150 A weld starting from the initiation of arc shut down. Case 3 of Table 19 [30].

Between $t=0$ to $t=7.2$ ms, the arc emission prevented the surface temperature reading from being taken. The first frame reported the surface temperature at 7.2 ms. The maximum weld pool temperature prior to arc extinction is projected backwards from $t=7.2$ ms as shown by the dashed line.
These are calculated to be 2,253 K, 2,506 K, and 2,820 K for the three cases mentioned and are also tabulated in Table 19.

If the mathematical model was to rigorously describe the actual experimental surface temperature, then the rate of energy input into the workpiece during arc decay must be known. This involves studying the characteristics of the transistor diversion banks [30] of the power supply. Such calculations were not done. Thus, the mathematical model will provide surface temperature results just prior to arc extinction.

5.1.3 Penetration Data and Surface Morphology

Concurrently, penetration studies of the same material were being performed at ORNL [138]. Although the original macrographs of the weld beads were not available to the author, photocopies of the macrographs were available and from which the schematics of the weld bead are shown in Fig. 68 to highlight the pertinent features. Figures 68 (a-c) were reproduced directly from those macrographs and confirmed verbally with Dr. Zacharia of ORNL [138].

Sulphur is considered to be the principal surface active element in AISI 304. Normally, this would result in a positive $\partial \gamma / \partial T$ in which one would expect a deeper penetration due to the inward flow. This is indeed observed for the 100 and 150 A cases. The 50 A case is rather unusual in that a rather shallow penetration (< 1 mm) was observed despite the positive $\partial \gamma / \partial T$.

Figure 69 shows the weld pool surface profile for the 150 A arc as obtained by Kraus [30]. The dome, which is caused by the thermal expansion of the liquid metal, can effectively reduce the distance between the electrode and the workpiece. At such a short arc length (~ 2 mm), this has important repercussion on the heat and current flux distributions. In order to account for the effect of the dome, the simulation is performed with the raised dome included in the arc model as shown in Fig. 70 (b). The purpose is to model the effect of the dome shown in Fig. 69 using an effective (shortened) arc length*. The reason is that although the height of the dome is reported (Table 19),

* Effective arc length = preweld arc gap – dome height.
Figure 68. Weld bead geometry for the 3 cases described in Table 19 [138].
(a) 50 A  (b) 100 A  (c) 150 A. The samples are heated for 25 seconds.
Figure 69. Weld pool surface profile in a plane perpendicular to top surface specimen and containing central axis through the length of electrode [30]. (150 A arc) The electrode has been added by this author to show its location relative to the weld puddle. The raised region is a liquid metal pool (dome) due to thermal expansion.
Figure 70. Velocity profile in the welding arc for (a) a flat surface with 1.5 mm arc gap and (b) a 2.0 mm pre-weld arc gap with a 0.5 mm-dome. (150 A arc)
the shape of the dome is not always reported. Figure 70 (a) shows the velocity profile of the welding arc with the effective arc length (1.5 mm) being modelled while Fig. 70 (b) shows the velocity profile with the pre-weld arc gap (2.0 mm) and the liquid dome (0.5 mm) included. Figures 71 (a-b) show the resulting heat and current flux distributions for the effective arc length and that for the raised dome. Except for the small difference in the peak heat flux (~ 6%), both results are comparable and the effective arc length will be used for simulating the welding process. The mathematical model will use the 1.5 mm arc gap as the reference case in order to indicate the upper limit of the power distribution. The 2.0 mm arc gap power distribution is also calculated so as to specify the lower limit of the power distribution.

Kraus [30] reports that the domes are generally more curve than flat but this is a generalization. In his study with AISI 8630 steel, the dome oscillates from side to side and is asymmetrical in nature. For AISI 304 steel as indicated in Fig. 69, the domes will be assumed to have flat surfaces.

5.1.4 Summary of the Reported Experimental Studies

From the experimental results, it can be seen that the weld pool characteristics are asymmetrical in nature. The instantaneous surface contour plots are asymmetric and the weld pool surface oscillates. It can be deduced that the arc is asymmetric too. However, the weld bead geometry appears symmetric. The mathematical model is formulated on the basis of symmetry. Thus, this is a limitation of the model. However, it is felt that under quasi-steady state condition (when the weld bead geometry does not change after long heating times), which is what the experiments are assumed [30], the observed weld bead should appear symmetric. This symmetry is the basis of this study and therefore, the mathematical model can be said to have a good representation of the transport phenomena in the workpiece if it can predict weld pool characteristics such as surface temperature, weld pool diameter, and weld pool depth (penetration).
Figure 71. Plot of (a) heat flux and (b) current flux distributions as a function of radial position corresponding to the weld pool surface geometry given in Fig. 70. (150 A arc)
5.2 Arc Modelling Results

5.2.1 Input Parameters and Cases Studied

The b.c.'s for the arc model are similar to Table A.1 in Appendix A. Two arc lengths of 1.5 mm and 2.0 mm are presented for completeness. The cathode spot current density is taken as $4.5 \times 10^7$ A/m$^2$ and three currents are tested, namely, 50 A, 100 A, and 150 A.

One of the limitations of the present arc model is its inability to deal with a pointed tip cathode. Although a step function may be prescribed to model the conic section of the tip, the boundary condition of this step function is not as straight-forward. The problem concerns the cathode current density at the step; how are $J_r$ and $J_z$ to be prescribed and whether $J_r$ and $J_z$ remain constant as the distance increases from the tip since the surface area also increases.

The choice of a flat cathode tip may be appropriate at longer arc lengths (> 3.2 mm) but at the arc lengths employed in the experimental studies, the radius of the electrode (1.6 mm) is beginning to approach the dimension of the arc length (1.5-2.0 mm). The primary effect is suspected to be the nature of the gas flow as driven by $J \times B$ at the cathode tip.

In order to circumvent this problem, a modified version of the cathode tip is used. Figure 72 (a) shows the flat tip that has been used so far. In the actual welding process, the tip is usually pointed with a given tip angle (Fig. 72 (b)). $R_e$ is the cathode spot radius as calculated from the specified cathode spot current density $J_e$ on the basis of the applied current. Figure 72 (a) basically simulates Fig. 72 (b) by means of an effective $R_e$. The principal difference between Fig. 72 (a) and (b) is the manner of gas flow. Clearly, Fig. 72 (b) is more streamline while Fig. 72 (a) has an abrupt change in the gas flow direction at the corner of the cathode. The concern here is how the gas flow may be affected despite the same $J \times B$ pinch force is applied. This flow pattern may not be that critical if the radius of the cathode is much smaller than the arc length in which case the gas can flow freely. The problem thus arises when the electrode radius approaches the arc length dimension such that flow is affected by the small constricted space.

The scheme employed to tackle this limitation is shown in Fig. 72 (c) where the radius of the electrode ($R_e$) is taken to be one node larger (~0.2 mm) than the cathode spot radius ($R_e$) such
Figure 72. Schematic diagram of the cathode tip.
(a) Flat cathode tip (mathematical model)  (b) Pointed cathode tip (experimental)
(c) Cathode tip that is employed with $R_c > R_e$
that the cathode impedes the gas flow as little as possible. This is to be contrasted with fixing the experimental cathode at 1.6 mm radius and choosing \( R_c \) to satisfy \( J_c \) (Fig. 72 (a)).

5.2.2 Computed Results for the Arc

Figures 73 (a-b) show a typical velocity and temperature profiles of a 100 A welding arc at 1.5 mm arc length while Figs. 74 (a-d) show the radial distributions of the heat flux, current flux, surface temperature, and surface velocity. The data for the 2.0 mm arc are also shown in Figs. 75 (a-d). The “surface” gas velocity and temperature are taken at 0.1 mm (first grid node above the workpiece) from the anode surface. This is assumed to be the edge of the anode boundary layer.

The calculated arc parameters are indicated in Table 20. The trends in the various arc parameters with increasing arc current are identical to those described in Chapter 2 and require no further elaboration. There is one minor point that needs to be highlighted; the efficiencies calculated for the 1.5 mm case are very close to 100 %. The reason is that the total voltage is taken to be the sum of the cathode fall voltage and arc column voltage (Appendix A). There is no reliable estimate of the anode fall voltage and it can vary from 2 to 10 volts depending upon process conditions [139]. Thus, the actual efficiencies should be slightly lower.

The boundary conditions for the weld pool are now available through Figs. (74-75). One more test still needs to be done and that is to compare the calculated values with the experimental data to ensure that the calculated results are within the same range or order of magnitude.

5.2.3 Comparison With Welding Arc Studies and Discussion

The experimental results for the welding arc are taken exclusively from Tsai and Eagar [22] as well as from Tsai’s doctoral thesis [140] since their studies parallel those that are being investigated here. Tsai and Eagar [22] measured the heat and current distributions for a wide range of conditions but only those pertinent to this study will be highlighted.
Figure 73. Calculated (a) velocity and (b) temperature profiles of a 100 A welding arc at 1.5 mm arc length. The maximum velocity vector (m/s) is shown at right of figure (a).
Figure 74. Plot of (a) heat flux and (b) current flux distributions as a function of radial position at 1.5 mm arc length for various arc currents.
Figure 74. Plot of (c) surface temperature and (d) surface velocity distributions as a function of radial position at 1.5 mm arc length for various arc currents.
Figure 75. Plot of (a) heat flux and (b) current flux distributions as a function of radial position at 2.0 mm arc length for various arc currents.
Figure 75. Plot of (c) surface temperature and (d) surface velocity distributions as a function of radial position at 2.0 mm arc length for various arc currents.
<table>
<thead>
<tr>
<th>Arc Length</th>
<th>1.5 mm arc length</th>
<th>2.0 mm arc length</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>50 A</td>
<td>100 A</td>
</tr>
<tr>
<td>Arc Current</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$Q_{a,\text{max}}$ (W/mm²)</td>
<td>65.2</td>
<td>104.6</td>
</tr>
<tr>
<td>$J_{a,\text{max}}$ (A/mm²)</td>
<td>9.0</td>
<td>12.9</td>
</tr>
<tr>
<td>$v_{\text{max}}$ (m/s)</td>
<td>33.1</td>
<td>72.4</td>
</tr>
<tr>
<td>$T_{\text{max}}$ (K)</td>
<td>15,950</td>
<td>17,590</td>
</tr>
<tr>
<td>$P_{a,\text{max}}$ (Pa)</td>
<td>58</td>
<td>172</td>
</tr>
<tr>
<td>$V_{\text{arc}}$ (V)</td>
<td>6.9</td>
<td>7.5</td>
</tr>
<tr>
<td>$\eta$ (%)</td>
<td>99</td>
<td>99</td>
</tr>
<tr>
<td>Electrode radius (mm)</td>
<td>1.01</td>
<td>1.01</td>
</tr>
</tbody>
</table>

Table 20. Calculated arc parameters at 1.5 mm and 2.0 mm arc lengths with $J_e=4.5 \times 10^7$ A/m².
5.2.3 (a) Comparison With Experimental Results

Figures 76 (a-b) show the experimentally obtained radial heat and current distributions for a 2 mm arc [22]. In comparison, Figs. 75 (a) and (b) reported a calculated peak heat and current values of 75 W/mm² and 9.5 A/mm². The corresponding experimental peak values are 52 ± 4 W/mm² and 7.6 A/mm². These result are obtained for a 75 degree tip tungsten electrode at 100 A with argon shielding. Although it seems that the calculated results give higher values, we need to compare it with other results to contrast the range of errors. In this respect, the empirical Gaussian formulas previously described in eqns. (72) and (73) are reproduced here:

\[
q(r) = \frac{3 \eta V I}{\pi a^2} \exp \left[ -\frac{3r^2}{a^2} \right] \tag{76}
\]
\[
J(r) = \frac{3 I}{\pi b^2} \exp \left[ -\frac{3r^2}{b^2} \right] \tag{77}
\]

These two functions have been used by many researchers [4,63,64] to model the weld pool and have reported to give good results. Using the process conditions described in Table 20, an arc efficiency of 80 %, and an effective radius of 3 mm [4,63,64], the maximum heat and current fluxes can be obtained as shown in Table 21:

<table>
<thead>
<tr>
<th>Case</th>
<th>I (A)</th>
<th>V (V)</th>
<th>Gaussian (eqn. 76)</th>
<th>Gaussian (eqn. 77)</th>
<th>Calculated (Fig. 75)</th>
<th>Calculated (Fig. 75)</th>
<th>Expt. (Fig. 76)</th>
<th>Expt. (Fig. 76)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>50</td>
<td>10.1</td>
<td>42.8</td>
<td>5.3</td>
<td>41.2</td>
<td>5.8</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>2</td>
<td>100</td>
<td>13.2</td>
<td>112.0</td>
<td>10.6</td>
<td>74.8</td>
<td>9.5</td>
<td>52</td>
<td>7.6</td>
</tr>
<tr>
<td>3</td>
<td>150</td>
<td>15.1</td>
<td>192.2</td>
<td>15.9</td>
<td>111.4</td>
<td>13.2</td>
<td>–</td>
<td>–</td>
</tr>
</tbody>
</table>

Table 21. Peak heat and current fluxes due to eqns. (76) and (77) and from the arc model in Fig. 75. The arc gap is assumed to be 2.0 mm.

It is noted that at 100 A, the calculated maximum heat flux from the arc model is about 50 % larger than the experimental value of Tsai and Eagar [22] while the Gaussian formulas of eqns. (76) and (77) are predicting more than twice the experimental peak heat input. Although the tip angle was slightly different, Tsai and Eagar [22] reported that the heat distribution parameter (effective arc
Figure 76. Experimental (a) heat and (b) current flux distributions at 2 mm arc length [22]. The error bar is given only for the heat flux.
radius) changed by only 14% when the tip angle increased from 30° to 120°. They argued that the heat distribution did not vary significantly with tip angle. However, this conclusion was based on the results of Fig. 56 (c) which was obtained for a 5.5 mm arc. It is not certain if the same conclusion can be reached for a 2.0 mm arc. In Chapter 2, it is noted the arc behavior is more sensitive to changes in process conditions at short arcs and therefore, it is suspected that the heat flux will be significantly modified by the tip angle at 2.0 mm arc length. Investigation into the heat and current flux variations with tip angle at short arc lengths (< 2 mm) is strongly recommended.

From Table 21, it can be seen that the Gaussian model tends to over-predict both the heat and current fluxes by a much wider margin. In fact, it does not appear to be in the right order of magnitude for the higher currents, especially the heat flux. The mathematical model shows better agreement even though it over-predicts the heat flux somewhat. There are reasons for concern regarding the disparity between the calculated arc results and the experimental results. It is suspected that the split anode method of measuring the arc power is reliable for long arc lengths (>> 2 mm). At short arcs, it is felt that the air gap (0.2 mm) between the two “Dee” split anodes may cause complication as the arc pass directly above them.

There is still a further problem with short arcs. Dinulescu and Pfender [141] reported that the anode boundary layer, which is not under local thermodynamic equilibrium, is beginning to approach the dimensions of the arc gap for the cathode spot current density employed. Although it appears that the problem may have gotten even more complicated as the anode boundary layer has to be fully modelled to account for the differences in electron and heavy particles temperatures, a first step approach might be reasoned that at such short arcs, the thermal energy is carried primarily by the electrons. As such, it may not even be necessary to account for the heavy particles contribution which Dinulescu and Pfender [141] described as primarily conductive.

5.2.3 (b) Effect of the Cathode Spot Current Density

The majority of the b.c. for the welding arc have been established on fundamental grounds except for one; the cathode spot current density. Although it has been discussed previously (Table
1) that $J_c$ does not vary substantially with arc current, the choice of $J_c$ remains. In this thesis, since the heat transfer in the cathode is not model, $J_c$ must be selected and this represents an adjustable parameter at this time. The sensitivity of this parameter is shown in Fig. 77 where two different $J_c$'s are used for a 150 A arc with 1.5 mm arc gap. Incidentally, the three contributions to the total heat flux are also shown. As noted, the higher $J_c$ results in a higher convective contribution. This is because as the current is the same, the actual electronic contribution is unchanged but the higher $J_c$ results in a stronger JxB term and thus the convective contribution is increased due to higher gas velocity. More critical is that as $J_c$ increases by 44 %, the peak heat flux increases by 23 % although the total power received by the workpiece remains the same. Certainly, the choice of $J_c$ can influence the weld pool behavior, particularly the peak surface temperature.

As a first approximation, the manner by which the unknown $J_c$ may be overcome is to model the heat transfer in the thermionic cathode via the Richardson-Dushman equation [142]:

$$J_c = 6 \times 10^8 T^2 \exp \left[ -\frac{\Phi_c e}{k_B T} \right]$$

(77)

where $\Phi_c$ is thermionic work function of the cathode surface. $\Phi_c$ for tungsten is about 4.4 volts [142] but modification may have to be made for a thoriated-tungsten electrode.

Figure 78 shows the heat and current flux distributions that have been calculated on the basis of $J_c=6.5 \times 10^7$ A/m². This should be contrasted with Fig. 74 where $J_c=4.5 \times 10^7$ A/m². Generally, the higher $J_c$ results in higher fluxes.

Another factor in which there is little control over is the integrity of the cathode tip. It is not certain if the cathode tip will maintain its shape during the entire welding operation. Firstly, vaporization does occur at the tungsten electrode [112,113] and some blurring of the tip may occur due to mass loss. Secondly, Hsu et al [20] in their experimental studies of the welding arc indicated that some deterioration of the tip occurred even for short welding durations. And thirdly, a brief survey of the Welding Handbook [143] showed that the electrode tip was generally not pointed after the welding operation although this could be case dependent.

The problem remains and the need to predict $J_c$ and the shape of the cathode tip must be
Figure 77. Plot of heat flux distribution as a function of radial position for (a) $J_c = 6.5 \times 10^7$ A/m$^2$ and (b) $J_c = 4.5 \times 10^7$ A/m$^2$ at 1.5 mm arc gap for a 100 A arc. The 3 contributions to $q_a$ are also shown.
Figure 78. Plot of (a) heat flux and (b) current flux distributions as a function of radial position for $J_c=6.5\times10^7$ A/m$^2$ at 1.5 mm arc length for various arc currents (50-150A).
addressed. The necessity to include the cathode in the modelling process seems all the more important as it has been mentioned countless times that the cathode spot is very critical in defining the heat transfer to the workpiece; for it is this spot where source of energy is emitted.

5.2.4 Summary of the Arc Modelling Studies

The arc model has been shown to provide the appropriate range of heat and current fluxes to the weld pool. Thus, there is confidence that the input boundary conditions to the weld pool are correct.

5.3 Weld Pool Modelling Results

5.3.1 Preliminaries

The surface temperature by Kraus [30] and the weld pool data by Zacharia and David [138] are obtained from the workpiece that has been heated for 25 seconds for each sample. This is an extremely long simulation time for a computer especially with fine grids. A 5-second simulation with 40x41 irregular grids requires about 33 hours on an Apollo DN 10000 or about 110 hours on a VAX Station 3100/30. Despite the long computational times, it is found that in many of the runs, the flow pattern, surface temperature, surface velocity, and weld pool shape are established very early (~ 1-2 s) during the welding process. This indicates that the general features of the pool remain unchanged although the weld puddle continues to grow in size. In this respect, the computational results can be used to compare with the experimental results on the basis of the surface temperature and the general shape of the weld pool. The specific details such as pool dimensions can be addressed once the general shape of the weld is established. All the results are presented at t=5.0 s unless otherwise noted.

It was briefly discussed in Chapter 4 (Section 4.8.5) that despite the extensive studies with the 100 A arc with the many variations of the heat flux distributions and $\partial \gamma / \partial T$, the calculated weld pools were seen to be very different from the experimental results (Fig. 68). The majority of the welds in Chapter 4 showed rather deep penetrations. It is thus suspected that the model may
not be simulating the proper mechanisms in the weld pool.

In this section, the basic elements of turbulent flows will be introduced but the details of the governing equations are given in Appendix B. A detailed examination of turbulent flow in the weld pool will not be made for reasons discussed in Appendix B.3. Furthermore, the weld pool flow is not predominantly turbulent but more of a laminar-transitional-turbulent type flow as the size of the pool increases as it grows. This makes the problem even more difficult to tackle as the two-equation K-ε turbulence model [144] is best suited for a predominantly turbulent flow. Despite the difficulties associated with turbulence modelling, insights and understanding can still be gained if parametric studies are done to establish the nature of the transport processes occurring in the weld pool.

A brief overview of the method of approach to the problem will give perspective to the nature of the task ahead. In the modelling of laminar flows, since all the transport properties are unique, there is really no empirical constant or adjustable parameter in either the governing equations or boundary conditions\(^*\). In the case of turbulence models, of which there are many varieties, the simplest is to assume some constant turbulent viscosity. Here, there are two adjustable parameters; the turbulent viscosity which can be arbitrary selected and the turbulent Prandtl which can vary between 0.9-1.1. The turbulent Prandtl number is used to determine the turbulent thermal conductivity. At this point, the calculated results become questionable since the turbulent viscosity, \( \mu_t \), is not a fundamental physical property. Although as a first approximation, one can estimate \( \mu_t \) on the basis of the type of flow (in this case - transitional), adjusting \( \mu_t \) to fit the experimental results defeats the purpose of the study. In spite of this, the critical observation developed from this initial attempt at turbulence modelling is that “will the calculated results provide correct the information in terms of pool shape and size?”. Fortunately, this is a resounding ‘yes’ and the suspicion that the flow may indeed be turbulent deserves further attention. At this point, the turbulence model must be refined to obtain more meaningful answers.

\(^*\) Although it was mentioned in Sections 5.2 that \( J_c \) is adjustable, fundamentally this parameter can still be determined by solving the Richardson-Dushman equation (eqn. 77).
The two-equation K-ε turbulence model [144] is the currently most popular model for simulating turbulent flow. The formulation of these governing equations are given in Appendix B. However, now, we have added a few more empirical constants‡ to the model. At first sight, it appears that empirical constants are again used to fit the experimental results. Fortunately, this is not always the case as these empirical constants are well tested with many flow situations and have withstand much criticism. It is certainly true that these constants depend on the flow situations [145]. Nevertheless, there is wide acceptance to the constants employed and in this study, the default constants and b.c.'s will be employed.

This is the state of affairs of the current analyses. We began with laminar flows and discovered that the calculated results differ widely from experiments. On conducting scoping studies using effective viscosity, the calculated results appear to provide the correct shape for the weld pool. Further analysis using the simplified K-ε model also provides similar results as that using the a constant effective viscosity. This observation confirms that flow in the weld pool is indeed turbulent. The analysis terminates here since further investigation using a constant effective viscosity does not have fundamental grounds while further analysis with the K-ε model requires major modifications of the boundary conditions at the solid-liquid interface (Appendix B).

5.3.2 Comparison With Experimental Weld Pool Results

Two sets of experimental results will be compared with; the first from Zacharia et al [63,64] and the second from Kraus [30] and Zacharia and David [138].

5.3.2 (a) Zacharia, David, Vitek and DebRoy's Results [63,64]

Figure 79 shows the computed and experimental results by Zacharia et al [63,64] of a 150 A arc at 2.0 mm arc length on a 30 mm by 30 mm by 6 mm AISI 304 steel. Although the calculated result shows excellent agreement with the experimental result, there are several major flows in

‡ Five in the governing equations and two more in the boundary conditions.
Figure 79. Comparison of the calculated and experimentally observed GTA weld fusion zone after 20 s [64]. (Heat contains 90 ppm sulphur).
their mathematical model:

i) No reason is given for the choice of the effective viscosity (0.05 kg/m-s). The laminar value is 0.006 kg/m-s which appears to be ten times smaller than the effective value.

ii) No reason is also given for the choice of the effective thermal conductivity (154.8 W/m-K). The laminar value is between 15 to 20 W/m-K.

iii) The turbulent Prandtl number for their case is 0.23 assuming $C_p$ is 753 J/kg-K. The correct turbulent Prandtl number is about 0.9. Thus, their rate of heat transfer is fundamentally incorrect.

iv) There is a cut-off temperature of 3,100 K which is assumed to be the boiling point. As a result, near the center of the pool, $\partial T/\partial r \sim 0$. Furthermore, Eagar [136] has strongly suggested against the boiling point ever being reached in arc welding.

One of the major criticisms of using a constant effective viscosity for the turbulence model is that the effective viscosity are both spatially dependent and velocity gradient dependent. Thus, the selection of a constant value is at best an order of magnitude assumption.

Employing the same boundary conditions* as those given by Zacharia et al [63] with the difference being that laminar physical properties are used, Fig. 80 (a) shows the computed weld pool result with a cut-off temperature of 3,100 K. No vaporization heat loss is assumed here. The two flow loops are due to $\partial y/\partial T$ changing from a positive to a negative value. The sample consists of 90 ppm sulphur in which case the temperature where $\partial y/\partial T=0$ is about 2,100 K. The region close to the center of the pool has negligible velocity (~ mm/s) as $\tau_{a,t}$ at the surface is almost zero. The primary observation is that although the calculated shape of the pool resembles the experimental data and that given by Zacharia et al [63] (Fig. 79), it cannot be justified due to the nature of the boundary conditions imposed.

A second test is made whereby the effective viscosity is taken at 0.05 kg/m-s and the effective thermal conductivity is taken at 42 W/m-K. These values are taken such that the

* One of the b.c., the penetration depth ($y_d$), is not defined.
Figure 80. Calculated weld pool flow field using (a) laminar physical properties and (b) assuming turbulent conditions with $\mu_{\text{eff}}=0.05$ kg/m-s and $k_{\text{eff}}=41.8$ W/m-K.

The sample is heated for 2.0 second.
effective viscosity is ten times the laminar value. The calculated result is shown in Fig. 80 (b). This figure gives a better agreement with the experimental result and in a way resembles the calculated flow field given in Fig. 79. The size of the pool is not expected to agree completely with the experimental data since the physical properties have been arbitrarily chosen.

The plot of the surface temperature and surface velocity for Figs. 80 (a) and (b) are shown in Figs. 81 (a-b). As the major portion of the surface is above 2,100 K, \( \partial \gamma / \partial T \) is negative and an outward flow field (positive velocity) is generated. The sharp temperature drop seen in both curves, around \( r \approx 2.75 \) mm for laminar and \( r \approx 3.4 \) mm for turbulent flows, is due to the change in flow direction caused by the change from positive to negative \( \partial \gamma / \partial T \). The change in flow direction is more pronounced for the laminar case.

5.3.2 (b) Kraus' [30] and Zacharia and David's [138] Results

The boundary conditions for the weld pool employed in this section is shown in Table 13 while most of the physical and transport properties are given in Tables 14-16. The additional material properties for turbulent conditions are shown in Table 22. Because of the large computational times required to simulate a 25-s run, all computed results are for 5.0 seconds. Thus, in general, the calculated pool is smaller than the experimental pool.

Figures 82-84 compares the calculated results with the experimental results for 50-150 A. Figure 82-84 (a)'s are reproduced from Fig. 68. Figures 82-84 (b)'s represent the computed results using a constant effective viscosity which is 10 times the laminar value. Figures 82-84 (c)'s show the calculated results using laminar physical properties and finally Figs. 82-84 (d)'s are the numerical results based on the K-\( \varepsilon \) turbulence model. The sizes and characteristic information of the weld pools for Figs. 82-84 are summarized in Table 23.
Figure 81. Plot of (a) surface temperature and (b) surface velocity corresponding to the case studied in Fig. 80 for laminar and turbulent physical properties.
Figure 82. Comparison of weld pool shape between (a) experimental result [138], (b) numerical result using a constant effective viscosity, (c) numerical result based on laminar properties, and (d) numerical result based on the K-ε turbulence model for 50 A.

The experimental data is for t=25 s while all the calculated results are for t=5 s.
Figure 83. Comparison of weld pool shape between (a) experimental result [138], (b) numerical result using a constant effective viscosity, (c) numerical result based on laminar properties, and (d) numerical result based on the K-ε turbulence model for 100 Å.

The experimental data is for t=25 s while all the calculated results are for t=5 s.
Figure 84. Comparison of weld pool shape between (a) experimental result [138], (b) numerical result using a constant effective viscosity, (c) numerical result based on laminar properties, and (d) numerical result based on the K-ε turbulence model for 150 A.

The experimental data is for t=25 s while all the calculated results are for t=5 s.
<table>
<thead>
<tr>
<th>Description</th>
<th>Nomenclature</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>effective dynamic viscosity</td>
<td>$\mu_{\text{eff}}$</td>
<td>0.060 kg/m-s</td>
</tr>
<tr>
<td>effective thermal conductivity</td>
<td>$k_{\text{eff}}$</td>
<td>45.18 W/m-K</td>
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</tbody>
</table>

Table 22. Material properties for turbulent conditions. These values supersede those given in Table 15.

<table>
<thead>
<tr>
<th>Case</th>
<th>Description</th>
<th>50 A (Figure 82)</th>
<th>100 A (Figure 83)</th>
<th>150 A (Figure 84)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experimental [30]</td>
<td>Pool radius (mm)</td>
<td>1.5</td>
<td>1.625</td>
<td>4.3</td>
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<td>Constant Effective Viscosity</td>
<td>Pool depth (mm)</td>
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<td>2.46</td>
<td>3.9</td>
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<td></td>
<td>Peak temperature (K)</td>
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<td>2506</td>
<td>2820</td>
</tr>
<tr>
<td>Laminar Properties</td>
<td>Pool radius (mm)</td>
<td>0.8</td>
<td>2.0</td>
<td>2.7</td>
</tr>
<tr>
<td></td>
<td>Pool depth (mm)</td>
<td>0.3</td>
<td>1.9</td>
<td>3.1</td>
</tr>
<tr>
<td></td>
<td>Peak temperature (K)</td>
<td>1959</td>
<td>2521</td>
<td>2941</td>
</tr>
<tr>
<td>K-ε model</td>
<td>Max pool velocity (cm/s)</td>
<td>15.5</td>
<td>31.6</td>
<td>40.6</td>
</tr>
<tr>
<td></td>
<td>Max surface velocity (cm/s)</td>
<td>11.0</td>
<td>31.6</td>
<td>40.6</td>
</tr>
<tr>
<td></td>
<td>Pool radius (mm)</td>
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</tr>
<tr>
<td></td>
<td>Peak temperature (K)</td>
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<tr>
<td></td>
<td>Max pool velocity (cm/s)</td>
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<td>69.7</td>
<td>67.5</td>
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<tr>
<td></td>
<td>Max surface velocity (cm/s)</td>
<td>49.3</td>
<td>62.0</td>
<td>67.0</td>
</tr>
</tbody>
</table>

Table 23. Description of weld pools for Figs. 82-84.
Firstly, there are large differences between the experimental results and the laminar results in terms of pool size and shape, especially as the current increases. The laminar results predict much too deep a penetration and do not resemble the experimental data at all. On introducing an effective viscosity which is 10 times the laminar value, the computed results now begin to resemble the experimental data in terms of pool shape and general size. Naturally, an exact comparison is not feasible for two reasons: 1) the simulated data is for 5.0-s while the experiment is for 25-s, and 2) the selected physical property is arbitrary. Despite the gross assumption used, the calculated weld pool do resembles the experimental data.

In order to provide some confidence to the constant effective viscosity model, the K-\(\varepsilon\) turbulence model is employed where the calculated weld pools do resemble weld pool results based on the effective viscosity in terms of pool shape and general size. Therefore, on the basis of the above observations, it is concluded that the flow phenomena in the weld pool for AISI 304 is indeed turbulent.

The overall velocity in the weld pool decreases as the viscosity increases as seen from, say Figs. 82 (b and c). However, the surface temperature distribution did not increase (Fig. 85 (a)) despite the lowered free surface velocity since the thermal conductivity of the liquid is now enhanced; thus conducting, as opposed to convecting in the laminar case, more thermal energy away from the free surface.

Figures 85 (a-c) show the surface temperature for the various models as compared with the experimental data (plotted as points). For the 50 A and 100 A cases, since the arc did not provide sufficient local power to heat the weld pool surface beyond the \(\gamma\) turning point temperature (2,400 K), the slope of the surface temperature is quite constant for all the three models (laminar, constant \(k_{\text{eff}}\), and K-\(\varepsilon\)). However, in the 150 A case, both the laminar and constant \(k_{\text{eff}}\) models showed a sudden drop in the surface temperature around \(r\sim 0.7 \text{ mm}\) because the surface temperature exceeds 2,400 K. The K-\(\varepsilon\) model predicts a slightly lower surface temperature distribution due to the

* Refers to Figs. 82-84 (c)'s where laminar physical properties are used.
Figure 85. Comparison of surface temperature between the experimental result and the different models (effective viscosity, laminar, K-ε) shown in Fig. 84.

(a) 50 A (b) 100 A (c) 150 A
Figure 85. Comparison of surface temperature between the experimental result and the different models (effective viscosity, laminar, K-ε) shown in Fig. 84.
(c) 150 A
enhanced thermal conductivity in turbulent flows.

In general, the experimental data do not show a sharp drop in surface temperature along the free surface; but rather a gradual change in the temperature distribution. The sudden change in the experimental surface temperature in Fig. 85 (b) for the 100 A may be due to an instantaneous snap-shot taken of the free surface. Examination of Kraus [30] data for the other weld pools indicates that some of the profiles are much more complicated. The surface temperatures for the other workpiece material (AISI 316L and AISI 8630) as reported by Kraus [30] are too chaotic to be explained by a simple model of one or two flow loops. Instead, he proposed multiple flow loops in the weld pool. This observation certainly lends support to the proposal that the flow in the weld pool is turbulent and chaotic.

5.3.3 General Observations and Discussion

First and foremost, the calculated results based on the K-ε turbulence model involves a gross assumption in that the boundary conditions at the solid-liquid interface are not imposed by a wall function. Instead, it is imposed by drag due to solidification as expressed by the drag term in the momentum equation. The used of a constant effective viscosity is unfavorable either since the turbulent viscosity should be spatially dependent. It follows that the analyses presented here are basically scoping studies of the welding problem.

Despite the multitude of mathematical modelling efforts described in Figs. 5 (a-c), there is really only one "authoritative" paper and that is by Zacharia et al [63]. The reason is that they attempt to correlate their model with experiments as rigorously as they can. This is not to say that all the other models are wrong but rather all the other models are "basically models" and did not really compare their calculations with experiments. Mathematical models can be used to describe trends in a process but mathematical models together with experiments certainly have a definite advantage if they correlate properly and correctly.

Since the initial treatment of the convective weld pool modelling efforts by Oreper and Szekely [44] using laminar transport equations, the majority of the later publications has employed
an identical set of laminar equations. The notion of turbulent flows for welding was first mentioned by Paul and DebRoy [54] for laser welding and later by Zacharia et al [63] for arc and laser welding; although both use a constant effective viscosity and thermal conductivity. In this thesis, a more in-depth sensitivity and parametric study of the heat source, the $\partial \gamma / \partial T$ variations, the gas shear stress, material composition, and material physical and transport properties have led to the conclusion that flow in the weld pool is turbulent.

5.4 Summary of Results

1. The calculated weld pool results based on laminar physical properties are unable to correlate with experimental data.

2. The calculated results based on constant effective viscosity are very similar to those based on the K-$\varepsilon$ model. Both of these results yield weld pool shapes that strongly resemble the experimental results.

3. It is concluded that the flow in the weld pool is indeed turbulent.
6. CONCLUSIONS

1. Vaporization does not control the surface temperature of the weld pool in gas tungsten arc welding (GTAW) of stainless steel if the surface tension coefficient, \( \frac{\partial \gamma}{\partial T} \), is of the order of \( 10^{-4} \) N/m-K. This conclusion is based on the studies of mixed control vaporization of Langmuir kinetics and mass diffusion across the anode boundary layer.

2. Mixed control vaporization predicts that the rate of heat loss is about 1/16th (about an order of magnitude) that due to Langmuir vaporization and so some other mechanism must be controlling the surface temperature of the weld pool.

3. Convective heat transfer due primarily to Marangoni shear is responsible for the surface temperature distribution. As \( |\frac{\partial \gamma}{\partial T}| \) increases, the surface tension shear stress, \( \tau_{s,t} \), also increases. This results in a stronger surface velocity, which translates to more thermal energy being removed from the free surface, and thus the surface temperature decreases.

4. If \( \frac{\partial \gamma}{\partial T} \) is greater than \( +1.0 \times 10^4 \) N/m-K or \( \frac{\partial \gamma}{\partial T} \) is less than \( -1.0 \times 10^4 \) N/m-K, then the rate of heat loss from the free surface will be limited by convective heat transfer. Otherwise, it will be limited by vaporization which is unlikely since \( |\frac{\partial \gamma}{\partial T}| \) for steel is of the order of greater than \( 10^4 \) N/m-K.

5. The weld pool is not very sensitive to changes in the welding arc power distribution. Small changes in the welding arc (say 10%) produce correspondingly small changes in the weld pool characteristics (~ 1-4%) (size, pool velocity, temperature); that is, the weld pool is rather insensitive to small fluctuations in the arc power distribution in the case of low current welding with a planar weld pool surface.
6. The material property of the base plate, particularly the concentration of the surface active element (in this case sulphur), is important in determining the pool shape. However, small variations (up to 20%) in the sulphur concentration do not affect the weld bead geometry substantially.

7. The gas shear stress, \( \tau_{\text{gas}} \), due to the plasma arc velocity over the weld pool is not an important driving force for weld pool convection in planar weld pool surfaces. The surface tension shear stress is much larger than \( \tau_{\text{gas}} \). In general, \( \tau_{\text{gas}} \) strengthens the flow direction if the surface is driven by negative \( \partial \gamma / \partial T \) flows and weakens it if it is driven by positive \( \partial \gamma / \partial T \) flows.

8. The flow in the weld pool is suspected to be turbulent. Laminar flows models are unable to correlate the calculated results with experimental data. However, with the use of constant effective viscosity and thermal conductivity which are both larger than the molecular values, the calculated results begin to resemble the experimental data.

7. Calculated results for turbulence based on the constant effective viscosity and that based on the simplified K-\( \varepsilon \) model yield similar results; both of which closely resemble the experimental data. It is proposed that the flow field in the weld pool is in fact turbulent.
7. FUTURE DIRECTIONS

The following observations are noted while developing the mathematical model. They indicate the areas in which the model has not given a rigorous treatment. In some cases, the information is not available while in others the treatment is too simple. These deserve further attention and where possible, suggestions are also given as to how they should proceed.

A. The Welding Arc

1. The size of the cathode spot radius should be calculated rather than pre-assigned. This involves modelling the heat transfer in the cathode itself. The Richardson-Dushman equation may be used to estimate the cathode spot size and cathode spot current density since it provides a direct relationship between temperature and current density.

2. In almost all welding operations, a pointed tip cathode is used. The arc model must be modified to account for this feature especially at short arc lengths. The conic section of the cathode is best modelled using body-fitted coordinates so as to avoid the problem of step functions in the finite difference scheme.

3. Vaporization of gaseous species from the cathode is known to modify the electrical and thermal conductivities of the plasma. Although the anode heat flux is not strongly affected since 80% of the heat is carried by the electrons, however, the temperature of the arc can affect the the rate of mass transfer at the weld pool free surface. This will in turn affect the peak surface temperature and thus the weld pool characteristics. It is recommended that the effect of the contaminating species be factored into the plasma such that the transport and physical properties of the arc are more accurately represented. In particular, the treatment suggested by Dunn et al [112,113] is recommended.
4. The effect of vaporization of gaseous species from the anode in affecting the anode boundary layer is not known. Also, the anode fall voltage must be predicted more accurately since negative anode fall voltages have been reported [108]. Dinulescu and Pfender [141] suggested that the anode fall voltage be included in the arc voltage only when it is positive. There is a further problem in that at short arcs (1-2 mm), the thickness of the anode boundary layer begins to be significant (0.2-0.4 mm). Although one may be inclined to solve for non-local thermodynamic equilibrium conditions in this layer, an easier alternative can be reasoned that at such short arcs, the primary mechanism of heat transfer may be electronic. This means that it may not be necessary to solve for the heavy particles temperatures.

5. Finally, in order to provide confidence to the arc model proposed here for short arcs typically found in GTAW, it is recommended that some experimental work be performed to compare with the calculated heat and current fluxes, particularly for those at 1.5 mm and 2.0 mm arc lengths.

B. The Weld Pool

1. The turbulence model must be further developed in order to address the weld pool flow field, particularly for the boundary conditions at the mushy zone. Since logarithmic velocity profile and Couette flow (standard wall functions) may be assumed near the solid-liquid boundary, adaptive meshes seem to be the best choice to model the weld pool. If adaptive meshes are not used, then one must be very careful of the choice of the wall function, particularly with respect to the orientation of the solid-liquid boundary layer. It should be quite evident that this boundary condition is the most critical component of the turbulence model. The reader is strongly advised to introduce as little uncertainties as possible into this boundary condition.
2. The effective mass transfer coefficient (or the heat transfer correlation as given by eqn. (37)) must be determined if it can be applied to the welding arc scenario. This is because the correlation is used for a nozzle flow imping onto a flat plate which may not be suitable as a correlation for a welding arc. In this study, there is a 16% error in the heat transfer correlation. In addition, there is also a 5% error in the latent heats of vaporization of Mn and Fe.

3. The reliability of the \( \partial y/\partial T \) relationship with temperature should be further explored; more specifically the estimation of the standard heat of adsorption, \( \Delta H^* \). How is \( \Delta H^* \) affected by multi-components surface active elements as well as how is Fe-S-O interaction be included the \( \partial y/\partial T \) relationship? The latter query refers to GTAW with argon shielding gas where some researchers [8] continually report that there is oxygen contamination (oxide particles) in the weld pool surface despite the argon shielding. The importance in establishing \( \partial y/\partial T \) is quite crucial in that \( \partial y/\partial T \) is a parameter that is strongly affected by the surface temperature.

4. The kinetic interaction of sulphur segregation at the free surface is not known. In particular, it is not certain if sulphur will remain segregated at the free surface after prolonged heating. The chemical interaction of S with other species must be quantified, if not be established, in order to ensure that there is no kinetic effect on the nature of the sulphur bonds.

5. It is desirable to be able to obtain the physical and transport properties of steel (or whatever the workpiece is) as a function of temperature. One of the problem is that these properties are dependent upon the chemical composition. The problem specification then becomes very specific and generalization may be difficult.
6. The end goal of the modelling effort is not only to predict the shape of the weld pool but also the type of microstructures that are produced since these structures determine the properties of the weld. The ability to predict the type of grains and segregation between the grains falls under the domain of “micro-modelling”. The desire to couple “macro-modelling” of the weld pool (characteristic dimension ~ 0.1 mm) with “micro-modelling” at the solid-liquid interface (characteristic dimension ~ 1 μm) is partly a matter of computational speed but mostly on the theory of solidification. Perturbation of the solidification fronts can result in secondary and tertiary dendrite arms. These perturbation studies fall under the umbrella of stability analyses. In addition, the complex interaction of double-diffusion between mass and thermal energy at the fronts may make interpretation of the results complicated. The most common prediction that can be obtained on the basis of the temperature gradient and growth rate of the solid-liquid interface is the dendrite arm spacing. This is at best an order of magnitude approximation. Some attempts perhaps can be made at addressing or initiating the macro-modelling of the weld pool with the micro-modelling of the solidifying fronts.

C. The Free Surface

1. Although the introduction began addressing a deformable free surface which was attempted using the SOLA-VOF model, the author had been unsuccessful in his attempt after 2 years. Yet, the deformable free surface still remains. Future work should try to include this free surface. The way to tackle the problem is to employ an algorithm that can solve the free surface problem using an implicit scheme and still be able to handle massive deformations of the surface. In addition, the free surface must be able to consider non-linear boundary conditions and heat transfer. The current free surface model is explicit and Marangoni shear b.c. is not so easily implemented.
2. If turbulence is to be included into the free surface problem, one must be cautious as there are additional terms in the K-ε equations for the dissipation of kinetic energy at the free surface. A good discussion of these additional terms can be found in Rodi [145]. The problem has become even more complicated. The reader is strongly advised to be very cautious before venturing into turbulence modelling with free surface capability. The Marangoni shear b.c. at the free surface is not as straight-forward for the K-ε equation.

3. At the writing of this thesis, direct simulation of turbulence has become quite popular as a result of faster and more powerful workstations. The 25 MIPS* 6000-series machine by IBM has just been recently unveiled. It is envisaged that within the next 5 years, massively parallel machine will be commercially viable to small research groups. Although this solves only part of the problem, it is nevertheless a major leap ahead. In other words, the problem is not as hardware limited as before but more software limited. Direct simulation with adaptive meshes appears to be an attractive alternative but should only be attempted at the very last resort. Although this method of modelling is fundamentally sound, it is not trivial. The reader is strongly advised to explore the K-ε model to the best of his abilities, making appropriate changes in the empirical constants on the basis of physical grounds, since this model may be adequate from a material processing perspective.

* Only 4 years ago, the author was struggling with a Vax Station II running on 1.0 MIPS.
APPENDIX A : MATHEMATICAL FORMULATION OF THE WELDING ARC

A.1 Welding Arc Model Development and Governing Equations

The computational domain is shown in Fig. A.1. The welding arc consists of an electric arc struck between a tungsten electrode and a steel workpiece. In GTAW the process is usually direct current straight polarity where the electrode is negative (cathode) and the workpiece is positive (anode) although other configurations are possible. The non-consumable electrode is either tungsten or thoriated-tungsten and shielding of the electrode and weld-zor.e is provided by an inert gas such as Ar, He, or Ar-He mixture. In this model, a tungsten electrode with Ar shielding gas is used on either a copper or a steel plate.

Based on the assumptions described in Chapter 2.1, the governing transport equations expressed in cylindrical coordinates are:

Conservation of Mass

\[
\frac{1}{r} \frac{\partial (\rho u)}{\partial r} + \frac{\partial (\rho w)}{\partial z} = 0 \quad (A.1)
\]

Conservation of Radial Momentum

\[
\frac{1}{r} \frac{\partial (\rho u^2)}{\partial r} + \frac{\partial (\rho uw)}{\partial z} = -\frac{\partial P}{\partial r} + \left[ \frac{2}{r} \frac{\partial}{\partial r} \left( \frac{\mu (\partial u)}{\partial r} \right) - \mu \frac{2u}{r^2} + \frac{\partial}{\partial z} \left( \frac{\mu (\partial u)}{\partial z} \frac{\partial w}{\partial r} \right) \right] - J_z B_\theta \quad (A.2)
\]

Conservation of Axial Momentum

\[
\frac{1}{r} \frac{\partial (\rho w u)}{\partial r} + \frac{\partial (\rho w^2)}{\partial z} = -\frac{\partial P}{\partial z} + \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( \eta \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial r} \right) \right) \right] + \frac{\partial}{\partial z} \left( \mu \frac{\partial w}{\partial z} \right) + J_r B_\theta \quad (A.3)
\]

Conservation of Thermal Energy

\[
\frac{1}{r} \frac{\partial (\rho u h)}{\partial r} + \frac{\partial (\rho w h)}{\partial z} = \frac{1}{r} \frac{\partial}{\partial r} \left( k \frac{h}{C_p} \frac{\partial h}{\partial r} \right) + \frac{\partial}{\partial z} \left( k \frac{h}{C_p} \frac{\partial h}{\partial z} \right) + \frac{J_r^2 + J_z^2}{\sigma_e} - S_r + \frac{5 k_b}{2} e \left( \frac{J_r}{C_p} \frac{\partial h}{\partial r} + \frac{J_z}{C_p} \frac{\partial h}{\partial z} \right) \quad (A.4)
\]

Conservation of Charge Continuity (Gauss Law)

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( \sigma_e r \frac{\partial \phi}{\partial r} \right) + \frac{\partial}{\partial z} \left( \sigma_e \frac{\partial \phi}{\partial z} \right) = 0 \quad (A.5)
\]

The momentum equations consist of, from left to right, the two convective terms, pressure gradient term, the diffusive term, and the electromagnetic body force term. The energy equation consists of, from left to right, the two convective terms, the two diffusive terms, the Joule heating term, the radiation loss term, and the transport of enthalpy due to electron drift (Thompson effect).
The current density can be obtained from:

\[ J_r = - \sigma_e \frac{\partial \phi}{\partial r} \]  
(A.6a)

\[ J_z = - \sigma_e \frac{\partial \phi}{\partial z} \]  
(A.6b)

while the self-induced azimuthal magnetic field is derived from Ampere’s law as:

\[ B_\theta = \frac{\mu_0}{r} \int_0^r J_z r \, dr \]  
(A.7)

The integration constant in eqn. (A.7) is assumed zero for \( B_\theta \to 0 \) as \( r \to 0 \) since the integrand approaches zero as \( r \to 0 \). Equations (A.5-7) complete the information required to determine the electromagnetic body force.

### A.2 Boundary Conditions for the Welding Arc

The boundary conditions (b.c.’s) are summarized in Table A.1.
A.2a Cathode Region (Regions ABCD and DE)

At the cathode region, the momentum boundary conditions are straightforward. $\partial (p w) / \partial z$ is the gradient of the mass flow and is assumed zero at the inflow (DE). This is analogous to $\partial w / \partial z$ except that the density term is included to ensure mass conservation since the density of the gas is temperature dependant.

<table>
<thead>
<tr>
<th>Region</th>
<th>$u$</th>
<th>$w$</th>
<th>$h$</th>
<th>$\phi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>AB</td>
<td>0</td>
<td>0</td>
<td>T = 3,000 K $Q_{\text{ionic}} =</td>
<td>I</td>
</tr>
<tr>
<td>BC</td>
<td>0</td>
<td>0</td>
<td>T = 3,000 K</td>
<td>$\frac{\partial \phi}{\partial z} = 0$</td>
</tr>
<tr>
<td>CD</td>
<td>0</td>
<td>0</td>
<td>T = 3,000 K</td>
<td>$\frac{\partial \phi}{\partial r} = 0$</td>
</tr>
<tr>
<td>DE</td>
<td>0</td>
<td>$\frac{\partial p w}{\partial z} = 0$</td>
<td>T = 1,000 K</td>
<td>$\frac{\partial \phi}{\partial z} = 0$</td>
</tr>
<tr>
<td>EF</td>
<td>$\frac{\partial u}{\partial r} = 0$</td>
<td>$\frac{\partial w}{\partial r} = 0$</td>
<td>T = 1,000 K</td>
<td>$\frac{\partial \phi}{\partial r} = 0$ (inflow)</td>
</tr>
<tr>
<td>FG</td>
<td>$\frac{\partial u}{\partial r} = 0$</td>
<td>$\frac{\partial w}{\partial r} = 0$</td>
<td>$\frac{\partial h}{\partial r} = 0$</td>
<td>$\frac{\partial \phi}{\partial r} = 0$ (outflow)</td>
</tr>
<tr>
<td>GH</td>
<td>0</td>
<td>0</td>
<td>T = 1,000 K (eqn. A.10)</td>
<td>$\phi = \text{const}$</td>
</tr>
<tr>
<td>HA</td>
<td>0</td>
<td>$\frac{\partial w}{\partial r} = 0$</td>
<td>$\frac{\partial h}{\partial r} = 0$</td>
<td>$\frac{\partial \phi}{\partial r} = 0$</td>
</tr>
</tbody>
</table>

Table A.1 Boundary conditions for the welding arc model.

The energy b.c.'s are given by a "free fall" type expression proposed by McKelliget and Szekely [A1] where:
\[ V_c = \frac{5}{2} \frac{k_B T_{c,\text{elec}}}{e} \]  
(A.8a)

\[ Q_{c,\text{ionic}} = |J_c| V_c \]  
(A.8b)

\( T_{c,\text{elec}} \) is the electron temperature and is approximated by the plasma temperature in the arc column adjacent to the cathode. \( V_c \) is used by eqn. (A.8b) to approximate the energy consumed in the cathode fall region to ionize the plasma. This b.c. is a positive source term to the energy equation. The cathode surface is assumed to be at 3,000 K which is the typical temperature observed for most GTAW at the cathode.

The electric potential b.c. at the cathode is given by:

\[ J_c = \frac{1}{\pi R_c^2} = 6.5 \times 10^7 \text{ A/m}^2 \quad r < R_c \]  
(A.9a)

\[ J_c = 0 \quad r \geq R_c \]  
(A.9b)

where \( R_c \) (AB) is the cathode spot radius. It is assumed that a single value of \( J_c \) is valid over a wide range of conditions. Zero gradient is assumed elsewhere for the electric potential. The inlet gas is assumed to be at 1,000 K. This boundary condition is not critical in affecting arc behavior as shown by Hsu et al [A2].

### A.2b Anode Region (Region GH)

The momentum b.c.'s are self-explanatory from Table A.1 where a no slip b.c. is imposed. In general, this is valid for both a solid surface and molten pool. In the case of the molten pool, the surface velocity of the pool (~ 0.5 m/s) is much less than the plasma gas surface velocity (~ 10 m/s) such that the molten surface appears stationary to the gas jet. This one way interaction ignores the effect of the weld pool velocity on the arc velocity. However, the effect of the gas shear stress on the weld pool surface is not ignored when the gas shear stress is of the same order of magnitude as the surface tension shear stress (see Chapter 4).

The anode temperature is assumed to be 1,000 K. It is felt that, in this instance, this assumption does not affect the arc substantially for the reasons outlined in Section 2.3.

The convective heat gained by the anode in the anode boundary layer is reflected as the
heat loss from the arc and is given by:

\[
Q_{\text{conv}} = \frac{0.515}{Pr_w} \left( \frac{\mu_e \rho_e}{\mu_w \rho_w} \right)^{0.11} \sqrt{\left( \frac{\mu_w \rho_w \frac{\partial u_e}{\partial r}}{\partial r} \right)} (h_e - h_w)
\]

(A.10)

where \( h_e \) is the enthalpy of the gas at the at the edge of the anode boundary layer and \( h_w \) is the enthalpy at the anode wall temperature (\( T_w = 1,000 \) K). This equation acts as a heat sink (negative source term) in the energy equation at the boundary layer. Equation (A.10) is derived from the correlations [A3,A4]:

\[
\frac{Nu_w}{\sqrt{Re_w}} = 0.515 \left( \frac{\mu_e \rho_e}{\mu_w \rho_w} \right)^{0.11}
\]

(A.11a)

\[
Q_{\kappa,\text{conv}} = \left( \frac{Nu_w}{\sqrt{Re_w}} \right) \frac{(h_e - h_w)}{Pr_w} \sqrt{\mu_w \rho_w \frac{u_e}{r}}
\]

(A.11b)

for stagnation point flow where the subscript \( e \) is for the properties evaluated at the electron temperature at the edge of the boundary layer and the subscript \( w \) for the wall temperature. Equation (A.11b) has been modified relative to eqn. (A.10).

The anode surface (Region GH) is taken to be isopotential (\( \phi = 0 \)). This is based on the assumption that the conductivity in the metal is much higher than the plasma and that the variation of the electric potential in the metal is much less than in the arc.

A.2c Arc Column (Regions EG and HA)

Symmetry is assumed for all the usual b.c.'s at the axis of symmetry. At the outflow, the inlet gas at DE and EF is assumed to be 1,000 K. Although this value is arbitrary, it is found that the computed arc behavior does not change significantly whether 1,000 K or 2,000 K is taken. This is because the specific heat variation outside the arc column is very small (520 J/kg-K at 1,000 K compared to 9,310 J/kg-K at 15,000 K) and does not pose a problem to the energy equation.

The inflow and outflow regions (EF and FG) are defined by the direction of the velocity \( u \) as calculated. In some instance, \( \partial u / \partial z \) or \( \partial h / \partial r \) gradients is used. The former is used to conserve mass as \( \rho \) may change due to temperature variation while the latter serves to indicate that heat loss by conduction and convection is zero.
A.3 Derived Arc Parameters

The anode heat flux to the work piece is calculated from:

\[ q_a = Q_{a,\text{elec}} + Q_{a,\text{conv}} + Q_{a,\text{rad}} \]  

(A.12)

where

\[ Q_{a,\text{elec}} = J_a \left( \frac{5}{2} + \frac{e \phi_a}{k_b \sigma} \right) \frac{k_b T_{a,\text{elec}}}{e} + J_a \Phi_a \]  

(A.12a)

\[ Q_{a,\text{rad}} = Q_{\text{rad},ij} = \int_{V_j} \frac{S_{R,ij}}{4 \pi r_{ij}^2} \cos \psi \, dV_j \]  

(A.12b)

\( Q_{a,\text{elec}} \) is the electronic contribution to the anode heat flux as derived from Pfender et al [A5,A6]. \( \phi_d \) is the thermal diffusion coefficient for electrons while \( T_{a,\text{elec}} \) is the electron temperature and is assumed to be equivalent to the film temperature such that \( T_f = 0.5(T_{a,\text{elec}} + T_w) \).

The term in parenthesis in eqn. (A.12a) is estimated to be 3.202 [A5]. The work function, \( \Phi_a \), of the anode wall is 4.3 V for Cu and 4.5 V for steel. \( Q_{a,\text{conv}} \) is the convective contribution and is given by eqn. (A.11b). \( Q_{a,\text{rad}} \) is the radiative contribution to the anode (Fig. A.2) The integral is re-written as an elliptic integral in azimuthal direction; the results of which is available from an integral table [A7]. The equation is then integrated numerically in r- and z-directions to obtain \( Q_{\text{rad},ij} \) for each location \( i,j \). At this juncture, vaporization from the anode is neglected from the arc modelling. However, it is included in the weld pool modelling. Experimental studies [A8,A9] have shown that vaporization from the anode is not as sensitive in affecting arc behavior as compared to vaporization from the cathode since the vapors from the anode are being swept away by the plasma jet once they leave the anode surface. This is certainly true for arc currents above 50 A [A8].

The arc voltage is given as:

\[ V_{\text{arc}} = V_c + V_{\text{col}} \]  

(A.13)

where

\[ V_{\text{col}} = (\phi_{c(\text{max})} - \phi_{c(\text{min})}) \]  

(A.13a)

\[ V_c = \frac{5}{2} \frac{k_b T_{c,\text{elec}}}{e} \]  

(A.13b)

The anode fall voltage is assumed to be zero. There is no reliable estimate of the anode fall voltages [A10] and even negative anode fall voltages have been reported [A5,A11]. For the current density encountered in arc welding, the negative anode drop voltage is calculated to be about 2 volts.
The arc efficiency is calculated as:

\[ \eta = \frac{L_r}{2\pi \int_0^L q_s (r) \, r \, dr} \]

\[ \eta = \frac{V_c + V_{col}}{V_c + V_{col}} \]  \hspace{1cm} (A.14)

The gas shear stress over the anode surface is given as:

\[ \tau_{gas} = -\mu_{gas} \frac{\partial u}{\partial z} \bigg|_{anode} \]  \hspace{1cm} (A.15)

The anode over-pressure is obtained from the pressure fields as calculated from the continuity equation.

![Anode Surface Diagram](image)

**Figure A.2** Configuration of radiation view factors.

- \( S_{R,i,j} \) is the view factor from the anode surface \( i \) to the volume element \( V_j \).
- \( r_{ij} \) is the distance from the anode surface \( i \) to the volume element \( j \).
- \( \Psi \) is the angle made by \( r_{ij} \) and the normal to the anode surface while \( \theta \) is the azimuthal direction with respect to the z-axis.

### A.4 Solution Technique

The governing equations and its associated b.c.'s were solved using 2/E/FIX, a finite-volume approached by Pun and Spalding [A12]. The difference equations were solved by iteration until convergence were satisfied to 99%. Variable grids are employed in all computations with the
smallest grids at the cathode fall region ($\Delta z=0.482$ mm, $\Delta r=0.15$ mm) and anode fall region ($\Delta z=0.2$ mm) and the largest near the mid-region of the arc ($\Delta z=0.65$ mm) and outflow ($\Delta r=1.2$ mm). A good discussion of the 2/E/FIX code is given by Patankar [A13].

A.5 Physical Properties of the argon plasma

The physical properties required for the argon plasma at atmospheric pressure are plotted in Fig. A.3–5. The plasma properties are obtained from Liu [A14] while the radiation source term is obtained from Evans and Tankin [A15]. It is important to note the highly non-linear properties of the argon arc with respect to temperature.

A.6 References

Figure A.3. Argon (a) density and (b) radiation source term as a function of temperature \([A14,A15]\).
Figure A.4. Argon (a) thermal conductivity and (b) specific heat as a function of temperature [A14].
Figure A.5. Argon (a) electrical conductivity and (b) viscosity as a function of temperature [A14].
APPENDIX B. MATHEMATICAL FORMULATION OF TURBULENCE MODEL

The two-equation K-\( \varepsilon \) turbulence model developed by Launder and Spaulding [B1] is employed in this work. However, several other texts and paper [B2-B6] are also consulted to establish the governing equations for cylindrical coordinates. The K-\( \varepsilon \) model employed have been simplified considerably. The reader should refer to Rodi [B7] for a more detailed description of the other terms in the turbulence equations.

Figure B1 shows the computational domain. The following assumptions are used for the turbulent model:

i) Isotropic turbulence is assumed but spatially variable turbulent viscosity is used.

ii) Density fluctuations due to turbulence are negligible.

iii) Heat capacity is assumed constant.

The symbols employed henceforth are local to this appendix and are given at the end of this appendix.

![Computational domain and boundary conditions](image)

Figure B1. Computational domain and boundary conditions.
B.1 Governing Equations

On the basis of the above assumptions, the governing equations in cylindrical coordinates are given as:

**Conservation of Mass**

\[
\frac{1}{r} \frac{\partial (ru)}{\partial r} + \frac{\partial w}{\partial z} = 0
\]  
(B.1)

**Conservation of Radial Momentum**

\[
\rho \left[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial r} + w \frac{\partial u}{\partial z} \right] = \left[ \frac{\partial}{\partial r} \left( \mu_{eff} \frac{\partial (ru)}{\partial r} \right) + \frac{\partial^2 u}{\partial z^2} \right] - \frac{\partial P}{\partial r} + J_2 B_0 - K_d u
\]  
(B.2)

**Conservation of Axial Momentum**

\[
\rho \left[ \frac{\partial w}{\partial t} + u \frac{\partial w}{\partial r} + w \frac{\partial w}{\partial z} \right] = \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( \mu_{eff} \frac{\partial w}{\partial r} \right) + \frac{\partial^2 w}{\partial z^2} \right] - \frac{\partial P}{\partial z} + J_r B_0 - K_d w + \rho g \beta (T - T_i)
\]  
(B.3)

**Conservation of Thermal Energy**

\[
\rho C_p \left[ \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial r} + w \frac{\partial T}{\partial z} \right] = \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( k_{eff} \frac{\partial T}{\partial r} \right) + \frac{\partial^2 T}{\partial z^2} \right] + \frac{\Delta H}{C_p} \frac{\partial T}{\partial t}
\]  
(B.4)

**Conservation of Turbulent Kinetic Energy**

\[
\rho \left[ \frac{\partial K}{\partial t} + u \frac{\partial K}{\partial r} + w \frac{\partial K}{\partial z} \right] = \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( \mu_{eff} \frac{\partial K}{\partial r} \right) + \frac{\partial}{\partial z} \left( \frac{\mu_{eff}}{\sigma_k} \frac{\partial K}{\partial z} \right) \right] + G_k - \rho e
\]  
(B.5)

**Dissipation Rate of Turbulence Energy**

\[
\rho \left[ \frac{\partial e}{\partial t} + u \frac{\partial e}{\partial r} + w \frac{\partial e}{\partial z} \right] = \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( \mu_{eff} \frac{\partial e}{\partial r} \right) + \frac{\partial}{\partial z} \left( \frac{\mu_{eff}}{\sigma_e} \frac{\partial e}{\partial z} \right) \right] + \frac{C_1 G_k \varepsilon}{K} - \frac{C_2 \rho e^2}{K}
\]  
(B.6)

**Generation of Turbulent Energy**

\[
G_k = 2 \mu_k \left[ \left( \frac{\partial u}{\partial r} \right)^2 + \left( \frac{\partial u}{\partial z} \right)^2 + \frac{1}{2} \left( \frac{\partial w}{\partial r} + \frac{\partial u}{\partial z} \right)^2 \right]
\]  
(B.7)

The terms in eqns. (B.1-B.4) have been previously examined in Chapter 3. Equations B.5 and B.6 consist of, from left to right, the convective term, the diffusive term, the generation term, and the destruction term. The rate of generation of turbulent kinetic energy, \( G_k \), given in eqn. (B.7) can be derived from the rate of irreversible conversion of mechanical energy to internal energy in the equation of mechanical energy [B5].

The effective viscosity and effective thermal conductivity are calculated as the sum of their molecular and turbulent components:
\[
\mu_{\text{eff}} = \mu + \mu_t \quad \text{(B.8)}
\]
\[
k_{\text{eff}} = k + k_t \quad \text{(B.9)}
\]

The turbulent viscosity in the K-\(\varepsilon\) model is given by:
\[
\mu_t = \rho C_{\mu} \frac{K^2}{\varepsilon} \quad \text{(B.10)}
\]

while the turbulent thermal conductivity can be derived from the turbulent Prandtl number:
\[
Pr_t = \frac{C_{\mu} \mu_t}{k_t} = 0.9 \quad \text{(B.11)}
\]

\(K\) and \(\varepsilon\) in eqn. (B.10) must be calculated from eqns. (B.5-7). The recommended values for the 5 empirical constants in these equations are:
\[
C_{\mu} = 0.09 \quad C_1 = 1.44 \quad C_2 = 1.92 \quad \sigma_k = 1.0 \quad \sigma_\varepsilon = 1.3 \quad \text{(B.12)}
\]

**B.2 Boundary Conditions**

For ease of discussion, the traditional boundary conditions for turbulent flows in a cylinder shall be first described following which the boundary conditions can be reduced to the welding problem. The typical boundary conditions for the K-\(\varepsilon\) model* are shown schematically in Figure B1. The b.c. for regions AB and AD are straight-forward where symmetry and free slip are assumed, respectively.

The K-\(\varepsilon\) model is best for flows in the regions that are strongly turbulent, that is \(\mu_t >> \mu\). For flow adjacent to a solid boundary (regions BC and CD), special treatment is required in order to avoid the use of extremely fine grids that would be needed to resolve the details of the transition from laminar-like flow at the wall to the viscous sub-layer and to the turbulent core. One way to bridge the viscous sub-layer and to impose solid wall b.c. on the K-\(\varepsilon\) model of strongly turbulent flows is to assume a "wall function". This is treated in further detail in Fig. B2 where a section of the solid wall is shown.

*The boundary conditions for the momentum and energy equations have been given in Chapter 3.*
The wall function approach assumes that at $y = y_c$, the velocity component parallel to the wall obeys the logarithmic law of the wall:

$$\frac{u_k}{u_*} = \frac{1}{K_v} \ln \left( \frac{u_* y_c}{v} \right)$$

where

$$u_* = \frac{\tau_o}{\rho}$$

$K_v$ is the von Karman's constant and is estimated to be 0.41 while $E$ is the roughness parameter which is 9.8 for smooth walls. If at the same location, the generation of $K$ is in equilibrium with the destruction of $K$, then it can be shown that

$$K_c = \frac{u_*^2}{\sqrt{C_\mu}}$$

$$\varepsilon_c = \frac{u_*^3}{K_v y_c}$$

The treatment so far is for smooth surfaces where experimental data shows that $K/u_*^2 \approx 3.3$ such that $C_\mu = 0.09$ from eqn. (B.15). For rough surface, experimental studies indicate that $K/u_*^2 \approx 5.5$ such that $C_\mu = 0.033$. Furthermore, for rough surface, there is an additional constant on the right side of eqn. (B.13).

Summarizing, from the velocity $u_c$ at the wall, the wall shear stress $\tau_o$ can be determined. Then using eqns. (B.15) and (B.16), both $K_c$ and $\varepsilon_c$ at point $y_c$ adjacent to the wall can be calculated and the boundary conditions are thus specified.
B.3 Boundary Conditions Particular to the Weld Pool

The above discussion can now be directed at the weld pool. The most pressing problem is the specification of the b.c. at the solid-liquid interface, specifically the mushy zone. Not only must \( u_c \) be parallel to the wall which can be a problem as the solid-liquid boundary curves, but also some velocity profile must be assumed in this region. If, as a first approximation, the temperature of a cell which is below the liquidus temperature is assumed to be solid, then a staircase solid-liquid profile will be obtained. This is not desirable as the flow can be impeded.

Ideally, the problem can best be handled by adaptive meshes or body-fitted coordinates that change as the pool grows. Firstly, this will take care of the wall functions as the mesh can change its size and shape to suit the solid-liquid contour. Secondly, it also overcomes the problem of the \( K-\epsilon \) equations in the solid phase as they need not be solved. Here, the governing equations may have to be formulated using porosity factors.

The boundary conditions for the weld pool is tedious to impose. As a first step towards the analysis of turbulent flow, a major assumption is invoked whereby no slip b.c.'s are imposed at regions BC and CD. The \( K-\epsilon \) equations are allowed to achieve convergence on the basis of the diminishing velocity due to drag in the mushy zone and solid phase. We understand that this is a serious drawback for this analysis but nevertheless, it will allow scoping studies to be performed.

B.4 References

B.5 Nomenclature

\[ B_0 \quad \text{azimuthal magnetic field (Wb/m}^2) \]
\[ C_1 \quad \text{constant in turbulence model (\(-\) \)} \]
\[ C_2 \quad \text{constant in turbulence model (\(-\) \)} \]
\[ C_\mu \quad \text{constant in turbulence model (\(-\) \)} \]
\[ C_p \quad \text{heat capacity (J/kg-K) \)} \]
\[ E \quad \text{roughness parameter = 9.8 \)} \]
\[ f_L \quad \text{fraction of liquid (\(-\) \)} \]
\[ G_k \quad \text{generation of turbulence energy (kg-m/s}^5) \]
\[ g \quad \text{gravitational acceleration (m/s}^2) \]
\[ J_r \quad \text{radial current density (A/m}^2) \]
\[ J_z \quad \text{axial current density (A/m}^2) \]
\[ K \quad \text{turbulent kinetic energy (kg-m/s}^5) \]
\[ K_d \quad \text{drag coefficient in source term for phase change source term (kg/m}^3s) \]
\[ k \quad \text{molecular thermal conductivity (W/m-K) \)} \]
\[ k_{\text{eff}} \quad \text{effective thermal conductivity (W/m-K) \)} \]
\[ k_t \quad \text{turbulent thermal conductivity (W/m-K) \)} \]
\[ K_v \quad \text{von Karman's constant = 0.41 \)} \]
\[ P \quad \text{pressure (Pa) \)} \]
\[ Pr_t \quad \text{turbulent Prandtl number = } C_p \mu_\kappa/k_\kappa (\cdot) \]
\[ r \quad \text{radial coordinate (m) \)} \]
\[ T \quad \text{temperature (K) \)} \]
\[ T_r \quad \text{reference temperature for Boussinesq approximation (K) \)} \]
\[ t \quad \text{time (s) \)} \]
\[ u \quad \text{radial velocity (m/s) \)} \]
\[ u_c \quad \text{velocity parallel to wall at } y_c \text{ (m/s) \)} \]
\[ u_* \quad \text{friction velocity (m/s) = } (\tau_o/\rho) \quad \text{\)} \]
\[ w \quad \text{axial velocity (m/s) \)} \]
\[ y_c \quad \text{location relative to wall (m) \)} \]
\[ z \quad \text{axial coordinate (m) \)} \]
\[ \beta \quad \text{coefficient of thermal expansion (T}^{-1}) \]
\[ \Delta H \quad \text{latent heat of fusion (J/kg) \)} \]
\[ \varepsilon \quad \text{turbulent dissipation rate (m}^4$s$^5) \]
\[ \mu \quad \text{molecular dynamic viscosity (kg/m-s) \)} \]
\[ \mu_{\text{eff}} \quad \text{effective dynamic viscosity (kg/m-s) \)} \]
\[ \mu_t \quad \text{turbulent dynamic viscosity (kg/m-s) \)} \]
\[ \rho \quad \text{density at } y_c \text{ (kg/m}^3) \]
\[ \nu \quad \text{kinematic viscosity (m}^2$s$) \]
\[ \sigma_k \quad \text{Prandtl number for K (\(-\) \)} \]
\[ \sigma_\varepsilon \quad \text{Prandtl number for } \varepsilon (\cdot) \]
\[ \tau_o \quad \text{actual wall shear stress (Pa) \)} \]
9. REFERENCES

35 N.N. Rykalin, Calculations of Heat Processes in Welding, printed in 1960 in Moscow, USSR.


104. see op. cit. [18], p. 188.


106. op. cit. [67], p. 132.

107. ibid., p. 140.


109. op. cit. [18], pp. 192-193.

110. op. cit. [67], p. 166.

111. op. cit. [105], p. 34.


124. op. cit. [121], pp. 139-140.


131. ibid., p. 746.

132. op. cit. [121], pp. 358-377.