Metal fusion using pulsed Gas Metal Arc: Melt pool modelling and CFD simulation

Pradip Aryal
Metal fusion using pulsed Gas Metal Arc: Melt pool modelling and CFD simulation

Pradip Aryal
dedication
To Maya and my family
Acknowledgments

First and foremost, I would like to express my sincere gratitude to my main supervisor Assoc. Prof. Isabelle Choquet for her extensive help, continuous support and encouragement. Her enthusiasm for the subject matter, combined with her adept mentoring skills, played a pivotal role in facilitating the successful completion of this thesis. I would also like to thank my co-supervisors Assoc. Prof Fredrik Sikström and Prof. Håkan Nilsson for for their unwavering guidance, thought-provoking discussions, meticulous reviews, and valuable feedback.

Many thanks to all the research engineers for sharing their invaluable knowledge. A special mention to Kjell Hurtig for his invaluable assistance and expertise in conducting experiments.

I would like to acknowledge the funding organisation EU project - Horizon 2020: INTEGRADDE for the financial support. Your contribution has empowered us to push the boundaries of knowledge and explore new frontiers. I would also like to extend my appreciation to our industry collaborators, with a special mention to the Loiretech group.

I would like to acknowledge the Swedish National Infrastructure for Computing (SNIC) at NSC for generously providing the computational resources essential for conducting the numerical simulations.

My heartfelt thanks for the wonderful support I have received from my friends in this research group, as well as from other groups. Your encouragement, discussions, and shared insights have been instrumental in this journey.

In addition, I would like to thank my family for their support. Their belief in me has been my strength, inspiring me to overcome challenges. And last but certainly not least, I want to express my deepest gratitude to Shiyaa. Your presence has brought a sense of balance, positivity, and harmony that has been transformative for me. Your unwavering support have added a new dimension of fulfillment, making each step of my journey more meaningful.

Pradip Aryal
Trollhättan, October 2023
Acknowledgments

First and foremost, I would like to express my sincere gratitude to my main supervisor Assoc. Prof. Isabelle Choquet for her extensive help, continuous support and encouragement. Her enthusiasm for the subject matter, combined with her adept mentoring skills, played a pivotal role in facilitating the successful completion of this thesis. I would also like to thank my co-supervisors Assoc. Prof Fredrik Sikström and Prof. Håkan Nilsson for their unwavering guidance, thought-provoking discussions, meticulous reviews, and valuable feedback.

Many thanks to all the research engineers for sharing their invaluable knowledge. A special mention to Kjell Hurtig for his invaluable assistance and expertise in conducting experiments.

I would like to acknowledge the funding organisation EU project - Horizon 2020: INTEGRADDE for the financial support. Your contribution has empowered us to push the boundaries of knowledge and explore new frontiers. I would also like to extend my appreciation to our industry collaborators, with a special mention to the Loiretech group.

I would like to acknowledge the Swedish National Infrastructure for Computing (SNIC) at NSC for generously providing the computational resources essential for conducting the numerical simulations.

My heartfelt thanks for the wonderful support I have received from my friends in this research group, as well as from other groups. Your encouragement, discussions, and shared insights have been instrumental in this journey.

In addition, I would like to thank my family for their support. Their belief in me has been my strength, inspiring me to overcome challenges. And last but certainly not least, I want to express my deepest gratitude to Shiyaa. Your presence has brought a sense of balance, positivity, and harmony that has been transformative for me. Your unwavering support have added a new dimension of fulfillment, making each step of my journey more meaningful.

Pradip Aryal
Trollhättan, October 2023

Det utförda modelleringsarbetet har gjort det möjligt att förklara hur flödet i smältan och dess geometri orsakar defekter vid ändringar av ett arbetsstyckes orientering så lite som 20° jämfört med horisontell positionering vid svets i V-fog. Dessutom använder moderna numeriska modeller för smältans fysik olika delmodeller för att beräkna den elektromagnetiska kraften och tidsberoendet hos en pulserande ljusbåge. Dessa delmodeller jämförandes i en analys för att förklara deras signifikanta skillnader vid simulering av smältflödet, termisk konvektion, ytvågor, smältans form och stelnade geometri. De föreslagna förbättringarna i modelleringen baserat på denna analys har gett mer noggranna förutsägelser av processens smältzon, vilket bidrar till utvecklingen av en sant prediktiv simuleringsmodell som kommer att vara användbar i den efterfrågade utvecklingen av gasmetallbågsprocessen.
Populärvetenskaplig
Sammanfattning

Sökord: Gasmetallbågsvetsning, Svetsläge, Elektromagnetiskkraftmodellering, Smältytans rörelser, Computational Fluid Dynamics, OpenFOAM

Gasmetallbågsprocessen har revolutionerat metallbearbetning och produktionsteknik under ett århundrade med sin påfallande effektivitet och mångsidighet, speciellt vid svetsning. På senare år har denna teknik också tillämpats alltmer inom additiv tillverkning (AM), även känt som 3D-printing. Gasmetallbågsbaserad AM har väckt ett stort industriellt intresse på grund av dess förmåga att tillverka stora och komplexa komponenter. Det finns dock problem, dels kring defekter i processen, dels kring numeriska modellers förmåga att simulera processen. Följaktligen finns det ett behov av en djupare förståelse och förbättrade modeller för att övervinna dessa utmaningar och frigöra den fulla potentialen i denna teknologi. För att angripa detta problem utvecklades och tillämpades modellering med hjälp strömningsmekaniska beräkningar (CFD) i detta avhandlingsarbete, tillsammans med fysiska experiment för att komplettera modelleringssARBETET.

Det utförda modelleringssARBETET har gjort det möjligt att förklara hur flödet i smältan och dess geometri orsakar defekter vid ändringar av ett arbetsstyckes orientering så lite som 20° jämfört med horisontell positionering vid svets i V-fog. Dessutom använder moderna numeriska modeller för smältans fysik olika delmodeller för att beräkna den elektromagnetiska kraften och tidsberoendet hos en pulserande ljusbåge. Dessa delmodeller jämförandes i en analys för att förklara deras signifikanta skillnader vid simulering av småtfloedet, termisk konvektion, ytvågor, smältans form och stelnade geometri. De föreslagna förbättringarna i modelleringen baserat på denna analys har gett mer noggranna förutsägelser av processens smältzon, vilket bidrar till utvecklingen av en sant prediktiv simuleringsmodell som kommer att vara användbar i den efterfrågade utvecklingen av gasmetallbågsprocessen.
Pulsed gas metal arc is a highly efficient technique used in manufacturing processes like welding and additive manufacturing. It offers high productivity and cost benefits but it is also prone to defect formation when process parameters are not properly controlled and optimized. A deeper process understanding can support achieving improved process control and mitigate these potential drawbacks. Nevertheless, there are still several challenges. For instance, the correlation between the input and output process parameters is non-linear and complex due to the multi-physics nature of the process. In addition, the elevated temperature and the intense radiative emission from the arc, along with the smoke, and the non-transparency of metal, make in-process observation challenging. Modelling and simulation offer a complementary approach to gain a deeper process understanding. In this study, a thermo- and fluid dynamics model was developed, focusing on the melt pool and metal deposition, while simplifying the arc to boundary conditions (decoupled approach). This model incorporates various forces and phenomena such as thermocapillary and electromagnetic forces, melting and solidification, and tracking of surface deformation and droplet coalescence.

In the first part of the thesis, the developed model was applied to investigate the effect of workpiece orientations on the melt pool dynamics and reinforced bead geometry in multi-layer gas metal arc welding of a V-groove joint. The comparison of the predicted fusion zone with macrographs obtained from the experiments showed good qualitative agreement. It was found that the force balance in the melt pool changes significantly when changing the workpiece orientation by as little as 20° relative to the flat position. This results in distinct melt flow...
Abstract

Title: Metal fusion using pulsed Gas Metal Arc: Melt pool modelling and CFD simulation

Language: English

Keywords: Gas metal arc, Electromagnetic force modelling, Free surface deformation, Computational Fluid Dynamics, OpenFOAM

ISBN 978-91-89325-45-6 (Electronic version)

Pulsed gas metal arc is a highly efficient technique used in manufacturing processes like welding and additive manufacturing. It offers high productivity and cost benefits but it is also prone to defect formation when process parameters are not properly controlled and optimized. A deeper process understanding can support achieving improved process control and mitigate these potential drawbacks. Nevertheless, there are still several challenges. For instance, the correlation between the input and output process parameters is non-linear and complex due to the multi-physics nature of the process. In addition, the elevated temperature and the intense radiative emission from the arc, along with the smoke, and the non-transparency of metal, make in-process observation challenging. Modelling and simulation offer a complementary approach to gain a deeper process understanding. In this study, a thermo- and fluid dynamics model was developed, focusing on the melt pool and metal deposition, while simplifying the arc to boundary conditions (decoupled approach). This model incorporates various forces and phenomena such as thermocapillary and electromagnetic forces, melting and solidification, and tracking of surface deformation and droplet coalescence.

In the first part of the thesis, the developed model was applied to investigate the effect of workpiece orientations on the melt pool dynamics and reinforced bead geometry in multi-layer gas metal arc welding of a V-groove joint. The comparison of the predicted fusion zone with macrographs obtained from the experiments showed good qualitative agreement. It was found that the force balance in the melt pool changes significantly when changing the workpiece orientation by as little as 20° relative to the flat position. This results in distinct melt flow
patterns, melt pool shapes, bead geometries, and in some cases, defect formation such as humping, undercut, and insufficient fusion. It was concluded that to avoid these defects a lower angle range is necessary for multilayer welding with the uphill orientation and side inclination.

The second part of the thesis focused on analyzing different variants of the model for the electromagnetic force with a decoupled approach. Three commonly used models were compared: (1) the analytical models proposed by Kou and Sun in integral form, (2) by Tsao and Wu in algebraic form, and (3) the partial differential equations governing the electric and magnetic fields. The comparative investigation was supported by experimental tests that also provided estimates of unknown model parameters and validation data. It was found that the distinct assumptions on which these models rely are not all justified. They resulted in predicting different melt flow patterns and amplitude of the free surface oscillations, as well as different melt pool shapes and bead geometries. Model (3) is recommended to advance to a predictive melt pool model and was subsequently used in the remaining work of the thesis.

Furthermore, the literature shows that modeling the effect of pulsed arc on the melt pool using a decoupled approach involves various simplifications. Arc pulsation affects energy and force balance in the melt pool through arc heat flux, arc pressure, and electromagnetic force. A systematic investigation of model variants considering pulsing was conducted using previously documented experimental test cases. The results showed that the influence of arc pressure was insignificant in those cases. However, model variants simplifying arc pulsing to a time-averaged effect underestimated the amplitude of the Marangoni flow and downward flow compared to a more comprehensive approach that considered the time dependence of arc pulsation. Thus, it is recommended to use a melt pool model that accounts for the time-dependent arc pulsation, which was also subsequently utilized in the remaining work of the thesis.

The electromagnetic force models discussed earlier assume a stationary free surface when computing the electromagnetic force. However, this force is often at leading order in the vicinity of the arc. In the same region, the metal drop transfer leads to a periodic deformation of the melt pool free surface. In the final part of the thesis, the model was extended to account for free surface deformation when computing the electromagnetic force. This extension was applied to experimental test cases, and a comparison was made with simulation results obtained using the stationary electromagnetic force model. Significant differences in the results were observed, particularly in predicting the experimentally observed fingertip-shaped fusion zone geometry. The proposed improvement in the electromagnetic force model provided better predictions in this regard.
Publications

Appended journal articles and manuscripts


IV. P. Aryal, I. Choquet, Melt pool electromagnetic force model extended to account for free surface deformation - Application to gas metal arc. (Submitted to International Journal of Heat and Mass Transfer).
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\vec{A})</td>
<td>Magnetic potential ([N/A])</td>
</tr>
<tr>
<td>(A)</td>
<td>Permeability coefficient of mushy zone ([-])</td>
</tr>
<tr>
<td>(as)</td>
<td>Activity of the surface element in % weight ([%])</td>
</tr>
<tr>
<td>(\vec{B})</td>
<td>Magnetic field ([T])</td>
</tr>
<tr>
<td>(B_\theta)</td>
<td>Azimuthal magnetic field ([T])</td>
</tr>
<tr>
<td>(B_0)</td>
<td>Bond number ([-])</td>
</tr>
<tr>
<td>(Ca)</td>
<td>Capillary number ([-])</td>
</tr>
<tr>
<td>(C_\alpha)</td>
<td>Interface compression factor ([-])</td>
</tr>
<tr>
<td>(c)</td>
<td>Specific heat capacity ([J/(kg K)])</td>
</tr>
<tr>
<td>(D_{\text{drop}})</td>
<td>Diameter of molten drop ([m])</td>
</tr>
<tr>
<td>(d)</td>
<td>Gaussian distribution factor ([-])</td>
</tr>
<tr>
<td>(\vec{E})</td>
<td>Electric field ([V/m])</td>
</tr>
<tr>
<td>(\vec{F})</td>
<td>(\vec{J} \times \vec{B}) Electromagnetic force ([N])</td>
</tr>
<tr>
<td>(f_{\text{drop}})</td>
<td>Frequency of drop transfer ([s^{-1}])</td>
</tr>
<tr>
<td>(f_l)</td>
<td>Liquid fraction ([-])</td>
</tr>
<tr>
<td>(\vec{g})</td>
<td>Gravitational acceleration ([m/s^2])</td>
</tr>
<tr>
<td>(\Delta H_0)</td>
<td>Standard heat of adsorption ([J/(kg mol)])</td>
</tr>
<tr>
<td>(h)</td>
<td>Specific enthalpy ([J/kg])</td>
</tr>
<tr>
<td>(h_{sf})</td>
<td>Latent heat of fusion ([J/kg])</td>
</tr>
<tr>
<td>(h_{fv})</td>
<td>Latent heat of vaporization ([J/kg])</td>
</tr>
</tbody>
</table>
## NOMENCLATURE

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\vec{A}$</td>
<td>Magnetic potential [N/A]</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Permeability coefficient of mushy zone [-]</td>
</tr>
<tr>
<td>$a_s$</td>
<td>Activity of the surface element in % weight [%]</td>
</tr>
<tr>
<td>$\vec{B}$</td>
<td>Magnetic field [T]</td>
</tr>
<tr>
<td>$B_\theta$</td>
<td>Azimuthal magnetic field [T]</td>
</tr>
<tr>
<td>$Bo$</td>
<td>Bond number [-]</td>
</tr>
<tr>
<td>$Ca$</td>
<td>Capillary number [-]</td>
</tr>
<tr>
<td>$C_\alpha$</td>
<td>Interface compression factor [-]</td>
</tr>
<tr>
<td>$c_p$</td>
<td>Specific heat capacity [J/(kg K)]</td>
</tr>
<tr>
<td>$D_{drop}$</td>
<td>Diameter of molten drop [m]</td>
</tr>
<tr>
<td>$d$</td>
<td>Gaussian distribution factor [-]</td>
</tr>
<tr>
<td>$\vec{E}$</td>
<td>Electric field [V/m]</td>
</tr>
<tr>
<td>$\vec{F}_{\vec{E} \times \vec{B}}$</td>
<td>Electromagnetic force [N]</td>
</tr>
<tr>
<td>$f_{drop}$</td>
<td>Frequency of drop transfer [s$^{-1}$]</td>
</tr>
<tr>
<td>$f_l$</td>
<td>Liquid fraction [-]</td>
</tr>
<tr>
<td>$\vec{g}$</td>
<td>Gravitational acceleration [m/s$^2$]</td>
</tr>
<tr>
<td>$\Delta H^0$</td>
<td>Standard heat of adsorption [J/(kg mol)]</td>
</tr>
<tr>
<td>$h$</td>
<td>Specific enthalpy [J/kg]</td>
</tr>
<tr>
<td>$h_{sf}$</td>
<td>Latent heat of fusion [J/kg]</td>
</tr>
<tr>
<td>$h_{fv}$</td>
<td>Latent heat of vaporization [J/kg]</td>
</tr>
</tbody>
</table>
NOMENCLATURE

$I$         Electric current [A]
$j$         Current density [J/m$^2$]
$j_r$       Radial component of current density [J/m$^2$]
$j_z$       Vertical component of current density [J/m$^2$]
$J_0$       Bessel function of zero order and first kind [-]
$J_1$       Bessel function of first order and first kind [-]
$k$         Thermal conductivity [W/(m K)]
$k_l$       Entropy factor [J/(kg K)]
$k_B$       Boltzmann constant [J/K]
$k_{electrical}$   Electrical resistivity [Ω·m]
$L_c$       Characteristic melt pool length [m]
$Ma$        Marangoni number [-]
$m$         Element atomic weight [kg]
$m_{vap}$   Mass flux of evaporation [kg/s]
$p$         Pressure [Pa]
$p_{arc}$   Arc pressure [Pa]
$p_{sat}$   Saturated vapor pressure [Pa]
$p_{amb}$   Ambient pressure at standard condition [Pa]
$Pe$        Peclet number [-]
$Pr$        Prandtl number [-]
$q_{arc}$   Energy source term due to arc [W/m$^2$]
$q_{drop}$  Energy source term due to metal drop [W/m$^2$]
$q_{rad}$   Rate of radiative cooling [W/m$^2$]
$R$         Universal gas constant [J/(mol K)]
$Ra$        Rayleigh number [-]
$Re$        Marangoni Reynolds number [-]
$Rm$        Magnetic Reynolds number [-]
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_w$</td>
<td>Wire radius [m]</td>
</tr>
<tr>
<td>$r$</td>
<td>Radius [m]</td>
</tr>
<tr>
<td>$t$</td>
<td>Time [s]</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature [K]</td>
</tr>
<tr>
<td>$T_m$</td>
<td>Melting temperature [K]</td>
</tr>
<tr>
<td>$T_l$</td>
<td>Liquidus temperature [K]</td>
</tr>
<tr>
<td>$T_s$</td>
<td>Solidus temperature [K]</td>
</tr>
<tr>
<td>$T_{amb}$</td>
<td>Ambient temperature [K]</td>
</tr>
<tr>
<td>$T_v$</td>
<td>Vaporization temperature [K]</td>
</tr>
<tr>
<td>$\Delta T$</td>
<td>Temperature difference [K]</td>
</tr>
<tr>
<td>$\bar{\bar{u}}$</td>
<td>Fluid velocity vector [m/s]</td>
</tr>
<tr>
<td>$U_c$</td>
<td>Characteristic melt flow velocity [m/s]</td>
</tr>
<tr>
<td>$\bar{U}_{wp}$</td>
<td>Workpiece travel velocity vector [m/s]</td>
</tr>
<tr>
<td>$V$</td>
<td>Electric voltage [V]</td>
</tr>
<tr>
<td>$WFR$</td>
<td>Wire feed rate [m/s]</td>
</tr>
<tr>
<td>$x$</td>
<td>x coordinate [m]</td>
</tr>
<tr>
<td>$y$</td>
<td>y coordinate [m]</td>
</tr>
<tr>
<td>$z$</td>
<td>z coordinate [m]</td>
</tr>
<tr>
<td>$x_0$</td>
<td>x coordinate of the arc centre on workpiece surface [m]</td>
</tr>
<tr>
<td>$y_0$</td>
<td>y coordinate of the arc centre on workpiece surface [m]</td>
</tr>
<tr>
<td>$z_0$</td>
<td>z coordinate of the arc centre on workpiece surface [m]</td>
</tr>
<tr>
<td>$x_{drop}$</td>
<td>x coordinate of the centre of molten drop [m]</td>
</tr>
<tr>
<td>$y_{drop}$</td>
<td>y coordinate of the centre of molten drop [m]</td>
</tr>
<tr>
<td>$z_{drop}$</td>
<td>z coordinate of the centre of molten drop [m]</td>
</tr>
</tbody>
</table>

**Greek Symbol**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\eta_{arc}$</td>
<td>Total thermal efficiency [-]</td>
</tr>
</tbody>
</table>
### NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\eta_{arc\rightarrow pool}$</td>
<td>Arc thermal efficiency</td>
<td>[-]</td>
</tr>
<tr>
<td>$\eta_{arc\rightarrow drop}$</td>
<td>Droplet thermal efficiency</td>
<td>[-]</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Surface tension coefficient</td>
<td>[N/m]</td>
</tr>
<tr>
<td>$\sigma_0$</td>
<td>Surface tension coefficient at melting temperature</td>
<td>[N/(m K)]</td>
</tr>
<tr>
<td>$\left(\frac{\partial \sigma}{\partial T}\right)_0$</td>
<td>Coefficient of surface tension temperature gradient</td>
<td>[N/m]</td>
</tr>
<tr>
<td>$\sigma_{SB}$</td>
<td>Stefan Boltzmann constant</td>
<td>[W/(m² K⁴)]</td>
</tr>
<tr>
<td>$\sigma_e$</td>
<td>Electrical conductivity</td>
<td>[1/(Ω m)]</td>
</tr>
<tr>
<td>$\sigma_{arc, j}$</td>
<td>Arc parameter for current density distribution</td>
<td>[m]</td>
</tr>
<tr>
<td>$\sigma_{arc, p}$</td>
<td>Arc parameter for arc pressure distribution</td>
<td>[m]</td>
</tr>
<tr>
<td>$\sigma_{arc, q}$</td>
<td>Arc parameter for heat flux distribution</td>
<td>[m]</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Dynamic viscosity</td>
<td>[Pa s]</td>
</tr>
<tr>
<td>$\mu_0$</td>
<td>Permeability of free space</td>
<td>[T m/A]</td>
</tr>
<tr>
<td>$\mu_m$</td>
<td>Permeability of medium</td>
<td>[T m/A]</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Volume fraction</td>
<td>[-]</td>
</tr>
<tr>
<td>$\alpha_{drop}$</td>
<td>Volume source term</td>
<td>[-]</td>
</tr>
<tr>
<td>$\alpha_T$</td>
<td>Thermal diffusivity</td>
<td>[m²/s]</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density</td>
<td>[kg/m³]</td>
</tr>
<tr>
<td>$\rho_{drop}$</td>
<td>Mass source term</td>
<td>[kg/m³]</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Thermal expansion coefficient</td>
<td>[1/K]</td>
</tr>
<tr>
<td>$\beta_r$</td>
<td>Retro-diffusion coefficient</td>
<td>[-]</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>Radiative emissivity</td>
<td>[-]</td>
</tr>
<tr>
<td>$\varepsilon_m$</td>
<td>Permittivity of medium</td>
<td>[N m²/C²]</td>
</tr>
<tr>
<td>$\varepsilon_0$</td>
<td>Permittivity of free space</td>
<td>[N m²/C²]</td>
</tr>
<tr>
<td>$\Gamma_s$</td>
<td>Surface excess at saturation condition</td>
<td>[J/(kg mol m²)]</td>
</tr>
</tbody>
</table>

### Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>AM</td>
<td>Additive Manufacturing</td>
</tr>
</tbody>
</table>

xii
<table>
<thead>
<tr>
<th>NOMENCLATURE</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>η</td>
<td>Arc thermal efficiency</td>
</tr>
<tr>
<td>η→pool</td>
<td>Droplet thermal efficiency</td>
</tr>
<tr>
<td>σ</td>
<td>Surface tension coefficient</td>
</tr>
<tr>
<td>σ0</td>
<td>Surface tension coefficient at melting temperature</td>
</tr>
<tr>
<td>(∂σ/∂T)0</td>
<td>Coefficient of surface tension temperature gradient</td>
</tr>
<tr>
<td>σSB</td>
<td>Stefan Boltzmann constant</td>
</tr>
<tr>
<td>σe</td>
<td>Electrical conductivity</td>
</tr>
<tr>
<td>σarc,⃗j</td>
<td>Arc parameter for current density distribution</td>
</tr>
<tr>
<td>σarc,p</td>
<td>Arc parameter for arc pressure distribution</td>
</tr>
<tr>
<td>σarc,q</td>
<td>Arc parameter for heat flux distribution</td>
</tr>
<tr>
<td>µ</td>
<td>Dynamic viscosity</td>
</tr>
<tr>
<td>µ0</td>
<td>Permeability of free space</td>
</tr>
<tr>
<td>µm</td>
<td>Permeability of medium</td>
</tr>
<tr>
<td>α</td>
<td>Volume fraction</td>
</tr>
<tr>
<td>αdrop</td>
<td>Volume source term</td>
</tr>
<tr>
<td>αT</td>
<td>Thermal diffusivity</td>
</tr>
<tr>
<td>ρ</td>
<td>Density</td>
</tr>
<tr>
<td>ρdrop</td>
<td>Mass source term</td>
</tr>
<tr>
<td>β</td>
<td>Thermal expansion coefficient</td>
</tr>
<tr>
<td>βr</td>
<td>Retro-diffusion coefficient</td>
</tr>
<tr>
<td>ε</td>
<td>Radiative emissivity</td>
</tr>
<tr>
<td>εm</td>
<td>Permittivity of medium</td>
</tr>
<tr>
<td>ε0</td>
<td>Permittivity of free space</td>
</tr>
<tr>
<td>Γs</td>
<td>Surface excess at saturation condition</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Abbreviations Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>CFL</td>
<td>Courant Friedrichs Lewy number</td>
</tr>
<tr>
<td>CSF</td>
<td>Continuum Surface Force</td>
</tr>
<tr>
<td>CTWD</td>
<td>Contact-tip to workpiece distance</td>
</tr>
<tr>
<td>DI</td>
<td>Diffuse Interface</td>
</tr>
<tr>
<td>DILU</td>
<td>Diagonal Incomplete LU</td>
</tr>
<tr>
<td>DNS</td>
<td>Direct Numerical Simulation</td>
</tr>
<tr>
<td>EMF</td>
<td>Electromagnetic force</td>
</tr>
<tr>
<td>FDM</td>
<td>Finite Difference Method</td>
</tr>
<tr>
<td>FCT</td>
<td>Flux Corrected Transport</td>
</tr>
<tr>
<td>FVM</td>
<td>Finite Volume Method</td>
</tr>
<tr>
<td>FZ</td>
<td>Fusion Zone</td>
</tr>
<tr>
<td>GAMG</td>
<td>Generalised Geometric Algebraic Multi-Grid</td>
</tr>
<tr>
<td>GMA</td>
<td>Gas Metal Arc</td>
</tr>
<tr>
<td>GMAW</td>
<td>Gas Metal Arc Welding</td>
</tr>
<tr>
<td>GTA</td>
<td>Gas Tungsten Arc</td>
</tr>
<tr>
<td>GTAW</td>
<td>Gas Tungsten Arc Welding</td>
</tr>
<tr>
<td>HAZ</td>
<td>Heat Affected Zone</td>
</tr>
<tr>
<td>LBW</td>
<td>Laser Beam Welding</td>
</tr>
<tr>
<td>LS</td>
<td>Level Set</td>
</tr>
<tr>
<td>MAC</td>
<td>Marker and Cell</td>
</tr>
<tr>
<td>MULES</td>
<td>Multidimensional Universal Limiter for Explicit Solutions</td>
</tr>
<tr>
<td>PDE</td>
<td>Partial Differential Equation</td>
</tr>
<tr>
<td>PISO</td>
<td>Pressure Implicit with Splitting of Operators</td>
</tr>
<tr>
<td>OpenFOAM®</td>
<td>Open Source Field Operation and Manipulation</td>
</tr>
<tr>
<td>RQ</td>
<td>Research Question</td>
</tr>
<tr>
<td>SIMPLE</td>
<td>Semi Implicit Method for Pressure-Linked Equations</td>
</tr>
</tbody>
</table>
### NOMENCLATURE

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SSF</td>
<td>Sharp Surface Force</td>
</tr>
<tr>
<td>VOF</td>
<td>Volume of Fluid</td>
</tr>
</tbody>
</table>
# Contents

Acknowledgments i  
Populärvetenskaplig Sammanfattning iii  
Abstract v  
Publications vii  
NOMENCLATURE ix  

## 1 Introduction  
1.1 Motivation ........................................ 1  
1.2 Research gaps ...................................... 5  
1.3 Research questions and objectives ............... 6  
1.4 Scope and limitations ............................. 7  
1.5 Methodology ...................................... 8  
1.6 Outline ........................................... 10  

## 2 Gas metal arc fusion  
2.1 A description of the method .................... 11  
2.2 Metal transfer modes .............................. 14  
  2.2.1 Short-circuit transfer mode .................. 14  
  2.2.2 Globular transfer mode ....................... 15  
  2.2.3 Spray transfer mode .......................... 15  
2.3 Heat transfer and melt pool driving forces ....... 17  
2.4 Typical defects in gas metal arc fusion .......... 22  

## 3 State of the art  
3.1 A brief history of melt pool modelling: early developments 27  
3.2 A brief history of melt pool modelling: extension to convection 29  
3.3 Melt pool modelling of non-flat welding orientation ........ 30  
3.4 Electro-magnetic force models applied to the melt pool .... 32  
3.5 Effect of arc pulsation on the melt pool flow .......... 35  
3.6 Effect of self-adaptable electromagnetic force .......... 37
List of Tables

A1.1 Nominal chemical composition of filler metal and workpiece used at University West ........................................... 64
A1.2 Chemical composition of Invar 36 alloy used with CompuTherm [165] ................................................................. 64
A1.3 Chemical composition of Invar 36 alloy used by Zhan et al. [97, 151] and Jiaming [152] ........................................ 64
A1.4 Chemical composition of Invar 36 alloy produced by Re-Steel 65
A1.5 Chemical composition of Invar 36 alloy produced by VDM metals [160] ................................................................. 66
A1.6 Solidus and liquidus temperature of Invar 36 alloy ............... 66
A1.7 Melting temperature of Invar 36 ........................................... 67
A1.8 Latent heat of fusion of Invar 36 ........................................... 67
A1.9 Density of Invar 36 alloy at solidus temperature ................. 70
A1.10 Thermal conductivity as function of temperature from VDM metals [160] ................................................................. 71
A1.11 Specific heat capacity at constant pressure in the solid state derived from the enthalpy; Seifter et al. [158] ................. 73
A1.12 Specific heat capacity at constant pressure as function of temperature; VDM metals [160] ........................................... 75
A1.13 Coefficient of thermal expansion as function of temperature; VDM metals [160] ................................................................. 77
A1.14 Surface tension and surface tension temperature gradient of iron, nickel and their binary alloy [157] ..................... 79
A2.15 Boundary condition for the test Case 1 ................................. 82
A2.16 Dimensionless Number for the test Case 1 ............................. 83
A2.17 Material properties of the steel alloy used for the test case 2 .. 86
A2.18 Material properties of argon ................................................ 87
A2.19 Parameters for calculation of interfacial surface tension of Fe-S binary alloy [49] ..................................................... 88
List of Figures

1.1 a) Picture of a use case mold with a support structure. b) CAD model of a use case mold showing the positioning of metal parts; on courtesy of Loiretech. Note: Figure (b) is upside down compared to (a). c) Illustration of typical orientations of the workpiece in relation to the gravitational acceleration across distinct sections of the mold surface, as indicated in (b).

2.1 Illustration of GMAW (side view along the travel direction). Adapted with permission from [21].
2.2 Illustration of GMA based AM [23].
2.3 Sketch of the main forces governing the metal transfer.
2.4 Current in pulsed-spray mode [44].
2.5 Set of sketches showing a force (red arrows) and its effect on the melt flow direction (green arrows). (a)-(c) Temperature gradient of surface tension between the melting temperature $T_m$ and the maximum melt temperature $T_{max}$ and thermocapillary force at (a): low, (b): moderate, and (c) elevated surfactant content. (d) Electromagnetic force. (e): Density between $T_m$ and $T_{max}$ and buoyancy force.
2.6 Humping defects [85].
2.7 Illustration of insufficient penetration in a cross-section perpendicular to the weld direction (a similar perspective is used in the following sketches).
2.8 Lack of fusion.
2.9 Undercut.
2.10 Underfill.
2.11 Excess reinforcement.
2.12 Overlap.
2.13 Burn through.
4.1 Classification of interface modelling methods. The methods used in this study are highlighted in green.
4.2 Free surface modeling method: (a) interface fitting, (b) interface tracking, and (c) interface capturing [51].
LIST OF FIGURES

4.3 FVM control volume with cell centroid P and volume $\Omega_P$. The coloured face centred in $f$ with the area $S_f$ is shared by the adjacent control volumes with cell centroid $P$ and $N$. [148] 46

4.4 Flow chart of the solution algorithm 52

A1.1 Density of Invar 36 alloy (Zhan et al. [97], Seifter et al. [158], CompuTherm [165], Thermo-Calc [166]), Pure iron [171] and pure nickel [171] as a function of temperature. 69

A1.2 Thermal conductivity of Invar 36 (Zhan et al. [97, 151], Seifter et al. [158], CompuTherm [165], VDM metals [160]) as a function of temperature. 72

A1.3 Specific heat capacity of Invar36 alloy (Zhan et al. [97], Seifter et al. [158], CompuTherm [165], Thermo-Calc [166], VDM metals [160]), pure iron [171], and pure nickel [171] as a function of temperature. 74

A1.4 Coefficient of thermal expansion of Invar 36 (Zhan et al. [97], Thermo-Calc [166], CompuTherm [165], Re-Steel [161], Experimental measurements, and High Temp Metals [163]) as a function of temperature. 76

A1.5 Viscosity of Invar 36 (CompuTherm [165]), pure iron [171] and pure nickel [171] as a function of temperature 77

A1.6 Surface tension data for levitated Fe-Ni alloys as a function of temperature. Adapted from [157] 78

A1.7 Electrical resistivity of Invar 36 as a function of temperature 80

A2.8 Schematic for the test Case 1. 83

A2.9 Steady state temperature distribution and velocity field of free surface Marangoni-driven flows with phase change. 84

A2.10 Melt front comparison between present test case and the results from Tan et al. [175]. 85

A2.11 Computational domain 87

A2.12 Variation of surface tension ($\sigma$) and the coefficient of surface tension temperature gradient ($d\sigma/dT$) with respect to temperature for different sulfur concentration; (a) 20 ppm and (b) 150 ppm. 89

A2.13 Boundary condition for the test Case 2. 90

A2.14 Comparison of melt front between present study and Saldi [51] at $t = 5$ s and post-weld fusion geometry of corresponding experiments by Pitscheneder et al. [177] for different sulfur concentration; (a) 20 ppm and (b) 150 ppm. 92
Chapter 1

Introduction

This doctoral thesis on metal fusion with Gas Metal Arc (GMA) focuses on modelling the behavior of the metal in the solid and liquid state, and its possible vaporization, using computational fluid dynamics (CFD). GMA is a heat source with a non-refractory electrode. Therefore, it transfers molten metal to the workpiece, in addition to heat. It has a long history of application in various production technologies, including welding, cladding, and, more recently, additive manufacturing (AM). These technologies are used in the production of metal parts for different industries such as energy (e.g., wind turbines), automotive, aerospace, and biomedical [1]. Nevertheless, there is still a need for process improvements to enhance efficiency, product quality, and promote a more sustainable utilization of resources. It is thus essential to reach a deeper process understanding. This knowledge is sought by complementing experimental observation with modelling. However, the CFD models that are commonly used to predict metal fusion with GMA present some knowledge gaps concerning their ability to capture the leading-order physics taking place in the process. This chapter introduces in more detail the background and motivation of this work, the identified research gaps, and the research questions formulated to address these gaps. The scope and limitations, methodology, and outline are then given.

1.1 Motivation

This study roots on a set of challenges faced by both the manufacturing industry and society as a whole. First, the limited availability of skilled welders prompts manufacturers to shift their production from manual to automated processes. Second, the usual approach to process design and improvement practiced in the industry for metal fusion heavily relies on the trial-and-error method. This method is time-consuming, and resource intensive. Third, a surge of interest in GMA heat sources is being driven by the development of additive manufacturing.
Chapter 1

Introduction

This doctoral thesis on metal fusion with Gas Metal Arc (GMA) focuses on modelling the behavior of the metal in the solid and liquid state, and its possible vaporization, using computational fluid dynamics (CFD). GMA is a heat source with a non-refractory electrode. Therefore, it transfers molten metal to the workpiece, in addition to heat. It has a long history of application in various production technologies, including welding, cladding, and, more recently, additive manufacturing (AM). These technologies are used in the production of metal parts for different industries such as energy (e.g., wind turbines), automotive, aerospace, and biomedical [1]. Nevertheless, there is still a need for process improvements to enhance efficiency, product quality, and promote a more sustainable utilization of resources. It is thus essential to reach a deeper process understanding. This knowledge is sought by complementing experimental observation with modelling. However, the CFD models that are commonly used to predict metal fusion with GMA present some knowledge gaps concerning their ability to capture the leading-order physics taking place in the process. This chapter introduces in more detail the background and motivation of this work, the identified research gaps, and the research questions formulated to address these gaps. The scope and limitations, methodology, and outline are then given.

1.1 Motivation

This study roots on a set of challenges faced by both the manufacturing industry and society as a whole. First, the limited availability of skilled welders prompts manufacturers to shift their production from manual to automated processes. Second, the usual approach to process design and improvement practiced in the industry for metal fusion heavily relies on the trial-and-error method. This method is time-consuming, and resource intensive. Third, a surge of interest in GMA heat sources is being driven by the development of additive manufactur-
ing for building large and complex metal parts layer upon layer. And last but not least, is the need to achieve sustainable manufacturing practices. This implies prioritizing the efficient use of energy and raw material, prolonging product life through repair technologies, and increasing productivity while maintaining quality. These different challenges require developing advanced process control models able to adapt in real-time the process parameters in order to counteract inherent process variations and prevent the formation of defects. This entails the need for in-depth process understanding.

Metal fusion with a GMA involves applying current or voltage between a metal wire and a workpiece separated by a shielding gas that protects the molten metal from atmospheric contamination. From a physical point of view, wire and workpiece are both electrodes. In welding and other metal fusion processes with GMA, the term "electrode" refers to the metal wire, and this terminology is used hereafter. The electric conduction between the electrode and the workpiece leads to the formation of an electric arc, which is essentially a thermal plasma. The shielding medium is thus partially ionized and its temperature reaches up to about 20 000 K. These two physical characteristics respectively imply magnetic field induction and intense radiation. The thermal plasma provides the heat needed to melt the wire, and to form a melt pool in the workpiece. Wire melting leads to the transfer of metal drops to the melt pool. The frequency of drop transfer can be controlled by pulsing the GMA electric signals and adjusting the pulse duration. Some of the important physical phenomena occurring in this process are therefore heat transfer, electromagnetism, phase changes, and the flow of molten metal with free surface deformation. Moreover, the material properties are temperature dependent. It is therefore a complex, non-linear, and multi-physics process that in addition involves multiple variables. For a given material composition, some of the notable process variables include electric current, travel speed, wire diameter, wire feed rate, and the composition and volume flow rate of the shielding gas. Comprehending the link between process input parameters and outputs is therefore non-intuitive. Furthermore, the intense radiation from the thermal plasma and the opacity of the metal limit the experimental observation. Modelling and simulation thus offer a complementary approach to understanding how the process conditions influence the convection in the melt pool and the geometry of the fusion zone.

The modelling of a melt pool produced by a GMA is either done with a coupled approach or with a decoupled one, the latter being the most common. The coupled approach includes in the model the physics of the thermal plasma. However, the coupled models often simplify the physics of the sheath and pre-sheath that are characterized by various non-equilibria (charge, chemical, and thermal) [2,3]. One of the reasons is the numerical difficulty in coupling the electromagnetic and
the thermo-fluid fields through these boundary layers constituting the interface between the thermal plasma and the molten metal while the interface (or free surface) deforms. The decoupled approach does not model the physics of thermal plasma. An advantage is its lower computational time compared to the coupled approach. Nevertheless, it accounts for the effect of thermal plasma on the metal through source terms and boundary conditions. This implies closing the model by supplying the effective arc radius as well as the electric current distribution, and voltage at the plasma/metal interface. These boundary data are needed to set the source terms of arc heat flux and arc pressure force, as well as the boundary conditions for the electromagnetic fields. The decoupled approach is used in this study, although it also raises some modelling issues that are described below.

This study was supported by the European project Integrade. It was more specifically conducted in collaboration with the industrial project partner Loiretech group. This company, located in Lorient (France), designs, and manufactures tooling such as large metallic molds to be used for producing aerospace components. Figure 1.1(a) illustrates a noteworthy use case with molds made of Invar 36 alloy. It is manufactured starting from thick and curved parts as illustrated in Figure 1.1(b). It necessitates V-groove joint preparation, followed by welding in a multi-layer technique as well as bridging the gaps using additive manufacturing. Both welding and AM are performed with a pulsed GMA heat source, with one pulse one drop (OPOD) metal transfer.

During metal fusion with a GMA in its basic configuration, i.e., the flat orientation shown in Figure 1.1(c)-(I), the torch is positioned above the workpiece, with its axis aligned with the force of gravity. However, as the parts of this use case have a large size and weight, their manipulation and positioning can suffer from poor accuracy. The parts are thus fixed prior to the welding and AM processes and are not repositioned during the processing. Instead, the GMA torch is oriented in multiple axes to permit adjusting its direction to the local changes in part curvature and maintain the torch axis normal to the workpiece surface. When the torch is repositioned, the relative orientation of the GMA axis with respect to the force of gravity changes. Typical paths of travel followed by the GMA torch across different sections of the workpiece surface are indicated by the arrows numbered (I) to (IV) in Figure 1.1(b). They correspond to the various local orientations of the gravitational acceleration ($\mathbf{g}$) with respect to the workpiece (and torch axis) that are sketched in Figure 1.1(c). Too large changes in relative orientation can lead to the formation of defects during the metal fusion process and the disqualification of the part. Examples of typical defects are humping and lack of fusion. The effect of the workpiece orientation on the melt flow during multi-layer welding of a V-groove joint is thus important to understand to avoid defect formation.
Besides, the reliability of a CFD model for metal fusion with GMA necessitates describing with relevant assumptions the leading-order physics governing
the process. The scientific community reached a long time ago a consensus regarding the heat fluxes and forces that govern the flow of molten metal with an electric arc. However, there is not yet a consensus on how to model some of these terms, especially the electromagnetic force (EMF) and the effect of pulsed power supply. The EMF can be among the leading order forces driving the melt flow and thus the heat transfer during metal fusion with a GMA [4]. Experimental studies showed that arc pulsing has a significant influence on the behavior of the melt pool, the fusion zone, and the reinforced bead geometry [5, 6]. Different models that have been proposed in the literature for the EMF are being used today [7–9]. Different models are also being applied in the literature to describe the effect of arc pulsation; moreover, they are combined with different EMF models [9, 10]. The motivation for choosing one variant over another, and the adequacy, limitations, or possible inadequacy of these models for the studied process are thus important to understand.

### 1.2 Research gaps

In this context, the following major research gaps were identified based on the literature review:

1. Changes in the relative orientation of the torch axis with respect to the force of gravity might modify enough the force balance in the molten metal to potentially influence the flow dynamics, the weld geometry, and the occurrence of defects. However, the effect of the workpiece orientation on the melt flow is poorly documented for multi-layer welding. Numerical simulation and experimental works in this field are restricted to single-layer welding and mostly investigated for challenging welding orientations that are overhead, vertical up, and vertical down [11, 12]. There is therefore a need for understanding the melt flow dynamics during multi-layer welding at various orientations of the workpiece.

2. Three different EMF models are mainly used in the literature for the CFD simulation (with a decoupled approach) of a melt pool produced using an electric arc. The first one is based on partial differential equations (PDE) governing a scalar and a vector field. The other two models, which are analytical, are defined through the integral function introduced by Kou and Sun [13], and the algebraic expression by Tsao and Wu [14]. The comparison of the EMF computed with the two analytical models was made by Kumar and Debroy [15]. However, the comparison to the EMF computed with the PDEs is yet to be conducted. More importantly, the effect of these
three EMF models on the predicted melt pool thermal flow is poorly documented; no published comparison could be found. Therefore, for each of these EMF models, the underlying assumptions and the influence of these assumptions on the prediction of the melt pool thermal flow are subjects that remain to be explored.

3. Arc pulsation imposes the time dependence of the boundary data (electric current, voltage, and effective arc radius) at the plasma/metal interface. The literature shows that this time dependence is often omitted. Instead, time-averaged values are predominantly used [16–18]. This requires conducting parametric studies to adjust some model parameters (described in more detail in the next chapter) to reproduce the penetration depth of the fusion zone. However, the nature of the problem and the model are three-dimensional and the potential impact on the predicted melt pool flow and geometry of neglecting the time dependence of these boundary data is not well understood. Some recent studies have incorporated time dependencies of these boundary data using Fourier curve-fitting functions [10, 19]. The authors emphasized that the main advantage was to avoid the parametric study mentioned above. To our knowledge, it is not established whether these models lead to the same simulation results, necessitating further investigation in this regard.

4. During metal fusion with GMA, the transfer of drops from the wire causes periodic oscillations of the free surface of the melt pool. The amplitude ($\delta z$) of these oscillations is the largest at the impact point, which is about the arc centre. It is of the order of the drop diameter, which is approximately the wire diameter in OPOD transfer mode. According to the study of Kumar and Debroy [15], the EMF could vary by one order of magnitude within $\delta z$. However, all the EMF models mentioned above assume a frozen free surface. In other words, they ignore the deformation of the free surface when computing the EMF fields even if the latter is included in the melt pool model. The effect of this assumption is poorly documented. To our knowledge, the relaxation of this assumption has not been attempted yet. Therefore, the influence of this assumption on the predicted melt pool dynamics is still an open question.

1.3 Research questions and objectives

The previously identified research gaps led to the formulation of the following four research questions:
CHAPTER 1. INTRODUCTION

The previous models of the predicted melt pool thermal flow are poorly documented; no published comparison could be found. Therefore, for each of these models, the underlying assumptions and the influence of these assumptions on the prediction of the melt pool thermal flow are subjects that remain to be explored.

Arc pulsation imposes the time dependence of the boundary data (electric current, voltage, and effective arc radius) at the plasma/metal interface. The literature shows that this time dependence is often omitted. Instead, time-averaged values are predominantly used [16–18]. This requires conducting parametric studies to adjust some model parameters (described in more detail in the next chapter) to reproduce the penetration depth of the fusion zone. However, the nature of the problem and the model are three-dimensional and the potential impact on the predicted melt pool flow and geometry of neglecting the time dependence of these boundary data is not well understood. Some recent studies have incorporated time dependences of these boundary data using Fourier curve-fitting functions [10, 19]. The authors emphasized that the main advantage was to avoid the parametric study mentioned above. To our knowledge, it is not established whether these models lead to the same simulation results, necessitating further investigation in this regard.

During metal fusion with GMA, the transfer of drops from the wire causes periodic oscillations of the free surface of the melt pool. The amplitude (δ_z) of these oscillations is the largest at the impact point, which is about the arc centre. It is of the order of the drop diameter, which is approximately the wire diameter in OPOD transfer mode. According to the study of Kumar and Debroy [15], the EMF could vary by one order of magnitude within δ_z. However, all the EMF models mentioned above assume a frozen free surface. In other words, they ignore the deformation of the free surface when computing the EMF fields even if the latter is included in the melt pool model. The effect of this assumption is poorly documented. To our knowledge, the relaxation of this assumption has not been attempted yet. Therefore, the influence of this assumption on the predicted melt pool dynamics is still an open question.

1.3 Research questions and objectives

The previously identified research gaps led to the formulation of the following four research questions:

RQ1 What are the effects of the workpiece orientation (relative to the arc axis) on the melt flow and resulting bead geometry during multi-layer GMAW of a V-groove joint?

RQ2 What are the effects of the three common electromagnetic force models on the prediction of GMA melt pool?

The research question RQ2 was decomposed into the following subquestions:

RQ2.1 What are the assumptions underlying these three models and their influence on the predicted electromagnetic force?

RQ2.2 What is the influence of these three models on the predicted melt flow, free surface oscillation, and bead geometry?

RQ2.3 In which circumstances and for predicting which aspect of a GMA melt pool is each of these models suited or questionable?

RQ3 When using pulsed GMA, what is the impact on the predicted melt pool of modelling time-dependent rather than time-averaged pulsing parameters?

RQ4 What are the effects on the prediction of GMA melt pool of taking into account the deformation of the free surface when modelling the EMF?

The objective of this research work is thus to answer these questions.

1.4 Scope and limitations

The present research on metal fusion with GMA was mainly based on a modelling methodology using CFD. The studied test cases include multi-layer welding on a V-groove joint (in relation to Loiretech’s mold application) and bead-on-plate deposit on a flat plate (for model analysis and improvement). These test cases were also carried out experimentally through collaborative studies. Argon was used as a shielding gas. The working material was Invar 36 alloy. It is a nickel-iron alloy consisting primarily of 36% nickel and 64% iron. In the experiments, GMA fusion was operated with an electric power set within the range of the conduction-deep penetration transitioning mode. Pulsating electric signal was applied with OPOD metal transfer mode.

Concerning the model, a decoupled approach addressing the melt pool was applied using CFD. The thermal plasma arc was thus modeled through source terms of arc heat flux, arc pressure, and current density at the gas-metal interface. Heat transfer due to metal vaporization was also modelled. The metal transfer was
simulated by injecting droplets in the computational domain. The numerical method for tracking the deformation of the free surface of the molten metal was the Volume of Fluid (VOF) method.

The model assumptions and limitations are as follows:

- The fluids are assumed to be incompressible.
- The fluid flow is assumed laminar.
- The thermo-physical properties of Invar 36 are not very well-documented in the liquid temperature range (see Appendix).
- Mass transfer with metal vaporization is ignored due to the neglectable mass fraction of vaporized metal for the process studied.
- The physics of the thermal plasma is not predicted by the decoupled model. As a result, the flow of the shielding gas is also ignored in the simulations.
- Metal detachment from the electrode wire is not modelled.
- The metal droplets transferred to the melt pool are assumed spherical with predefined volume, temperature, velocity, and frequency.
- The metal is assumed uniform in chemical composition. Therefore, the diffusion of the species within the alloy is neglected.
- Time-averaged values of the pulsating electric signals were used in paper I and II. The time dependence of these signals was reproduced in the simulations of the cases investigated in Paper III and Paper IV.

1.5 Methodology

The methodology adopted to investigate the identified research questions included the following main parts:

- Bibliographic studies were performed at different stages of the work.
- A number of experiments were designed and conducted in collaboration with other PhD. students and engineers to obtain data for testing the model. The experimental setup included a high-speed camera that was used to capture the metal transfer.
- Temperature-dependent material data for Invar 36 were collected from the literature, compared, and for model implementation convenience, they were interpolated when available only as data points.
A computational fluid dynamic solver (or initial solver) available at the beginning of the thesis was further developed in the open-source CFD software OpenFOAM®. The initial solver was a melt pool solver for stationary laser beam heat source and autogeneous conduction mode welding developed in an earlier project starting from the native OpenFOAM® solver interfoam. As those earlier developments can be found in [20], they are not repeated here. The developments were resumed in this study devoted to GMA fusion of Invar 36. The main implementations made in the present work include

- Temperature-dependent thermo-physical properties of Invar 36.
- Surface tension and thermocapillary (or Marangoni) force accounting for the presence of surfactant.
- Arc heat source and arc pressure force acting on the free surface.
- Relative motion between the arc heat source and the workpiece.
- EMF model based on partial differential equations (PDE) for the electric potential and the magnetic potential vector.
- EMF model based on Kou and Sun model [13].
- EMF model based on Tsao and Wu model [14].
- Metal transfer model leading to periodic source terms of metal volume fraction, mass, momentum, and energy.
- Time-dependent arc parameters accounting for variations in heat flux, arc pressure and EMF during pulse cycle.
- Self-adaptable EMF model accounting for the deformation of the melt pool free surface.

Preliminary numerical test cases were executed to evaluate as independently as possible specific parts of the model.

Project applications to the Swedish National Infrastructure for Computing were written, and the software preliminary tested at University West was installed on a SNIC cluster.

Experimental results in the form of high-speed images showing the metal transfer and melt free surface from side view were used to collect information for closing the metal transfer model.

Domain and mesh convergence studies were conducted to investigate the quality of the numerical solution.
CHAPTER 1. INTRODUCTION

- Parametric studies were conducted to prepare the arc heat source boundary model.
- The computational results were confronted to available experimental results (mainly macrograph images at this stage).
- The results were analyzed and selected for preparing publications.

This research was not a linear journey consisting in the succession of the activities above listed. Several of these parts were indeed re-iterated to deepen the knowledge because new questions arose as the understanding of the problem progressed.

1.6 Outline

The rest of this thesis is organized as follows. To complete this introductory chapter, the GMA welding and AM process, the modes of metal transfer with GMA, the forces driving the flow in the melt pool, and typical defects are described in the forthcoming Chapter 2. Next, Chapter 3 gives a summary of the state of the art relevant to the research questions. A brief description of aspects of the numerical methods used in this study that are not reported in the appended Papers is given in Chapter 4. The rest of the research work is available in the appended Papers. Therefore, it is not repeated here and only the summary of the Papers is presented in Chapter 5. The answers to the research questions and proposed future work are highlighted in the Conclusion (Chapter 6). The data collected from the literature and compared to select the thermo-physical and transport properties of the Invar 36 alloy used in this research work are presented in Appendix A1. Finally, two examples of test cases computed while developing the model and not included in the appended Papers are reported in Appendix A2.
Chapter 2

Gas metal arc fusion

This chapter presents the fundamental aspects of GMA-based metal fusion particularly, GMA welding and GMA-based AM (GMA-AM). The associated metal transfer modes are also presented. Next, this chapter discusses the heat transfer and forces that are active in the melt pool, along with their order of magnitude. The main defects associated with these processes are finally recalled, including some that have been predicted in this work.

2.1 A description of the method

GMA is a heat source commonly used in welding to join two or more metal parts. The other most common arc welding processes include gas tungsten arc welding (GTAW), and plasma arc welding (PAW). Overall, the main differences between these three processes are the type of electrode, the type of shielding gas, and the level of precision and control that can be achieved. GMAW is typically utilized for welding thick materials and for high-speed applications. This process is illustrated in Figure 2.1. Shielding gas is supplied through the nozzle of the GMA torch (or welding gun) to provide an inert atmosphere. It protects the melted metal transferred from the electrode to the melt pool (or molten puddle) from oxidation by the surrounding air. The electric arc is established between the wire and the workpiece when a sufficiently high electrical current is passed through the shielding gas to self-sustain its ionization. The resulting thermal plasma thus permits the electrical conduction between the electrode and the workpiece.

Arc-based AM, commonly known as Wire Arc AM (WAAM), is an extension of the welding process that uses the same principles and equipment. As illustrated in Figure 2.2, it aims at building three-dimensional (3D) objects by depositing material layer upon layer onto a metal base. AM, in general, offers several advantages over traditional manufacturing methods, including increased design flexibility, reduced material waste, and reduced lead times and costs for
expensive tooling. WAAM offers additional advantages including the ability to cost-effective fabrication of large components with strong mechanical properties. Furthermore, it is also known for low tooling, equipment, and manufacturing costs compared to AM with laser or electron beam for melting either wire or powder. Although all the aforementioned arc welding processes using GMA, gas tungsten arc, and plasma arc have been applied to build 3D geometry, the GMA-based AM is the most common WAAM process and thus also the focus of this thesis. The most unique advantage of GMA-based AM is its high deposition rate and high productivity [22]. For this reason, GMA-AM has recently emerged as a groundbreaking approach for developing and manufacturing high-performance components for a wide range of industries, including aerospace, automotive, medical, and energy. However, the process also poses some challenges, such as the need for accurate control of the wire feed rate, travel speed, and the shielding gas flow, to ensure consistent quality and dimensional accuracy [22].

The major process parameters in GMAW and GMA-AM include arc current and voltage. At least one of these parameters is controlled by the power source. The other controlled parameters are the wire feed rate, travel speed, contact-tip to workpiece distance (CTWD), as well as composition, and volume flow rate of the shielding gas. Achieving a successful GMA weld and GMA-based AM requires understanding and mastering the interrelation between these parameters. For instance, it is known that the power density of the arc is proportional to the current and arc voltage. The heat input per unit length is inversely proportional to the travel speed. The current is crucial to reach a selected penetration while the proper wire feed rate ensures good bridgeability of the joint gap in the case of GMAW. The shielding gas composition influences the arc behaviour, the metal transfer mode, the formation of slag, the level of smoke, and spatter as well as
CHAPTER 2. GAS METAL ARC FUSION

Figure 2.1: Illustration of GMAW (side view along the travel direction). Adapted with permission from [21].

expensive tooling. WAAM offers additional advantages including the ability to cost-effective fabrication of large components with strong mechanical properties. Furthermore, it is also known for low tooling, equipment, and manufacturing costs compared to AM with laser or electron beam for melting either wire or powder. Although all the aforementioned arc welding processes using GMA, gas tungsten arc, and plasma arc have been applied to build 3D geometry, the GMA-based AM is the most common WAAM process and thus also the focus of this thesis. The most unique advantage of GMA-based AM is its high deposition rate and high productivity [22]. For this reason, GMA-AM has recently emerged as a groundbreaking approach for developing and manufacturing high-performance components for a wide range of industries, including aerospace, automotive, medical, and energy. However, the process also poses some challenges, such as the need for accurate control of the wire feed rate, travel speed, and the shielding gas flow, to ensure consistent quality and dimensional accuracy [22].

The major process parameters in GMAW and GMA-AM include arc current and voltage. At least one of these parameters is controlled by the power source. The other controlled parameters are the wire feed rate, travel speed, contact-tip to workpiece distance (CTWD), as well as composition, and volume flow rate of the shielding gas. Achieving a successful GMA weld and GMA-based AM requires understanding and mastering the interrelation between these parameters. For instance, it is known that the power density of the arc is proportional to the current and arc voltage. The heat input per unit length is inversely proportional to the travel speed. The current is crucial to reach a selected penetration while the proper wire feed rate ensures good bridgeability of the joint gap in the case of GMAW. The shielding gas composition influences the arc behaviour, the metal transfer mode, the formation of slag, the level of smoke, and spatter as well as the deposited bead profile.

Shielding gases commonly utilized in GMAW and GMA-AM are argon (Ar), carbon dioxide (CO₂), and oxygen (O₂). They are either used as a single gas or in a mixture depending on the chemical composition of the metal. The blend of nitrogen (N₂), hydrogen (H₂), and helium (He) is also used in some cases. The type of chemical species constituting the shielding gas and their proportions have a significant effect on metal transfer and arc stability [24]. The most commonly used shielding gas in Europe is Ar. However, pure Ar causes arc instability when manufacturing steel workpieces [25]. Furthermore, Ar provides relatively low heat flux from the arc to the workpiece, which also limits the penetration depth [24]. By contrast, He has a higher ionization potential than Ar. Thus a high arc voltage is required to ionize He resulting in a hotter arc compared to pure Ar [24]. However, He is more expensive than Ar. Therefore, a mixture of Ar and He is often preferred to gain advantages of each individual gas. Shielding with CO₂ for carbon steel fusion also offers advantages such as higher travel speed, deeper penetration, and reduced cost [26]. However, pure CO₂ is not preferred due to associated issues with spatter and element losses caused by oxidation [26], in addition to being a greenhouse gas. Shielding gas mixtures of Ar with 5-20% CO₂ are most commonly used for low alloyed steel. It indeed presents the advantages of stabilizing the arc and reducing imperfections such as inclusion and porosity [25].

GMAW and GMA-AM mostly operate in DC (direct current) and typically require the wire electrode to be positive relative to the negatively grounded workpiece. This arrangement is also known as direct current electrode positive (DCEP). Electrode negative polarity (DCEN) is quite uncommon because of its adverse effect on the metal transfer from the electrode wire to the workpiece [27].
2.2 Metal transfer modes

The balance between the forces acting on the melted tip of the electrode wire governs droplet detachment and the type of metal transfer. This last one has a significant influence on the melt pool behavior and the resulting bead quality. The transfer mode typically depends on the arc current, wire feeding rate, shielding gas composition, electrode wire diameter, and the contact-tip to workpiece distance. Various modes of metal transfer can be achieved by adjusting process parameters that act on the forces applied to the melted wire. The most significant of these forces are illustrated in Figure 2.3. Depending on their relative intensity, three basic modes of metal transfer are usually distinguished with GMA. These are the short circuit, globular, and spray transfer modes.

![Figure 2.3: Sketch of the main forces governing the metal transfer.](image)

2.2.1 Short-circuit transfer mode

This mode uses the lowest range of current and voltage compared to the other modes. The electromagnetic (or Laplace) force is then very weak. The consumable electrode with a built-up molten droplet at its end comes in direct contact with the melt pool creating an electrical short-circuiting. The arc voltage drops...
to zero and it extinguishes the arc which also reduces the heat input. The surface tension of the melt pool pulls the droplet off the electrode. Next, when the droplet is detached to the melt pool, the arc is quickly reignited with a rise in current. This sequence is periodically repeated with a frequency typically ranging between 20 to 200 Hz [28]. Typical shielding gas compositions for short-circuit transfer include 100 % CO₂ and mixture of 75% - 85% Ar with balance CO₂. This mode generates low heat input and is suitable for welding thin sections. Furthermore, it can be used in all welding orientations including overhead, vertical up, and vertical down because of precise control over a small melt pool volume [29]. The notable drawbacks of this transfer mode include insufficient fusion due to low current and welding generally limited to thin metal sheets. Short circuit transfer mode has occasionally been used in GMA-AM process. This mode in its most basic form offers improved control of the melt pool. However, it is not the preferred choice since it has limited deposition rates which reduce productivity.

### 2.2.2 Globular transfer mode

The globular transfer takes place at a current level that is higher than for short-circuiting transfer but lower than for spray transfer. The EMF is then larger than in the short-circuit transfer mode, but not the leading order one. Gravity plays a dominant role in droplet detachment and transfer in this mode. The droplet shape is often irregular with a diameter larger than the diameter of the filler wire. Occasionally, the large size droplets also touch the melt pool creating a short-circuiting, which detaches the build-up molten droplet from the filler wire. The impact of the large-size droplets into the melt pool causes a large amount of spatter [30]. CO₂-rich shielding gas results in characteristically globular transfer even at a high current [31]. When used in GMAW, the main advantages of this mode are high wire feed rate and heat input which result in a high deposition rate with deep penetration, especially when welding thick workpieces [32]. It is also inexpensive when used with a CO₂-rich shielding gas. The major drawbacks include spatter, poor finish and mostly limited to flat position [31]. These disadvantages also make this transfer mode unsuitable for GMA-AM.

### 2.2.3 Spray transfer mode

The spray transfer occurs at the highest level of current and voltage compared to the previous modes. The EMF is then at leading order so that the induced pinching effect governs droplet detachment and transfer [32]. This mode is characterized by the transfer of tiny molten droplets, similar to spray, through a stiff stable arc. Then, the droplet diameter is usually smaller than the diameter of
the electrode wire [30]. A true spray transfer mode is achieved when an Ar-rich shielding gas is used. Some notable advantages of the spray transfer mode compared to the two other transfer modes include high deposition rate, fast travel speed, sufficient fusion with better-looking bead profile [33], less spatter, and smoke formation [34]. The variations in the arc length in this mode lead to fluctuations in the electromagnetic field strength around the arc. If these variations are not controlled, they could have an adverse effect on spatter level and bead appearance. The major disadvantage of the spray transfer mode is its high heat input, as the current must remain above the transition current, which can cause distortion and burn through in a thin workpiece.

The high current, high wire feed rate, and fast travel speed with spray transfer can lead to a number of defects when the process parameters are not sufficiently controlled. These defects include lack of fusion, porosity, humping, burn-through, and undercut [35] which are common to both GMAW and GMA-AM. Several methods have been adopted to mitigate the risks of such defects while at the same time benefiting from the characteristic advantage of a high deposition rate and thus high productivity. Some commonly employed methods include changing the composition of the shielding gas, using a hybrid laser beam and GMA [36], or using tandem arc [37]. Another one consists in using a controlled pulse current waveform, leading to a so-called pulsed-spray transfer mode. It has been proven to offer several advantages including improved control over droplet size, reduced heat input, reduced spatter, and improved deposition efficiency [38, 39].

In pulsed-spray mode a current waveform pulsing between peak current and background current is supplied by the power source, as illustrated in Figure 2.4. The peak current raises the amperage above the transition current for spray transfer. It is applied for a short period in the cycle, which is then overtaken by the background current. The background current ensures that the arc is maintained while lowering the overall average value of the current. The pulse provides a stable arc with very little spatter [40]. The pulsing frequency can vary between 100 to 400 Hz. Ideally, one droplet is generated and transferred at each pulse cycle (OPOD). This is also the mode used in this study. The melt pool is allowed to cool slightly during the background period of the cycle which makes the process suitable for the out-of-position welding and AM [41]. The reduced overall heat input with pulse-spray transfer mode also reduces the size of the heat-affected zone (HAZ) [42]. Despite these advantages, pulse-spray transfer mode suffers from some drawbacks like adequate shielding gas is required to maintain a stable arc, and repeatability and controllability is not guaranteed [43].

The three fundamental modes of metal transfer explained above are extensively utilized in welding and AM. However, with the constant advancement in technology, new variations in metal transfer modes have been developed. These
innovations have enabled better control of the process and improved the quality of the deposited bead, resulting in more efficient and effective welding and AM operations. These new variants are mostly proprietary, patent protected, and designed to address specific work requirements. A variant called Cold Metal Transfer (CMT) developed by Fronius company in 2004 has been proven to be efficient in AM. It is characterized by oscillating wire feeding controlled by a high-speed digital system [45]. This allows for keeping low heat input and facilitates the control of the metal transfer. It ensures consistent part geometry [46] and improved bead aesthetics [47]. A drawback is the relatively high cost of equipment. CMT can also suffer from poor dilution with metals requiring a high heat input to reach melting. Nevertheless, the different transfer modes influence also the driving forces in the melt pool through the action of the thermal plasma on the free surface, the electromagnetic force, and the momentum transferred by the droplets.

2.3 Heat transfer and melt pool driving forces

During GMA fusion, the heat is transferred from the arc to the surface of the melt pool through conduction, convection, as well as radiation and further within the pool through conduction and convection. For metals, radiation is indeed limited to the surface. The rate of heat transfer also influences the temperature distribution in the HAZ. Therefore, it is important to quantify the dominant heat transfer mechanism in the melt pool. The relative strength of the convective to the conductive heat transfer is quantified by the heat Péclet number ($Pe$), given by:

$$ Pe = \frac{U_c L_c}{\alpha T} \tag{2.1} $$
where $U_c$ and $L_c$ are the characteristic flow velocity and length of the melt pool, respectively, and $\alpha_T$ is the thermal diffusivity. For typical GMA fusion, the Péclet number is in the vicinity of 100 [4], which means that the liquid metal convection plays a dominant role in the heat transfer. Therefore, the forces governing the flow of melted metal play an important role in transferring the heat in the workpiece.

There are several forces active in the melt pool during GMA fusion that are induced by either gradient of density, pressure, temperature, or velocity, and external forces. They include the force of gravity, buoyancy, viscous force, arc pressure force, arc shear force, EMF, drop impact force, and forces due to surface tension. These last ones include the surface tension force, which is normal to the free surface, and the thermocapillary force which is tangential. The thermocapillary force arises as a result of the variation of surface tension due to temperature gradient, $d\sigma/dT$. Its amplitude and direction can change with the concentration in surface active element (surfactants) [48]. The surface active elements, such as sulfur and oxygen, can thus significantly influence the direction of the convective flow [49]. In the absence of surface active elements or at low concentration, the coefficient $d\sigma/dT$ is negative i.e., the surface tension decreases with increasing temperature. It results in an outward thermocapillary flow from the heat source center to the melt pool edges, as illustrated in Figure 2.5 (a). During processing, a dominant outward flow causes the melt pool to become shallow and wide [49,50]. Increasing sufficiently the concentration of surface active element results in introducing a temperature range $T_m < T < T_c$ in which the coefficient of surface tension temperature gradient is positive instead of negative. The critical temperature $T_c$ is the inflection point of $\sigma$ with respect to the concentration in surfactant, and $T_m$ is the melting temperature. The thermocapillary flow then becomes inward at the edge of the melt pool, while it remains outward in the centre where $T > T_c$, as sketched in Figure 2.5 (b). It results in counter-rotating thermocapillary flow that deepens and narrows the melt pool [20,51]. If the concentration of surface active element is so high that $T_c$ reaches or exceeds the maximum temperature in the melt pool, the thermocapillary flow becomes fully inward, leading to an even deeper and narrower melt pool, as shown in Figure 2.5 (c) [49,50].
The electromagnetic force depends on the current density and the induced magnetic field. It accelerates the molten metal mainly downward along the centreline of the arc. Therefore, it leads to inward flow recirculation as well as an increased penetration depth; this effect is sketched in Figure 2.5 (d). Besides, the flow in the thermal plasma induces pressure and shear forces on the melt pool. The former, which is normal to the free surface, causes its deformation while the latter, which is tangential, enhances the outward flow. These forces are generally small and often ignored in the simulation models, particularly for current levels less than 200 A [52].

The variation of the temperature inside the melt pool leads to the variation in the density ($\rho$) of the liquid metal. It induces the buoyancy force, as illustrated in Figure 2.5 (e) [53]. If this force was at leading order, it would cause an outward flow and contribute to a shallow and wide melt pool. The relative strength of these different driving forces determines the melt pool geometry. It can be established using the following dimensionless numbers.

The relative strength of the thermocapillary force with respect to the viscous friction force in the liquid metal is quantified by the Marangoni number ($Ma$),

$$Ma = -\frac{(\frac{d\sigma}{dT})L_c \Delta T}{\mu \alpha_f}$$

(2.2)

where $\frac{d\sigma}{dT}$ is the change in surface tension with temperature, $L_c$ is the characteristic melt pool length, $\Delta T$ is the difference between the maximum temperature inside the pool and the solidus temperature of the metal ($T_s$), and $\mu$ is the dynamic viscosity. For a melt pool during GMA fusion, the Marangoni number is typically in the range of $10^2$ - $10^5$.

The Rayleigh number compares the buoyancy force (related to natural convection) to the viscous friction force. The strength of the buoyancy force compared to the surface tension force can thus be characterized using the ratio of the Rayleigh number ($Ra$) to the Marangoni number, which is also known as the Bond (or Õtvtös) number ($Bo$),

$$Bo = \frac{Ra}{Ma} = \frac{\rho g \beta \Delta T L_c^3 / (\mu \alpha_f)}{(\frac{d\sigma}{dT})L_c \Delta T / (\mu \alpha_f)} = \frac{\rho g \beta L_c^2}{(\frac{d\sigma}{dT})}$$

(2.3)

where $\rho$ is the density of the metal, $g$ is the gravitational acceleration, and $\beta$ is the thermal expansion coefficient. For a typical GMA fusion process, the bond number ($Bo$) is in the range of $10^{-4}$ - $10^{-3}$. 
CHAPTER 2. GAS METAL ARC FUSION

Figure 2.5: Set of sketches showing a force (red arrows) and its effect on the melt flow direction (green arrows). (a)-(c) Temperature gradient of surface tension between the melting temperature $T_m$ and the maximum melt temperature $T_{\text{max}}$ and thermocapillary force at (a): low, (b): moderate, and (c) elevated surfactant content. (d) Electromagnetic force. (e): Density between $T_m$ and $T_{\text{max}}$ and buoyancy force.

20
2.3. HEAT TRANSFER AND MELT POOL DRIVING FORCES

The magnetic Reynolds number \( (R_m) \) [15] is the magnetic analogue of the Reynolds number which is associated with the electromagnetic-driven flow in the melt pool. It compares the strength of the EMF to the viscous force:

\[
R_m = \frac{\rho \mu_m I^2}{4 \pi^2 \mu^2}
\]  

(2.4)

where \( \mu_m \) is the magnetic permeability of the alloy, and \( I \) is the current. For a typical GMA fusion process, the magnetic Reynolds number \( (R_m) \) is in the range of \( 10^3 - 10^5 \) [4, 15].

The resultant ordering

\[
R_m \geq Ma > Ra
\]  

(2.5)

obtained in the melt pool for typical GMA fusion applications implies that the EMF is larger than or of the same order as the thermocapillary force. In fact, this depends on the electric current applied and holds in the vicinity of the arc column. Cho et al. [54] reported that a large EMF (thus a large magnetic Reynolds number) is associated with the recirculation of molten metal under the arc that is dominantly inward and downward and subsequently enhances the penetration depth. It was also reported by Murphy et al. [55] that increasing the current density increases the EMF which enhances the downward convective flow. Away from the vicinity of the arc column, the EMF weakens and the thermocapillary force becomes the dominant force driving the flow in the melt pool [56]. A high value of the Marangoni number implies that the thermocapillary force is of much larger order than the viscous friction force and the buoyancy force [4]. For a multi-layer GMA fusion, it also ensures proper interlayer fusion and hence low porosity [57].

It is often believed that the rate of heat transfer during GMA fusion is enhanced due to fluctuating velocity and turbulent behaviour of the melt pool [48]. However, it has not been clearly understood whether the melt pool behaviour is indeed turbulent. When authors assume a turbulent melt pool flow, the effect of the turbulence is often taken into account through enhanced value(s) of the viscosity and/or the thermal conductivity [4]. Different ways of estimating an enhancement factor are reported in the literature. Some authors [58] arbitrarily enhance the value of the viscosity and/or thermal conductivity until the simulation and experimental results match, while other authors [48, 59] calculate the effective properties using a turbulence model based on Prandtl’s mixing length. In this framework, the turbulent viscosity is expressed as:
\[ \mu_t = \rho l_m v_t \]  

(2.6)

where \( l_m \) is the mixing length and \( v_t \) is the turbulence velocity. The effective viscosity \( (\mu_{\text{eff}} = \mu_t + \mu_m) \) is then defined as a sum of turbulent viscosity \( (\mu_t) \) and molecular viscosity \( (\mu) \). The effective thermal conductivity is then calculated using the equation of Prandtl number as:

\[ Pr = \frac{\mu c_p}{\kappa_t} \]  

(2.7)

where \( c_p \) is the specific heat capacity of the liquid metal, and \( \kappa_t \) is the turbulent thermal conductivity. The effective thermal conductivity \( (\kappa_{\text{eff}} = \kappa_t + \kappa_m) \) is then defined as a sum of turbulent thermal conductivity \( (\kappa_t) \) and material thermal conductivity \( (\kappa) \). A typical value of the Prandtl number is commonly prescribed as 0.9 [60, 61].

The turbulent behaviour of the flow in the melt pool has been investigated in arc welding in several works using experimental [62] and computational [63, 64] approaches. In GMAW, the melt pool is further agitated by the droplet impact [65]. Yang and Debroy [59] used the \( k - \varepsilon \) turbulence model to simulate turbulent flow and heat transfer in a GMA melt pool. The computed fusion zone (FZ) geometry that did include a unique finger penetration agreed fairly well with the experimental results. However, the obtained agreement might have been influenced by the use of the cylindrical volumetric heat source model where the penetration depth was predetermined rather than predicted. On the other hand, a great number of numerical simulations [35, 66–68] in recent years have obtained equally satisfactory results assuming laminar flow and also without using an enhancement factor. It shows that there is a great disparity regarding turbulence and its modelling in the melt pool. Therefore, a laminar flow field is assumed in this thesis and no enhancement factor is used for the viscosity and thermal conductivity.

### 2.4 Typical defects in gas metal arc fusion

There are several types of defects associated with GMA fusion. Most of them are a consequence of a combination of improper process parameters, e.g., too low/high current, too slow/fast travel speed, contact-tip to workpiece distance, electrode orientation, workpiece orientation, shielding gas composition, and its flow rate. Some defects can also result due to metal composition and contaminants present in the working metal and shielding gas [69]. The most common defects encountered in GMAW are cracks, porosities, inclusions, spatters, inclusions present in the working metal and shielding gas [69]. The most common defects encountered in GMAW are cracks, porosities, inclusions, spatters, inclusions present in the working metal and shielding gas [69]. The most common defects encountered in GMAW are cracks, porosities, inclusions, spatters, inclusions present in the working metal and shielding gas [69]. The most common defects encountered in GMAW are cracks, porosities, inclusions, spatters, inclusions present in the working metal and shielding gas [69]. The most common defects encountered in GMAW are cracks, porosities, inclusions, spatters, inclusions present in the working metal and shielding gas [69]. The most common defects encountered in GMAW are cracks, porosities, inclusions, spatters, inclusions present in the working metal and shielding gas [69]. The most common defects encountered in GMAW are cracks, porosities, inclusions, spatters, inclusions present in the working metal and shielding gas [69]. The most common defects encountered in GMAW are cracks, porosities, inclusions, spatters, inclusions present in the working metal and shielding gas [69]. The most common defects encountered in GMAW are cracks, porosities, inclusions, spatters, inclusions present in the working metal and shielding gas [69]. The most common defects encountered in GMAW are cracks, porosities, inclusions, spatters, inclusions present in the working metal and shielding gas [69]. The most common defects encountered in GMAW are cracks, porosities, inclusions, spatters, inclusions present in the working metal and shielding gas [69]. The most common defects encountered in GMAW are cracks, porosities, inclusions, spatters, inclusions present in the working metal and shielding gas [69]. The most common defects encountered in GMAW are cracks, porosities, inclusions, spatters, inclusions present in the working metal and shielding gas [69].
2.4. Typical defects in gas metal arc fusion

defects encountered in GMAW are cracks, porosities, inclusions, spatters, insufficient fusion, insufficient penetration, undercut, under-fill, excess reinforcement, humping, burn-through, and overlap [70]. These defects cover a wide range in both shape and size. The size of the cracks and porosities usually range from micro-scale ($10^{-8} \text{ m} - 10^{-5} \text{ m}$) to low mesoscale ($10^{-5} \text{ m} - 10^{-1} \text{ m}$) [71]. Therefore, cracks and porosities are often much smaller than the grid size used for the simulations conducted in this work. Furthermore, material shrinkage upon solidification and material composition affect the formation of weld cracks (solidification and hot cracking) [72]. Since incompressible flow conditions and uniform material composition are assumed for the model of this study, the prediction of crack and micro-scale porosity is not feasible. The defects in bead geometry which are usually between mid-mesoscale ($10^{-5} \text{ m} - 10^{-1} \text{ m}$) and macro-scale ($10^{-1} \text{ m} - \text{ higher}$) mainly result from the processes, joint configurations [73], and welding position [74]. They can be predicted with the numerical model developed in this work and the mesh size used in the computations, as shown in the appended Paper I. The major geometrical defects related to GMAW and GMA-AM include

- **Humping** - It is one of the most common defects while using GMA fusion at a high travel speed. This defect can be observed when the deposited bead surface presents periodic undulations, as illustrated in Figure 2.6. A typical undulation sequence consists of a hump and a valley [75]. Humping has been a topic of investigation in all kinds of metal fusion processes [76–78]. Several theories were developed to predict and interpret the mechanism of hump formation, e.g., Rayleigh instability model [79], hydraulic jump model [80], arc induced model [81], thermocapillary model [82]. The CFD approach with free surface tracking was also used to quantitatively analyze hump formation [76, 77, 83, 84]. There is a general agreement within these studies that hump formation is a result of a high travel speed, strong back-flow of liquid metal, and premature solidification of a thin and elongated channel in the melt pool.

Hump formation is also common when welding a workpiece that is not horizontal, as shown by Hu et al. [74], Cho et al. [12], and Park et al. [41]. These investigations were performed for challenging workpiece orientations, leading to vertical up, vertical down, and overhead welding positions. It was also agreed in these studies that a strong backward flow of the molten metal prevents backfilling of the front portion of the melt pool, which leads to hump formation. Nguyen et al. [75] showed that it is possible to weld carbon steel at a higher travel speed and prevent hump formation by downhill welding a workpiece inclined at 5° and 10° compared to
the standard horizontal (flat) position. However, this may not be general-
izable to other conditions, such as other materials, due to the nonlinearity of the process.

**Figure 2.6: Humping defects [85]**

- **Insufficient penetration** - This defect is illustrated in Figure 2.7 with a single pass bead sketched in a cross-section perpendicular to the weld direction. The workpiece is shown in grey, the fusion zone (FZ) in light blue, while the HAZ is not reproduced. This defect occurs when the fusion zone (FZ) does not reach the root of the joint. Generally, this defect is caused by too low amperage and too high travel speed.

**Figure 2.7: Illustration of insufficient penetration in a cross-section perpendicular to the weld direction (a similar perspective is used in the following sketches).**

- **Lack of fusion** - Insufficient fusion occurs when the deposited bead fails to completely fuse with the joint edge or the previously deposited bead. A gap between the deposited bead and the workpiece can then be observed along the transverse cross-section, as can be seen in the sketch of Figure 2.8. Generally, this defect is caused by too high travel speed, too low current, or too narrow a groove joint.
2.4. TYPICAL DEFECTS IN GAS METAL ARC FUSION

• Undercut - Undercut is generally defined as a depression located at the toe of a weld bead. It can severely affect the bead properties as it causes stress concentrations and can also initiate cracks. Mendez and Eagar [81] and Mills and Keene [82], studied this defect experimentally with high sulphur steel. They attributed the undercut to the inward thermocapillary convection. However, it is not easy to deduce quantitative explanations for undercut through experimental observation because of the difficulty in measuring the temperature distribution and fluid flow in the melt pool [86]. Cho and Farson [77] used a 3D numerical model and suggested that insufficient liquid metal backfilling was responsible for the undercut. Ohji et al. [87] also used a transient 3D numerical model and suggested that the surface deformation due to arc pressure force was responsible for the undercut. Diverse hypotheses, therefore, coexist regarding the cause of undercut.

Figure 2.9: Undercut.

• Underfill - This defect occurs when the height of the reinforced bead is below the adjacent height of the workpiece, as shown in Figure 2.10. It can be intermittent or occur continuously along the longitudinal surface of a bead due to insufficient deposition of filler metal. It is an external defect and can be easily detected by visual inspection. Generally, this defect is caused by high travel speed or low wire feed rate.

Figure 2.10: Underfill.
Chapter 2. Gas metal arc fusion

• Excess reinforcement - In contrast to a underfill, the excess reinforcement occurs when the height of the reinforced bead is larger than the allowable height; see the sketch in Figure 2.11. Excess reinforcement may sometimes also come out from the root side of the joint. Generally, this defect is caused by excessive current, too slow travel speed, too high wire feed rate, or due to an incorrect joint configuration.

Figure 2.11: Excess reinforcement.

• Overlap - The overlap is sketched in Figure 2.12. It occurs when the filler material at the weld toe overflows the surface of the workpiece without fusing well with it. Generally, this defect is caused by too low current, too long arc, too slow travel speed, too high wire feed rate, or inappropriate angle relative to the workpiece.

Figure 2.12: Overlap.

• Burn through - The burn through occurs when a hole is blown through the weld joint, as illustrated in Figure 2.13. It is also referred to as meltthrough. It is usually encountered when joining thin parts. However, it also occurs with thick parts when using too high current or too wide root opening.

Figure 2.13: Burn through.
Chapter 3

State of the art

This chapter presents some key steps along the development of models of GMA fusion. This process involves a number of physical phenomena specific to the different regions which are the filler wire, the thermal plasma arc, the melt pool, the mushy zone (i.e. the alloy solid-liquid transition region), and the solid part of the workpiece. These phenomena are also non-linearly coupled within and between the different regions. They include among all various forms of heat and mass transfers, phase changes, changes in microstructure and material properties, distortions, and residual stresses. Self-consistent and unified modelling of these multi-scale phenomena is difficult and would require huge computational resources. Thus, modelling and simulation of GMA fusion is usually divided into sub-models that focus on specific aspects of the process and simplification of the rest. This is also the approach used in this study, focusing on the melt pool. In this respect, the history of melt pool modelling shows that two main development steps, which are presented below, can be distinguished: the early developments that focused on heat conduction and the more recent ones that account also for convection. Next, a state-of-the-art more specifically devoted to the modelling of the EMF in the melt pool is discussed. Finally, some studies that did model the melt pool to investigate GMAW at different non-flat welding orientations are reviewed.

3.1 A brief history of melt pool modelling: early developments

The earliest numerical models of welding started to be developed approximately in the 1970s [88]. These models focused mainly on the thermo-mechanical aspects of welding and investigated the temperature field and distortions in the workpiece. The arc and the melt pool thermal flow were not taken into account. Their effect was instead approximated through a heat source in the form of a
boundary condition. Calibration of the heat source model was required to match the experimental results in each separate case. These models have undergone rigorous development over several years, particularly in reference to the heat source model. Pelvic et al. [89] first suggested the use of a 2-dimensional Gaussian disc to describe the spatial distribution of the heat flux from the arc to the surface of the workpiece. Pelvic’s heat source model was then combined with the Finite Element Method (FEM) by Friedman [90] to predict a significantly improved temperature field in the FZ and the HAZ. The calibrated Gaussian distribution heat source is still widely used today. For instance, Tian et al. [91] recently applied it to predict angular distortion and transverse shrinkage during bead-on-plate GTAW.

The surface heat source model by Pelvic et al. [89] is quite successful when applied to predict welding with a small effective penetration depth e.g., in GTAW. However, when using a high power density heat source, e.g., plasma arc, this surface model cannot replicate the digging action of the heat source that transports the heat deep into the workpiece. High power density heat sources indeed induce intense vaporization of the liquid metal leading to free-surface deformation and keyhole formation that cannot be predicted when convection is ignored. To overcome this issue, Paley and Hibbert [92] developed a volumetric heat source model with a constant power density distribution in the FZ. However, soon after it was pointed out that the assumption of constant power density throughout the FZ leads to a mathematical solution (spherical molten pool shape) which is non-physical. To overcome these limitations, the double-ellipsoidal heat source model was proposed by Goldak et al. [93]. This 3-dimensional distribution provides a sufficient number of adjustable parameters to accommodate shallow as well as deep penetration welding. Moreover, it is also capable of handling non-axisymmetric heat distribution in workpieces with V- or U-groove joints or when joining dissimilar metals. So far, the double-ellipsoidal model is the most widely used for predicting the temperature field and its evolution with time while neglecting liquid metal convection within the melt pool; see e.g., [94,95]. More advanced models combining different forms of heat source distributions were also developed to accommodate various types of hybrid welding processes. For instance, circular disk, line, and double ellipsoidal models were combined for predicting laser-GTAW hybrid welding [96], double-ellipsoidal and conical models for laser-GMAW hybrid welding [97], and Gaussian planar and conical models for multi-layer laser-GMAW hybrid welding [94]. As far as the melt pool is concerned, another crucial step in model development was the extension to account for the convection phenomenon inside the melt pool.
3.2 A brief history of melt pool modelling: extension to convection

The fluid flow in the melt pool and its possible influence on the heat transfer and the properties of the weld was experimentally reported in the context of GTAW as early as in 1971 by Woods and Milner [98] and by Kublanov and Erokhin in 1974 [99]. The numerical simulation of the melt pool accounting for convection was initiated during the same decade. One of the earliest models was developed by Atthey [100] using a pre-determined hemispherical melt pool shape and a pre-determined EMF that was then the only driving force considered. Then, Oreper et al. [101] developed a quasi-steady model of the melt pool where a combined effect of the buoyancy and the EMF was considered. They found that under certain conditions, convective flow driven by the EMF could be crucial in determining the melt pool shape. However, the level of modelling at this stage was not yet sufficient to establish a satisfying correlation between the computed results and the experimental observations. In 1982, Heiple and Roper [102] experimentally observed that in many cases surface tension driven flow dominates the convection at the melt pool free-surface. These authors did also observe that the presence of surface active impurities can substantially alter the Marangoni flow and locally change its direction. Oreper et al. [103] developed a model of the melt pool that included the surface tension force for the first time. Their numerical results confirmed the above findings and observations by Heiple and Roper [102]. Although the melt pool model developed by Oreper et al. [103] was an important step towards understanding the effect of heat convection in the melt pool, several critical simplifications were still made such as the prior specification of the melt pool shape. Kou and Sun [13] introduced in 1985 a model solving the liquid alloy velocity and temperature fields simultaneously, therefore permitting predicting the shape of the melt pool. All these models were two-dimensional (2D) and assumed an arc heat source stationary with respect to a semi-infinite workpiece. However, in industrial manufacturing, the welding and AM applications mostly involve moving heat source and finite workpiece thickness. Kou and Wang [104] did extend the model of Kou and Sun [13] to 3D and a moving heat source. Their simulation results showed that the flow pattern is not symmetric with respect to the arc axis and hence cannot be properly predicted with a 2D approach.

All the melt pool models described above (until 1988) were developed for autogenous GTAW. The physics of GMAW involves additional phenomena such as metal transfer in the form of droplets that impinge on the melt pool and coalesce with the free surface. It is accompanied by deformation and oscillation of the free surface. The earliest melt pool model for GMAW was developed by Tsao
and Wu [14]. They also incorporated electromagnetic, buoyant, and surface tension forces. The metal transfer was simplified to a source term for the droplet enthalpy in the energy conservation equation. Mass and momentum transferred with the droplet were still ignored. Another important limitation did consist in assuming that the free surface of the melt pool was non-deformable while metal drop impingement is known to significantly influence the free surface dynamics. Furthermore, the arc pressure, which might also produce deformation of the free surface, was also neglected. An important subsequent step was to model the deformation of the free surface. The first approach did consist in applying the principle of free surface energy minimization. This was first applied in the melt pool model for GTAW by Zacharia et al. [105,106]. Kim and Na [107] proposed another variant with boundary-fitted coordinates that could be applied to large surface deformation and complex weld geometry. It was then employed to study GMAW. However, the effect of droplet impact and arc pressure on the free surface deformation were not yet considered. Ushio and Wu [108] further improved Kim and Na free-surface model with a non-orthogonal boundary-fitted coordinate system. The effect of the metal transfer was partly included through a heat source term and a constant force exerted on the surface of the melt pool. However, droplet impingement implies also mass transfer and variation with time of the force that was not yet taken into account. It was the introduction of the volume of fluid (VOF) method in the melt pool simulation in early 2000 that set the foundation for the modern CFD models. The VOF method allows tracking of the free surface of the droplet, the melt pool, their coalescence, and the build-up geometry of the reinforced bead. It was used by Cao et al. [109] to simulate the impact of a transferred metal droplet on the melt pool in GMAW. Other free surface tracking methods are also used today, such as the Level Set method. They are discussed in Chapter 4. As far as the process physics is concerned, other aspects further discussed hereafter are related to the modelling of the EMF and arc pulsation (see Sections 3.4 - 3.6).

### 3.3 Melt pool modelling of non-flat welding orientation

Several studies investigated the melt pool behaviour and resultant bead geometry when welding at various non-flat (non-horizontal) orientations. As underlined in Chapter 1 (Figure 1.1c), in this context the force of gravity is no longer aligned with the axis of the heat source (which is normal to the workpiece). These studies used both experimental and modelling approaches. Such studies applied to GMAW are now reviewed.

Park et al. [41] investigated experimentally the influence of the workpiece ori-
3.3. MELT POOL MODELLING OF NON-FLAT WELDING ORIENTATION

Orientation (relative to the gravitational force) on the molten pool, bead geometry, and microstructure using synchronized high-speed imaging and data acquisition. The welding was performed with flat, overhead, and vertical down workpiece orientations. The authors concluded that the overhead orientation resulted in a larger bead height with a convex shape. Increasing the rate of metal transfer in this position increased the backward flow of the molten pool, which resulted in humping. Furthermore, the vertical down workpiece orientation provided cushioning effect due to the accumulation of molten metal near the arc center. It resulted in a reduced penetration depth and a concave bead shape.

Kumar and Debroy [11] used a CFD approach to investigate the welding of V- and L-fillet joints at horizontal, uphill, and downhill orientations. The free surface deformation was estimated by minimizing the total surface energy. The metal transfer was modelled through a time-averaged volume heat source. The impact of the droplet was not simulated. These authors found that the joint configurations and workpiece orientation had a significant influence on the free surface of the melt pool. For the L-shaped fillet joint and each of the investigated orientations, asymmetric melt pool profiles were predicted, which affected the strength of the weld bead. The geometrical parameters of weld bead such as the horizontal and vertical fusion length (also known as the leg length in an L-shaped fillet joint) increased during downhill orientation while they decreased during uphill orientation. The computed FZ geometry, finger penetration shape, and solidified surfaces agreed fairly well with the experimental results.

Cho et al. [12] studied the melt pool, bead shape, and weld defects for various flat and non-flat orientations of a V-groove butt joint workpiece. The investigated workpiece orientations were flat, overhead, vertical up, and vertical down with and without the root gap. These authors found that full penetration was difficult to achieve without the root gap for the flat and overhead orientations of the workpiece. For the vertical-up orientation, intermittent humping and melt-through of the reinforced bead were observed. Furthermore, the vertical down orientation resulted in melt overflow which was later improved by increasing the welding travel speed. While such weld defects were previously predicted with the CFD model for the flat workpiece, the work performed by Cho et al. [12] was the first attempt to study this behaviour with CFD for a non-flat workpiece orientation.

Hu et al. [74] investigated the melt pool behaviour and reinforced bead shape for a bead-on-plate deposit using a robotic GMAW system for various flat and non-flat workpiece orientations. They found that the flat workpiece orientation generated continuous and uniform reinforced beads whereas the vertical down orientation generated reinforced beads with increased width and reduced height compared to the flat orientation. On the other hand, the vertical up workpiece
orientation resulted in an uneven splitting of the melt pool in the middle and generated beads with periodic humps.

The literature study shows that most researchers who did investigate the influence of the non-flat workpiece orientation on the melt pool did it for the challenging positions which are vertical up, vertical down, and overhead. Furthermore, these investigations focused on the melt pool in the first layer (root pass) only. The melt pool behaviour within the root pass and second layer can be remarkably different. The effect of non-flat workpiece orientation in the second layer (or multi-layer) GMAW is to our knowledge poorly documented. It was thus investigated in this study (see Appended Paper I).

3.4 Electro-magnetic force models applied to the melt pool

The EMF field is defined as the vector product of the current density field and the magnetic field. Its modelling, needed to account for the effect of the EMF on the melt pool convection, thus consists in computing the current density and the magnetic field distributions in the workpiece. This requires knowing the current density distribution at the free surface, which depends on the arc’s effective radius.

In the early days of the melt pool modelling accounting for the convection, Kou and Sun [13] developed a model for the EMF field using Maxwell’s equations with a magnetohydrodynamics approximation. These authors reduced the mathematical problem from the resolution of PDEs to the calculation of an integral equation involving the Bessel functions. To obtain an expression of the EMF field that had the advantage of a reasonable computational time, they did introduce some simplifications. For instance, they neglected the deformation at the free surface of the melt pool and assumed an axi-symmetric force field. A list of simplifications and the derivation of the Kou and Sun EMF model was detailed by Kumar and Debroy [15]. However, one of the simplifications was not clearly formulated, and it has consequences in melt pool modelling, as underlined in the appended Paper II.

The EMF model of Kou and Sun has been widely applied in the literature and is still commonly used. Considering, for instance, some recent studies, limited here to GMAW, it was applied by Cheon et al. [16] to study the finger-shaped penetration in bead-on-plate GMAW, by Wu et al. [17] to simulate the melt pool formed during GMAW of horizontal fillet joints, and by Zhu et al. [19] to compute the melt pool in narrow-gap GMAW of 5083 Al-alloy. Kou and Sun EMF
3.4. ELECTRO-MAGNETIC FORCE MODELS APPLIED TO THE MELT POOL

model was used by Zhu et al. [110] to study the influence of swing arc on the melt pool during narrow-gap GMAW. In this study, the EMF model was modified with a rotated coordinate system to compensate for the discrepancy between the vertical workpiece axis and the arc axis. These authors did use the effective arc radius as an adjustable parameter and set it to reproduce the penetration depth observed on the experimental macrograph. Cho et al. [12] applied the Kou and Sun EMF model to simulate the melt pool in a V-groove GMAW at various workpiece orientations. In this case, the effective radius of the electric current density distribution, needed for computing the EMF, was also adjusted to reproduce the elliptical symmetry characteristic of the arc in the V-groove. More recently, Cho et al. [35] investigated the transient behaviour of the melt pool in OPOD GMAW and proposed another approach to set the effective arc radius. They conducted experiments synchronizing high-speed imaging of the arc with the welding electrical signals and curve-fitted the data to obtain a Fourier series of the effective arc radius as a function of pulsing time. The Kou and Sun EMF model was also applied in several other 3D studies of the melt pool such as in laser-GMA hybrid welding [36], submerged arc welding [111], tandem submerged arc welding [112], and hollow GTAW [113].

Tsao and Wu [14] further simplified the EMF model of Kou and Sun [13]. They proposed a model necessitating even less computational time, being given by an algebraic analytical expression rather than an integral one. On top of the assumptions made by Kou and Sun [13], Tsao and Wu [14] indeed added two more simplifications: i. The radial component of the current density is reduced to an average value independent of the position in the workpiece. ii. The axial component of the current density and the angular component of the magnetic field are assumed to decrease linearly with the workpiece thickness. It is now known that this decrease is closer to exponential than linear. The derivation and final expression of the Tsao and Wu EMF model are given by Kumar and Debroy [15] and are not repeated here.

The EMF model of Tsao and Wu [14] has also been widely used in the literature and is still applied today, as can be seen with the next examples that focus only on GMAW. Chen et al. [114] applied it to study the transient melt pool dynamics during ForceArc® GMAW on a V-groove joint at various groove angles. Xu et al. [115] used it to study swing arc narrow gap GMAW, and Hu et al. [116] to investigate the weld bead abnormality at the weld start and the stop in GMAW. Hu et al. [116] found that the abnormal bead geometry at the start was mainly due to the depressed melt pool surface which presented a tendency for backward flow whereas the abnormality at the stop was attributed to the sudden stop of heat input. However, as underlined earlier, both EMF models discussed until now were derived assuming no deformation of the melt pool surface, i.e., the
same flat surface for the melt pool as for the original solid workpiece. The Tsao and Wu EMF model was also used for simulating the melt pool with a variety of other arc heat sources such as a plasma arc [117–119], GTA [83, 86, 120], and underwater wet flux-cored arc [121]. It was also applied to study hybrid applications of the GMA heat source. For instance, Zhang and Wu [122] as well as Gao et al. [123] used it to study the melt pool behaviour in hybrid GMA-laser beam welding and Park et al. [37] in tandem GMAW.

About a couple of decades ago, thanks to the significant increase in computational capabilities, some authors started also modelling the EMF field by solving the system of Maxwell’s equations with the magnetohydrodynamics approximations. However, even with this numerical approach, the assumption of a flat melt pool surface is still commonly used by most authors. Different variants of the numerical EMF model exist today. They share in common to solve the Laplace equation for the scalar electric potential and Ohm’s law to compute the current density field in the workpiece. The calculation of the magnetic field varies depending on the variants of the numerical EMF model. Hu et al. [124] and Rao et al. [125] used the integral form of Ampere’s law [126] to calculate the self-induced magnetic field. An advantage of this formulation is that it eliminates the need to define the boundary conditions for the magnetic field. A drawback is that it only calculates its azimuthal component. It turns out that the magnetic field distribution for a typical welding application is not simply azimuthal, as shown in the appended Paper II. Xu et al. [127] used the differential form of Ampère’s law to solve the magnetic field in a 3D cartesian coordinate system. A slightly different approach was used by Zhou et al. [128] who solved instead for the magnetic potential, \( \vec{A} \), and then derived the magnetic field, \( \vec{B} \), from the rotational of the magnetic potential. To obtain a unique solution for \( \vec{A} \), the Lorentz gauge, \( \nabla \vec{A} = 0 \), was chosen. Thus, the simulation of the melt pool with the numerical EMF model generally requires solving two additional PDEs in addition to the equations of conservation of mass, momentum, and energy, and the transport governing the metal volume fraction.

The literature review reveals that in the past most studies have adopted the analytical EMF expressions of Kou and Sun [13] and Tsao and Wu [14] (called hereafter analytical models for simplicity). These analytical models continue to be widely applied even today. As mentioned earlier some authors use also the numerical EMF model. Going back to the original developments, it can thus be seen that these models consider different levels of simplifications. However, the possible effect of these simplifications is seldom addressed. Kumar and Debroy [15] did provide the comparison of the distribution of the current density, magnetic field, and EMF force in the workpiece between different analytical models (i.e., Kou and Sun model, Tsao and Wu model, and a variant proposed...
3.5 Effect of arc pulsation on the melt pool flow

The variant of GMA fusion that uses a pulsed power supply (GMA-P) offers several advantages [6]. It is widely used for joining thin sheet metal parts and welding joints in non-flat orientations, which are often difficult with other processes. It has proven to improve joint quality and reduce hot cracking, spatter, and fusion defects [129, 130]. This process also has the advantages of both axial spray transfer of OPOD and a lower mean heat input which improves stability and quality [41]. The pulse parameters can indeed affect the microstructure, HAZ, and porosity formation via the arc behavior, thermal cycle, and flow field. However, the selection of these parameters is not straightforward. Several research works have investigated the effect of pulse parameters in GMAW-P. The majority of them were experimental and focused mostly on the influence of the weld quality, material microstructure, and mechanical properties. For instance, Ghosh et al. [131] suggested that the variation of the arc pressure during a pulsing cycle leads to the formation of a vortex in the shielding gas that causes the entrapment of gas in the melt pool resulting in the occurrence of porosity. Wang et al. [132] suggested that the melt pool has a very fast response to the varying electric current during the pulsing cycle. They showed that the plasma jet induces a significant surface depression at high current and the EMF is more effective at peak current than at background current. Zhao et al. [133] investigated drop dynamics in GMAW-P and showed that the pulsing parameters with varied peak current and peak duration, albeit with identical average current, strongly affect the dynamics of the drop transfer. They showed that a high current and
short pulse increase the drop velocity by nearly threefold while the increase in the drop temperature is much less significant.

Despite that many researchers have confirmed the influence of pulsing parameters on weld properties, the models intended for an in-depth analysis of the melt pool behavior using CFD usually ignore the time-dependence due to pulsing in the electric current, voltage, and arc radii. Therefore, they do not reflect the related time variations in the applied heat flux, arc pressure, and EMF. For instance, Zargari et al. [9] used CFD simulations to investigate melt pools in tandem-pulsed GMAW with a workpiece subjected to vibration. These authors computed the effective arc radius using an empirical relation [134] where the time-averaged value of the electrical current was used as an input. An enhancement factor $\beta$ was also incorporated in the computed EMF field to increase the agreement between computed and measured results. Muhammad et al. [135] developed a CFD model for a melt pool produced with a hybrid heat source composed of a laser and a GMA. They applied it to investigate the mixing of the filler and base metal when the GMA torch was operated in both the leading and trailing configurations with respect to the laser beam. The results were also compared with experiments. Although the experiments were performed pulsing the GMA, their model used the time-average value of the electrical quantities. Similar simplifications were made by Cho et al. [18] who investigated the melt pool dynamics using CFD simulation of V-groove joints and Wu et al. [17] for a complex V-shaped fillet joint. Cheon et al. [16] also ignored the time variations of the electric signals when studying, with CFD, the flow dynamics in the fingertip produced with a pulsed DC-GMA. Yet, in all these studies the reliability of the simulation results was confirmed by the authors comparing the predicted FZ with metallographic cross-sections. Such modelling simplifications are not limited to the simulation of welding; they are also made to simulate the melt pool in AM [136].

In recent years, some researchers did also take into account the time-dependencies of the quantities related to the pulsing of a GMA when modeling the melt pool. For instance, Zhu et al. [19, 110] used four terms Fourier series to curve fit the measured waveform of the electric current and voltage and one term Fourier series to curve fit the measured effective arc radius. They applied the curve-fitted data as a function of time and to investigate the melt pool behavior and defects formation in narrow-gap GMAW. Park et al. [10] used a similar approach with up to eight terms in Fourier series to investigate the molten pool dynamics and bead geometry in the vertical-downward position with pulsed GMAW. Applying the same method, Cho et al. [35] concluded that the time-dependent effective arc radii plays an important role in driving the molten metal. It can induce a significantly different melt flow in comparison to the time-average effective arc radius. The authors also suggested that a small effective arc radius
drives the flow deep into the melt pool even at lower electric current due to high arc force density.

All the aforementioned CFD models that did consider the time dependence related to arc pulsation used an analytical EMF model. It is shown in the appended Paper II that the analytical EMF model is not consistent with the more general (numerical) EMF model and consequently leads to different predictions of the melt pool properties. To the best of the author’s knowledge, the effect of the pulsation when computing the EMF with the numerical model has not been considered yet.

Furthermore, there are other concerns with the approaches currently adopted in the literature regarding the effect of pulsation on the melt pool dynamics. Cho et al. [35] highlighted that a model that approximates pulsation with, time-averaged values cannot reasonably reproduce the penetration depth observed in experiments. On the contrary, several other researchers (e.g., [9, 16, 17]) did not report such issue. They could validate reasonably their simulation results against the experiment despite using a pulsation model simplified to the time-averaged values. It was possible because the simplified models were iteratively calibrated, using the trial and error approach, until the predicted results gave the best match with the experimental data. Various means of calibration are commonly applied in the literature to make the simulation results comply with the experimental data. For instance, Zargari et al. [9] used an enhancement factor in the vertical component of the EMF that parabolically increased from 1 at 1 mm below the surface to 4 at the free surface to enhance the stirring action of the molten metal and better reproduce the penetration depth observed experimentally. Zhang et al. [122] did similar adjustments. The need to make these adjustments raises several questions. Is it sufficient to set the adjustable parameter once to obtain a predictive model, or should the parameter be adjusted again if a process condition is changed? Is the adjustment needed because the modelling of arc pulsation is simplified, or is it because of the analytic EMF mode or both? These aspects are addressed in Paper III.

### 3.6 Effect of self-adaptable electromagnetic force

The EMF models described in Sections 3.4 and 3.5 (including the analytical models) are the state-of-the-art models applied for the CFD simulation of a GMA melt pool using a decoupled approach. There is, however, a simplification made by each of these models. It consists in neglecting the deformation of the free surface when computing only the EMF field. For simplicity, these EMF models are
now called EMF models with frozen free surface or solely frozen EMF models.

The literature shows that the arc pressure and drop impact can significantly deform the free surface during metal fusion with GMA [118,137]. It is also known from the literature that the EMF changes exponentially and can vary by an order of magnitude in the vicinity of the arc axis within melt pool [15,137]. Therefore, the assumption of frozen free surface when computing the EMF field might need to be questioned.

In fact, the problem is even more restrictive for the two analytic models in their original formulation. They assume not only that the free surface is frozen but also that it is flat. The application of this model is thus suited for e.g., bead-on-plate while it is inappropriate when simulating a melt pool in a V-groove joint as the surface is then inclined. Therefore, Cho et al. [18] suggested a coordinate mapping method to estimate the free surface elevation in a V-groove joint. They compared the melt pools computed with the original Kou and Sun EMF model for a flat surface and its variant mapped to a volume with an inclined surface. These authors concluded that the elevation of the inclined free surface is critical to consider when computing the EMF since it affects not only the fusion profile but also the molten pool volume. However, they estimated the free surface elevation only at the beginning of the simulation. They further suggested that the coordinate mapping method is only necessary when simulating the melt pool produced with the GTA. They also presumed that it is not strictly required when a GMA is used since the metal deposited from the filler wire would fill the joint groove resulting in a nearly flat surface.

Wu et al. [17] developed another algorithm to estimate the elevation that the free surface should reach and used this elevation to compute the EMF. This algorithm was applied to investigate the melt pool behavior in a horizontal fillet joint. Later Zhu et al. [19] and Han et al. [138] used a similar approach to investigate also defects in a narrow gap GMAW. However, the free surface was still assumed frozen when computing the EMF (although frozen to the condition after rather than before deposition). In addition, these implementations were applied to the analytical EMF model whose limitations are already outlined in the appended Paper II.

In the context of the numerical EMF model, Zhou et al. [128] simulated separately the thermal arc plasma and imported the steady state distribution of the EMF fields into the metal sub-domain to simulate the melt pool behavior. This weakly coupled model was applied to simulate melt pool dynamics for BOP as well as for overlapping beads. Zhou et al. [128] showed that, for overlapping beads, the distribution of the EMF field is asymmetric due to differences in the
3.6. Effect of self-adaptable electromagnetic force

elevation of the free surface. They also concluded that the EMF field for the overlapping bead was lower in comparison to the bead-on-plate case due to a larger contact area of the thermal arc plasma with the melt free surface which reduced the current density. Furthermore, the EMF field that was imported into the metal sub-domain was steady and did not take into account either the transient effect of arc pulsation or the effect of the free surface deformation. Therefore, this model, as well as the previous ones, all assume a frozen free surface when computing the EMF.
The free surface thermo-fluid model of this study (and related assumptions) is provided in the appended Papers and therefore not repeated here. It is made of a set of PDEs supplemented with constitutive relations (e.g. temperature-dependent transport properties), initial and boundary conditions. These PDEs are time-dependent, non-linear, coupled, and solved in 3D space. In general, this type of problem has no analytical solution. Its resolution thus relies on a numerical method based on CFD. The three main discretization methods are commonly used in CFD. They are i) the Finite Element Method (FEM), ii) the Finite Difference Method (FDM), and iii) the Finite Volume Method (FVM). The FVM method is the most common discretization method [139]. These methods are applied in various commercial as well as open-source CFD software currently available. Well-known examples are Ansys, FLOW 3D, STAR CCM+, COMSOL, OpenFOAM, Palabos [140]. OpenFOAM, which is based on the FVM, is the software used in this work. It is an open-source object-oriented library for numerical simulation of CFD and solid mechanics based on C++ programming language [141]. Some notable advantages of OpenFOAM are highlighted below:

• Large number of in-built native solvers with extensive capabilities and a number of tutorials.
• Equation syntax closely representing the mathematical notation, which allows complex PDEs to be written in a clear, concise, and readable form.
• Algorithms and models that can be customized and extended according to the user's problem.
• Open architecture with complete access to the source code for all the users at no cost.

The model of this study was implemented based on the native OpenFOAM solver interFoam.
Chapter 4

Numerical methods

The free surface thermo-fluid model of this study (and related assumptions) is provided in the appended Papers and therefore not repeated here. It is made of a set of PDEs supplemented with constitutive relations (e.g. temperature-dependent transport properties), initial and boundary conditions. These PDEs are time-dependent, non-linear, coupled, and solved in 3D space. In general, this type of problem has no analytical solution. Its resolution thus relies on a numerical method based on CFD. The three main discretization methods are commonly used in CFD. They are i) the Finite Element Method (FEM), ii) the Finite Difference Method (FDM), and iii) the Finite Volume Method (FVM). The FVM method is the most common discretization method [139]. These methods are applied in various commercial as well as open-source CFD software currently available. Well-known examples are Ansys, FLOW 3D, STAR CCM+, COMSOL, OpenFOAM, Palabos [140]. OpenFOAM, which is based on the FVM, is the software used in this work. It is an open-source object-oriented library for numerical simulation of CFD and solid mechanics based on C++ programming language [141]. Some notable advantages of OpenFOAM are highlighted below:

- Large number of in-built native solvers with extensive capabilities and a number of tutorials.

- Equation syntax closely representing the mathematical notation, which allows complex PDEs to be written in a clear, concise, and readable form.

- Algorithms and models that can be customized and extended according to the user’s problem.

- Open architecture with complete access to the source code for all the users at no cost.

The model of this study was implemented based on the native OpenFOAM solver *interFoam*. The *interFoam* is a solver for two incompressible, isothermal and
immiscible fluids that models the evolution with time of the interface (or free surface) between the two fluids. The extension of interFOAM towards a solver for a melt pool was initiated in a former project with stationary laser beam heat source and steel S705 by Svenungsson [20]. The following major additional features were then added to the interFoam solver:

- Buoyancy force using Boussinesq approximation.
- Energy conservation equation.
- Phase change due to melting/solidification.
- Mushy zone model for implicit tracking of solid/liquid transition region.
- Temperature and surfactant dependence of the surface tension.
- Thermocapillary (or Marangoni) force.

The developments were resumed in this study devoted to GMA fusion of Invar 36 alloy adding

- Temperature-dependent thermo-physical properties.
- Arc heat source and arc pressure force acting on the free surface.
- Relative motion between the arc heat source and the workpiece.
- EMF model based on PDEs for the electric potential and the magnetic potential vector.
- EMF model based on Kou and Sun model.
- EMF model based on Tsao and Wu model.
- Metal transfer model leading to periodic source terms of metal volume fraction, mass, momentum, and energy.

This chapter gives a brief description of numerical methods important for this study, namely free surface modelling and the discretization of the transport equations with the FVM. It concludes with the solution method and algorithm. The numerical schemes applied are indicated in the appended Papers, and therefore not repeated here.
4.1 Free surface modelling methods

The problem of this study involves two phases: the metal alloy (solid and liquid) and the gas atmosphere. The classification of the main methods for modelling the evolution of the interface between two phases, or free surface problems, is illustrated in Figure 4.1. These methods include: (1) interface fitting, (2) interface tracking, and (3) interface capturing.

![Figure 4.1: Classification of interface modelling methods. The methods used in this study are highlighted in green.](image)

Interface fitting is based on a Lagrangian grid. The free surface is then described as an interface boundary, which is embedded in the grid, as shown in Figure 4.2(a). The grid and the interface boundary move with the fluid. Most finite-element solvers for multiphase flow use this approach. If there is no mass transfer between the two fluid phases in the physical problem (i.e. no vaporisation/condensation or diffusion of elements), the equations governing the fluid flow do not need to be supplemented with advection terms to describe a mass flow across the interface boundary as this one then coincides with the (physical) free surface. Interface fitting has thus the advantage of effectiveness and simplicity in the solution process [142, 143]. However, this method is prone to significant numerical errors due to severe element distortion when the free surface undergoes large deformation. It can also lead to negative element volume, which could abruptly terminate the solution process. Furthermore, this method struggles with tracking surfaces that break apart or coalesce. It is therefore poorly suited to model the metal transfer taking place in GMA fusion.

The two other classes of interface modelling methods use a fixed Eulerian grid, which eliminates the problem of element distortion associated with the interface
fitting method. They are based on a one-fluid (or mixture model) description of the two phases. Therefore, only one momentum equation is solved for two fluids. The thermodynamic and transport properties of the one-fluid are determined through volume-weighted averaging of the properties of the two fluids locally present. The interface tracking class is exemplified in Figure 4.2(b). The interface is then marked by a set of points that are explicitly tracked in time as they undergo topological changes because of the fluid motion. The first numerical method developed for interface tracking is the marker and cell (MAC) method that uses a volume marker [144]. The markers track the fluid volumes and the free surface is then made up of boundaries of the volumes. However, interface tracking is computationally demanding, particularly in 3D space due to the large number of markers whose motion needs to be followed [142]. It is therefore mostly limited to 2D CFD simulations. Moreover, it can lead to non-physical free surface in the presence of converging or diverging flow. For instance markers pulled apart might develop non-physical voids. Melt pool flow can be the location of converging flow in the presence of surfactant.

Figure 4.2(c) presents an example of the application of the interface capturing class. This class, which belongs also to the one-fluid formulation and is based on an Eulerian grid, employs a scalar transport equation in addition to the flow equations. The evolution of the interface is then marked by an indicator function via the solution of the scalar transport equation. This class is used for the computation of a wide variety of free surface flow problems since it is better suited than the previous methods to predict the evolution of a complex interface. It is also the method used in this study, as it is suited to predict the coalescence of transferred metal droplets with the melt pool free surface. However, interface capturing gives a less accurate representation of a free surface than interface tracking methods.

The commonly used interface capturing methods are the VOF method [145], and the level-set (LS) method [146]. With the LS method, a distance function is used as an indicator function [147]. This indicator function is smooth, continuous, and easier to solve compared to the VOF method. It is well known for its ability to predict sharper interface than the VOF method that suffers from numerical diffusion and smearing of the interface. However, the disadvantage with the LS method is that it requires periodically resetting the indicator function. As a result, mass conservation is not strictly ensured with the LS method [147], while the VOF method ensures better mass conservation [51]. In the VOF method, the volume fraction of a primary phase is used as an indicator function. This volume fraction is convected through the fluid domain by solving a scalar transport equation. This method is robust enough to handle complex fluid behavior such
as breakup and coalescence of fluid masses [142]. The performance of the VOF method for modelling the free surface of a melt pool has been widely evaluated in many previous simulation studies [35, 66–68]. In a way, the VOF method has become the standard free surface modelling method in this area of research. Therefore, the VOF method is also employed in this study.

4.2 Discretization of the transport equation

As OpenFOAM is based on the FVM, the main aspects of this discretization method are presented in this section. With this method, the space of the computational domain is partitioned into small control volumes or mesh cells. Each control volume is convex and has a cell centroid $P$ where the discrete solution is sought and stored. An example of control volume can be seen in Figure 4.3.

Each control volume is surrounded by a set of planar faces that constitute a closed surface. The faces that are shared between two control volumes are classified as internal faces, whereas the faces that belong to only one control volume located at a boundary of the domain are classified as boundary faces. In OpenFOAM, the control volumes can be irregularly ordered, and thus compose an unstructured grid mesh. The connectivity between faces and neighbouring control volumes are thus stored to be accessible during the computations. The control volumes can also have arbitrary polyhedral shapes and therefore have different numbers of enclosing faces.

For the thermo-fluid problem of this study, the metal and the gas atmosphere are assumed to be incompressible. The one-fluid density ($\rho$) is then a function of the local volume fraction in the metal ($\alpha$) and in gas ($1 - \alpha$), while the mass conservation (or continuity) equation becomes an additional constraint on the

![Figure 4.2: Free surface modeling method: (a) interface fitting, (b) interface tracking, and (c) interface capturing [51].](image-url)
velocity field. Then, the transported properties to be determined aim at computing the one-fluid pressure \((p)\) that is obtained so as to satisfy continuity, the one-fluid velocity vector \((\vec{u})\), temperature \((T)\), the alloy volume fraction \((\alpha)\), plus the electric potential \((V)\) and the magnetic potential vector \((\vec{A})\) when the numerical electromagnetic model is used. For simplicity, the transported properties are represented by a generic variable \(\phi\) in the rest of this section. With the space discretization of the finite volume method, \(\phi\) is determined at the centre \(P\) (located in \(\bar{x}_P\)) of each control volume and it represents the following (mean) cell value:

\[
\phi_P = \bar{\phi}(\bar{x}_P) = \frac{1}{\Omega_P} \int_{\Omega_P} \phi(x) d\Omega \quad (4.1)
\]

With the FVM, the PDEs governing the melt pool dynamics are expressed in a conservative form over each control volume and time step \(\Delta t\) to proceed to their discretization. They can be written in the following generic form:

\[
\int_{\Delta t} \left[ \frac{\partial}{\partial t} \int_{\Omega_P} (\rho \phi) d\Omega + \int_{\Omega_P} \nabla \cdot (\rho \vec{u} \phi) d\Omega - \int_{\Omega_P} \nabla \cdot (\rho \Gamma_\phi \nabla \phi) d\Omega \right] dt = \int_{\Delta t} \left[ \int_{\Omega_P} S_\phi d\Omega \right] dt \quad (4.2)
\]

where \(\Gamma_\phi\) denotes the diffusivity of the variable, and \(S_\phi\) is a source term. It should be noticed that when the EMF is computed with the numerical EMF model, Eq.
4.2. Discretization of the Transport Equation

4.2 is reduced to two terms: the diffusive term and the source term. In a preliminary set of the FVM discretization, the volume integrals with the divergence operator \( \nabla \cdot \) (i.e. the convective and the diffusive terms) are transformed to surface integrals applying the generalized form of Gauss theorem [149], leading to

\[
\int_\mathcal{N} \left[ \frac{\partial}{\partial t} \int_{\Omega_P} (\rho \phi) \, d\Omega + \int_{\partial \Omega_P} d\vec{S} \cdot (\rho \vec{u} \phi) - \int_{\partial \Omega_P} d\vec{S} \cdot (\rho \Gamma_\phi \nabla \phi) \right] \, dt
\]

\[
= \int_\mathcal{N} \left[ \int_{\Omega_P} S_\phi \, d\Omega \right] \, dt
\]

(4.3)

Next, the discretization of the transport Eq. 4.3 is made term by term to convert this integral form over differential volumes into discrete algebraic equations over finite volumes.

**Time discretization**

In this study, the time derivative that captures the rate of change of \( \phi \) is approximated over the volume \( \Omega_P \) using the temporal variation in a point according to a first-order Taylor expansion

\[
\phi(t + \Delta t) = \phi(t) + \Delta t \left( \frac{\partial \phi}{\partial t} \right)
\]

(4.4)

The variable known at the previous discretized time level, \( \phi^n = \phi(t) \), and the variable sought at the present time level, \( \phi^{n+1} = \phi(t + \Delta t) \), then lead to the first order approximation of the temporal derivative (Euler scheme, that is implicit). It results in the following expression that is used in the volume integral approximation

\[
\int_{\Omega_P} \frac{\partial \phi}{\partial t} \, d\Omega = \frac{\phi^{n+1}_P - \phi^n_P}{\Delta t} \Omega_P
\]

(4.5)

**Convective term**

The control volume \( \Omega_P \) being enclosed in a bounded set of flat faces, the integral over the surface of the control volume in the convective term is transformed into a sum over all the enclosing faces
where \( F_f = \vec{S}_f \cdot (\rho \vec{u}) \) is the mass flux through the face \( f \) of the control volume. This flux can be estimated with face interpolated values of \( \rho \) and \( \vec{u} \). However, the interpolation might introduce an error in the computation of the mass flux through \( f \). The assembly of the face flux over all the faces of a control volume is thus a critical step of the discretization to satisfy mass conservation. It is performed by calculating the conservative face flux from the solution of the pressure equation (itself derived from the continuity equation).

The value \( \phi_f \) of the variable at the face centre \( f \) is calculated from \( \phi \) at cell centres of control volumes applying interpolation schemes that take into account the flow direction through \( F_f \). In OpenFOAM, a scheme is specified by the user for each convective term. In this study, the convective discretization scheme used when solving for the alloy volume fraction is based on a second-order van Leer scheme strictly bounded between 0 and 1. When solving for the momentum and for the thermal energy, a blended convective discretization scheme is used. It is based on a second-order central-differencing scheme that is limited towards upwind in regions of rapidly changing gradient using a Sweby limiter that makes the solution total variation diminishing. The user specifies a coefficient that ranges between 0 and 1 to enforce either central differencing or upwinding. Coefficient 1 corresponds to the best convergence while coefficient 0 corresponds to the best accuracy. In this study this coefficient is set to 1.

### Diffusive term

Similar to the convective term, the integral over the surface of the control volume in the diffusive term is transformed into a sum over all the enclosing faces

\[
\oint_{\partial \Omega_p} d\vec{S} \cdot (\rho \vec{u} \phi) = \sum_f \vec{S}_f \cdot (\rho \vec{u}) \phi_f = \sum_f F_f \phi_f
\]  (4.6)

The terms \( (\rho \Gamma \phi) \) and \( \vec{S}_f \cdot (\nabla \phi) \) need additional treatment. In this study, the different test cases computed use orthogonal mesh. Therefore, the normal to the face \( f \) that is along \( \vec{S}_f \) (see Figure 4.3) is parallel to the vector \( \vec{d} \) joining the centres of the cells adjacent to the face. As a result, the discretization of the fluid property gradient at the face centroid is applied using the surface normal gradient scheme according to:

\[
\oint_{\partial \Omega_p} d\vec{S} \cdot (\rho \Gamma \phi \nabla \phi) = \sum_f \vec{S}_f \cdot (\rho \Gamma \phi \nabla \phi) = \sum_f (\rho \Gamma \phi) \vec{S}_f \cdot (\nabla \phi)
\]  (4.7)
\[
\n\nabla \phi_f = f_x (\nabla \phi)_P + (1 - f_x) (\nabla \phi)_N
\]

where \( f_x = \frac{|\vec{x}_N|}{|\vec{x}_N - \vec{x}_i|} \). This calculation is second-order accurate. A Gauss discretization is then applied to obtain the gradient \( \nabla \phi_P \) and \( \nabla \phi_N \) at the centroid of the cells \( P \) and \( N \), respectively. Thus, the Gauss discretization together with a linear interpolation scheme fully discretizes \( (\nabla \phi)_f \).

**Source term**

The source term \( S_\phi \) is made of all the terms in the equation that cannot be treated as a convective or a diffusive term. If this term is non-linear in \( \phi \), it is first linearized leading to

\[
S_\phi = S_u + S_P \phi
\]

After integration over the control volume centred in \( P \), it gives the following discretized source term

\[
\int_{\Omega_P} S_\phi d\Omega = S_u \Omega_P + S_P \Omega_P \phi_P
\]

### 4.3 Solution method and algorithm

The spatial and temporal discretizations above described are applied to the transport Eq. 4.3 accounting also for the boundary conditions. In this study, these conditions are either of Neumann or Dirichlet type. It leads to the following linear algebraic equation of unknown \( \phi_P^{n+1} \)

\[
\frac{\rho_P^{n+1} \phi_P^{n+1} - \rho_P^n \phi_P^n}{\Delta t} \Omega_P + \sum_f \left( \bar{S}_f \cdot (\rho \vec{u})_f^{n+1} \phi_f^{n+1} + (\rho \Gamma_\phi)_f^{n+1} \bar{S}_f \cdot (\nabla \phi)_f^{n+1} \right) = S_u \Omega_P + S_P \Omega_P \phi_P^n,
\]

For convenience this equation is now re-organised in a condensed form

\[
ap_P \phi_P^{n+1} + \sum_N a_N \phi_N^{n+1} = b
\]

49
where the coefficients $a$ are functions of the convective and diffusive fluxes through the faces of the control volume centred in $P$. The index $N$ indicates the control volumes neighbouring $P$ that contribute to the fluxes. The coefficient $b$ groups all the terms that are known because they do not depend on $\phi^{n+1}$. The system made of the equation at each of the $i = 1, \ldots, N_{cv}$ control volumes is assembled in a matrix form to be solved,

$$A\phi = b$$

(4.13)

where $A$ is the matrix of elements $a$, $\phi$ and $b$ are vectors of elements $\phi^{n+1}$ and $b$, respectively. By construction, the matrix $A$ is sparse. However, the size of the algebraic systems of equations (thus of $A$) being large, an iterative solution method is applied as usually done for CFD problems. To increase the rate of convergence of this solution process, a preconditioner is applied that propagates the information faster through the computational mesh. The assembled Eq. 4.13 with preconditioner can be expressed as:

$$M^{-1}A\phi = M^{-1}b$$

(4.14)

with $M$ being the preconditioner matrix. The solution algorithm is repeatedly applied to reduce iteratively the residuals until a pre-assigned level of convergence is achieved. The residual is basically a measure of the error in the solution. The smaller the residual, the more accurate the solution. The residuals are re-evaluated in each control volume after each solver iteration. The iterative solution is completed when the maximum (over the set of control volumes) residual is lower than the pre-assigned value of absolute tolerance, or of relative tolerance, or if the maximum number of iterations prescribed is reached. The solution algorithm is applied successively to the different variables of the problem, except for pressure and velocity whose strong coupling requires a special treatment. Then, the iterative solution advances to the next time step.

In the transient GMA fusion melt pool simulations in this study, the residuals (final) for the solution of the alloy volume fraction ($\alpha$), pressure $p$, velocity $\vec{u}$, and temperature $T$ was set to $10^{-12}, 10^{-8}, 10^{-8},$ and $10^{-10}$, respectively. The relative tolerance at the final iteration (before time incrementation) was set to 0 to force the solution to converge to the solver tolerance in each time step. The maximum number of iteration corresponds to OpenFOAM’s default value of 1000, which is far beyond the number of iterations needed for the test cases computed. Furthermore, an adjustable time step size was used, which is controlled by a CFL number. The maximum allowable CFL number (0.1) and corresponding time...
where the coefficients \( a \) are functions of the convective and diffusive fluxes through the faces of the control volume centred in \( P \). The index \( N \) indicates the control volumes neighbouring \( P \) that contribute to the fluxes. The coefficient \( b \) groups all the terms that are known because they do not depend on \( \phi_{n+1} \).

The system made of the equation at each of the \( i = 1, \ldots, N_{cv} \) control volumes is assembled in a matrix form to be solved, \( A \phi = b \) (4.13), where \( A \) is the matrix of elements \( a \), \( \phi \) and \( b \) are vectors of elements \( \phi_{n+1} \) and \( b \), respectively. By construction, the matrix \( A \) is sparse. However, the size of the algebraic systems of equations (thus of \( A \)) being large, an iterative solution method is applied as usually done for CFD problems. To increase the rate of convergence of this solution process, a preconditioner is applied that propagates the information faster through the computational mesh. The assembled Eq. 4.13 with preconditioner can be expressed as:

\[ M^{-1}A \phi = M^{-1}b \] (4.14)

with \( M \) being the preconditioner matrix. The solution algorithm is repeatedly applied to reduce iteratively the residuals until a pre-assigned level of convergence is achieved. The residual is basically a measure of the error in the solution. The smaller the residual, the more accurate the solution. The residuals are re-evaluated in each control volume after each solver iteration. The iterative solution is completed when the maximum (over the set of control volumes) residual is lower than the pre-assigned value of absolute tolerance, or of relative tolerance, or if the maximum number of iterations prescribed is reached. The solution algorithm is applied successively to the different variables of the problem, except for pressure and velocity whose strong coupling requires a special treatment. Then, the iterative solution advances to the next time step.

In the transient GMA fusion melt pool simulations in this study, the residuals (final) for the solution of the alloy volume fraction (\( \alpha \)), pressure \( p \), velocity \( \vec{u} \), and temperature \( T \) was set to \( 10^{-12}, 10^{-8}, 10^{-8}, \) and \( 10^{-10} \), respectively. The relative tolerance at the final iteration (before time incrementation) was set to 0 to force the solution to converge to the solver tolerance in each time step. The maximum number of iteration corresponds to OpenFOAM’s default value of 1000, which is far beyond the number of iterations needed for the test cases computed. Furthermore, an adjustable time step size was used, which is controlled by a CFL number. The maximum allowable CFL number (0.1) and corresponding time step size \( 10^{-5}s \) were specified to achieve a stable solution. This low CFL value was imposed by the free-surface part of the model.

Concerning the pressure-velocity coupling, three main algorithms are available in OpenFOAM: 1) pressure-implicit split-operator (PISO), 2) the semi-implicit method for pressure-linked equations (SIMPLE), and 3) PIMPLE which is a hybrid between PISO and SIMPLE. The SIMPLE algorithm is formulated for steady-state simulations whereas the PISO and PIMPLE algorithms are formulated for transient simulation. In this thesis, the PISO algorithm is used as it is more stable and faster in terms of computational time. Figure 4.4 shows a general flow chart of the solution algorithm applied to perform the simulations.
Paper I: Effect of Substrate Orientation on Melt Pool during Multi-Layer Deposition in V-Groove with Gas Metal Arc

The effect of changing the substrate orientation on the second layer GMAW pass of Invar 36 deposited in a V-groove joint was investigated experimentally and using numerical simulation. A thermo-fluid model with free surface deformation was developed to investigate the influence of the substrate orientation on melt flow behavior and resulting bead geometry. The results showed that even at an angle as low as 20 degrees relative to the flat position, the orientation significantly changed the force balance in the melt pool, resulting in different melt flow patterns and bead geometry. Specifically, the flat substrate resulted in a deeper penetration with a smooth reinforced bead, while the downhill orientation resulted in a shallow-penetration with a wider pool width and reduced reinforced height. The uphill orientation resulted in a narrow channel flow of the melt pool, leading to humping at solidification, and the sideway orientation resulted in an asymmetric melt pool. The predicted FZ and bead geometry agreed well with the experimental measurements.

Paper II: Comparative study of the main electromagnetic models applied to melt pool prediction with gas metal arc: effect on flow, ripples from drop impact, and geometry

The effects of the three different EMF models commonly applied to simulate the melt pool were comparatively investigated starting from the underlying assumptions. Each model was uniquely implemented into a the thermo-fluid simulation to predict the behavior of the melt pool for a bead-on-plate GMAW. It was concluded that the analytical models (i.e., Kou and Sun model as well as Tsao and...
Chapter 5

Summary of the appended Papers

Paper I: Effect of Substrate Orientation on Melt Pool during Multi-Layer Deposition in V-Groove with Gas Metal Arc

The effect of changing the substrate orientation on the second layer GMAW pass of Invar 36 deposited in a V-groove joint was investigated experimentally and using numerical simulation. A thermo-fluid model with free surface deformation was developed to investigate the influence of the substrate orientation on melt flow behavior and resulting bead geometry. The results showed that even at an angle as low as 20 degrees relative to the flat position, the orientation significantly changed the force balance in the melt pool, resulting in different melt flow patterns and bead geometry. Specifically, the flat substrate resulted in a deeper penetration with a smooth reinforced bead, while the downhill orientation resulted in a shallow-penetration with a wider pool width and reduced reinforced height. The uphill orientation resulted in a narrow channel flow of the melt pool, leading to humping at solidification, and the sideway orientation resulted in an asymmetric melt pool. The predicted FZ and bead geometry agreed well with the experimental measurements.

Paper II: Comparative study of the main electromagnetic models applied to melt pool prediction with gas metal arc: effect on flow, ripples from drop impact, and geometry

The effects of the three different EMF models commonly applied to simulate the melt pool were comparatively investigated starting from the underlying assumptions. Each model was uniquely implemented into a the thermo-fluid simulation to predict the behavior of the melt pool for a bead-on-plate GMAW. It was concluded that the analytical models (i.e., Kou and Sun model as well as Tsao and
Wu model) are not suited to the study of a thin workpiece (about 4 mm thickness) if the ground of the electric potential is imposed at the bottom of the workpiece. Furthermore, the three models lead to significantly different proportions of the force components in the radial and vertical directions. They also resulted in clearly different predictions of several crucial aspects of melt pool including the recirculation pattern, the thermal convection, the pool morphology, the bead geometry, and the oscillation of the free surface during metal transfer. It is also inferred that the enhancement applied to the EMF to reproduce the experimental fusion geometry, in particular with Tsao and Wu model, cannot be expected to counterbalance the observed discrepancies. Finally, it is believed that the most comprehensive of the three models, which involved solving for two additional PDEs governing electric potential and magnetic potential field, should be further extended to e.g., take into account the effect of the free surface local condition and its evolution with time on the EMF.

**Paper III:** Systematic analysis of the effect on the simulated melt pool of different approaches for modelling arc pulsation

This Paper aimed at comparatively investigating different approaches applied to transient modelling of the pulsation of the arc during the thermo-fluid simulation of melt pool. The results showed that the EMF during pulsing can be almost four times higher compared to when it is estimated using the time-average value of the arc parameters. The time evolution of the heat flux acting on the melt pool free surface during pulsing enhances the Marangoni force leading to slightly wider distribution of the thermal flow field in comparison to applying the constant heat flux. Furthermore, the transient modelling of the time-evolution of the pressure force on the surface of the melt pool was found to have weak effect with negligible variations in the temperature distribution, flow field and melt pool geometry compared to when estimating the pressure force using the time-average value of the arc parameters.

**Paper IV:** Melt pool electromagnetic force model extended to account for free surface deformation - Application to gas metal arc

This paper investigates the influence of the EMF that follows the local orientation of the free surface interface on the predicted melt pool. Previous models, which are currently the state-of-the-art, assumed a flat melt pool surface when calculating the EMF field. In contrast, the thermo-fluid model developed in this paper takes into account the deformation of the free surface when computing the EMF field. The results showed that when the deformation of the free surface of the melt pool is ignored, the computed electric potential isolines are distributed...
wider within the region of the melt pool. Similarly, the computed EMF field is distributed slightly deeper into the melt pool and their amplitude when measured on the same plane, is larger, resulting in noticeable differences in the predicted melt pool geometry.
Chapter 6

Conclusion

A thermo-fluid model of the melt pool in GMA fusion was developed and implemented in the open-source CFD software OpenFOAM. Several test cases were simulated for various types of GMA fusion (e.g. V-groove joint, bead-on-plate). Experiments were also conducted in parallel to obtain the parameters needed for the simulations as well as to validate the thermo-fluid model. The conclusions drawn based on the obtained results are presented below as an answer to the research questions.

6.1 Response to the research questions

RQ1. What are the effects of the workpiece orientation (relative to the arc axis) on the melt flow and resulting bead geometry during multi-layer GMA W of a V-groove joint?

This research question was addressed in the appended Paper I. The main elements of answer are now summarized:

• Flat orientation: in this position a stable melt pool with a large recirculation flow is predicted underneath the arc column. The recirculation enhances the heat transfer leading to a deep penetration. A stable melt pool produces a continuous and smooth reinforced bead.

• 20° downhill orientation: the contribution of the gravity along the direction parallel to the workpiece surface is then large enough to decelerate the Marangoni flow along the trailing edge of the melt pool and accelerate it on the forefront of the melt pool as compared to the flat orientation. A large swirl beneath the surface of the trailing region of the melt pool indicates stronger returning flow towards the melt front which also provides preheating of the workpiece. The melt pool tends to flow forward (towards the downward inclination) which reduces the melt pool length but...
Chapter 6

Conclusion

A thermo-fluid model of the melt pool in GMA fusion was developed and implemented in the open-source CFD software OpenFOAM. Several test cases were simulated for various types of GMA fusion (e.g. V-groove joint, bead-on-plate). Experiments were also conducted in parallel to obtain the parameters needed for the simulations as well as to validate the thermo-fluid model. The conclusions drawn based on the obtained results are presented below as an answer to the research questions.

6.1 Response to the research questions

RQ1. What are the effects of the workpiece orientation (relative to the arc axis) on the melt flow and resulting bead geometry during multi-layer GMAW of a V-groove joint?

This research question was addressed in the appended Paper I. The main elements of answer are now summarized:

- Flat orientation: in this position a stable melt pool with a large recirculation flow is predicted underneath the arc column. The recirculation enhances the heat transfer leading to a deep penetration. A stable melt pool produces a continuous and smooth reinforced bead.

- 20° downhill orientation: the contribution of the gravity along the direction parallel to the workpiece surface is then large enough to decelerate the Marangoni flow along the trailing edge of the melt pool and accelerate it on the forefront of the melt pool as compared to the flat orientation. A large swirl beneath the surface of the trailing region of the melt pool indicates stronger returning flow towards the melt front which also provides preheating of the workpiece. The melt pool tends to flow forward (towards the downward inclination) which reduces the melt pool length but
increases the melt pool width. The resulting effect is a bead with larger width and lower height.

- **20° uphill orientation**: in this position, the contribution of the gravity along the direction parallel to the workpiece surface enhances the Marangoni force and the flow towards the melt pool rear in the narrow channel of the V-groove. It, therefore, narrows the melt pool width and accumulates the molten metal at the melt pool rear resulting in humping upon solidification.

- **20° side inclined orientation**: the contribution of the gravity towards the lateral direction of the workpiece is large enough to push the trailing part of the melt pool towards the direction of the inclination resulting in an asymmetric melt pool flow along the travel direction. Furthermore, this causes incomplete fusion on the V-groove wall opposite to the inclination direction resulting in undercut defect.

Therefore, with these conditions, flat and downhill 20° inclined multi-layer deposition using GMAW can be performed while uphill 20° and side inclined 20° multi-layer deposition are not recommended.

**RQ2. What are the effects of the three common electromagnetic force models on the prediction of GMA melt pool?**

This research question was addressed in the appended Paper II. The answer to RQ2 is made of the answers to its sub-questions whose main points are summarized:

**RQ2.1. What are the assumptions underlying these three models and their influence on the predicted electromagnetic force?**

- The three electromagnetic models share in common the magnetohydrodynamics approximation.

- At the workpiece surface, the analytical models of Tsao and Wu and Kou and Sun (at least in their original and standard version) assume a flat melt pool free-surface and a Gaussian distribution of the current density.

- In the workpiece, the current density distribution predicted/assumed by the analytical models is axi-symmetric. This is not an obligatory condition with the numerical model, but it can be a special condition when the arc axis is symmetric about the workpiece.
• The analytical models neglect the contribution of the radial component of the current density in the melt pool. As a result, for the studied test case Kou and Sun model leads to approximately 50% overestimation of the EMF field in the melt pool region compared to the more general numerical model.

• The simplifying assumptions specific to Tsao and Wu model change significantly the components of the EMF in the melt pool region to an extent that can reach up to one order of magnitude.

RQ2.2. What is the influence of these three models on the predicted melt flow, free surface oscillation, and bead geometry?

The different electromagnetic models result in clearly distinct recirculation patterns, thermal convection, melt pool morphology and free surface oscillation. For the studied test case, the melt flow in the vicinity of the arc axis is predominantly downward with Kou and Sun model and with the numerical model whereas it is predominantly radially outward with Tsao and Wu model. When comparing the predicted results with the experimental data:

− The penetration is significantly shallow with Tsao and Wu model, significantly deep with Kou and Sun model, and it is in good agreement with the numerical model.

− On the other hand, the predicted melt pool width is slightly wide with Tsao and Wu model, slightly narrow with Kou and Sun model, and in good agreement with the numerical model.

− The computed bead height is significantly large with Kou and Sun model and it is in good agreement with the numerical model and Tsao and Wu model.

RQ2.3. In which circumstances and for predicting which aspect of a GMA melt pool is each of these models suited or questionable?

• The three EMF models could indifferently be used to fit the penetration depth to experimental macrographs provided that the model parameters are adjusted using a trial and error method. This would imply enhancing the vertical component of the EMF field when using Tsao and Wu model and properly adjusting the arc radius when using Kou and Sun model.

• The analytical model of Tsao and Wu is not recommended for the analysis of free surface oscillation as it can potentially overestimate the oscillating amplitude in the downstream of the melt pool.
For comprehensive analysis of the melt pool with a model able to predict thermal flow, pool morphology, and bead geometry, the numerical model is recommended.

**RQ3. When using pulsed GMA, what is the impact on the predicted melt pool of modelling time-dependent rather than time-averaged pulsing parameters?**

This research question was addressed in the appended Paper III. The answer to RQ3 is summarized as follows:

- The EMF field during pulsing cycle reached up to 4 times higher than when estimating it using time-averaged value of electric current and effective arc radii resulting in an enhanced recirculating flow of molten liquid underneath the arc.
- The modelling of time-dependent heat flux resulted in the evolution of local peak temperature on the melt pool surface in consistent with the evolution of the electrical waveform, albeit with a larger range of fluctuation in comparison to the time-averaged heat flux model. The thermocapillary flow is also enhanced resulting in slightly wider melt pool width.
- The modelling of time-dependent arc pressure showed weak effect with negligible differences in temperature distribution, flow field and melt pool geometry compared to the time-averaged arc pressure model.

**RQ4. What are the effects on the prediction of GMA melt pool of taking into account the deformation of the free surface when modelling the EMF?**

This research question was addressed in the appended Paper IV. The answer to RQ4 is summarized as follows:

- The EMF field is generally lower when taking into consideration the deformation of the free surface compared to frozen free surface case.
- The EMF field is asymmetric due to variations in the free surface elevation on each side of the arc axis despite maintaining symmetry in the position of the arc axis relative to the metal subdomain boundary.
- The effect of the free surface deformation on the EMF field results in a noticeable differences in the thermal flow field and also enhances improved prediction of the finger-tip shaped fusion zone. The re-circulating volume of molten liquid beneath the arc axis is lower which also causes reduced penetration depth and increased melt pool length in comparison to the frozen free surface model.
6.2 Future work

The CFD model of the melt pool developed in this doctoral thesis was primarily used to simulate melt pool behavior with the GMA heat source with or without considering the temporal variations characteristics of the thermal arc plasma during pulsing. Within this context, the model as it is can be used for other new applications involving melt pool simulation with the GMA and GTA heat source. Further developments of the model including the process physics that is currently simplified would ensure its application on a even wider spectrum. Several avenues for potential future research in this area are:

- Apply the model selected from the studies of papers II and III and improved in paper IV to simulate the test cases of paper I and perform a comparative analysis of the earlier results (i.e., in paper I) with the new ones.

- Extend the model to investigate the diffusion of alloying elements, since the effect of EMF on the element diffusion has not been investigated.

- Investigate the thermal flow field during multi-pass and multi-layer metal deposition e.g., GMA-AM.

- Extend the model to include material deformation and evolution of material microstructure, as a step towards investigating some typical defects formed during resolidification.

- Extend the model from decoupled to coupled by including the physics of the thermal arc plasma as well as of the sheath and pre-sheath layers at the metal/plasma interface. This could not only improve the accuracy of the simulation model but also eliminate the trial and error technique needed to calibrate the heat source model.
Appendices

A1 Material properties

The working material in this project is Invar which belongs to a set of nickel-iron alloys. Based on the proportion of iron and nickel, this set of alloys is broadly categorized into three sub-sets, all of which exhibit uniquely low thermal expansion. They are:

(i) Invar 36 (64% Fe in weight and 36% Ni)
(ii) SuperInvar (63% Fe in weight, 32% Ni and 5% Co)
(iii) Kovar (54% Fe in weight, 29% Ni and 17% Co)

The focus of this thesis is Invar 36, also commonly known as Invar or FeNi36. The name Invar is derived from the word invariable, referring to its lack of thermal expansion or contraction over a temperature range in the vicinity of 200°C. The thermal expansion of Invar alloy is indeed far below most kinds of alloys and is close to zero at room temperature, usually less than $2.0 \times 10^{-6} \, \text{C}^{-1}$ in the temperature range of 20 - 200°C [150]. Owing to this unique characteristic and excellent mechanical properties, Invar 36 alloy has been widely used in the fabrication of precision instruments and big molds for aerospace [97].

Although, the major elements of Invar 36 alloy are iron and nickel, several minor elements are used in varied proportions. The composition of the Invar 36 alloys collected from various sources for this study are thus recalled in Section A1.1. The thermophysical and transport properties of interest during melt pool simulation of Invar 36 alloy are mainly the density ($\rho$), the specific heat capacity ($c_p$), the thermal conductivity ($k$), the viscosity ($\mu$), the coefficient of thermal expansion ($\beta$), the latent heat of fusion ($\Delta h_f$) and the solidus ($T_{\text{sol}}$) and liquidus ($T_{\text{liq}}$) temperatures. These data are collected from various sources such as in-house experimental measurement, research article [94, 96, 97, 151–158], technical datasheet [159], datasheet of commercial companies [160–164], and thermodynamic databases e.g., CompuTherm [165], Thermo-Calc [166]. The temperature dependent properties of Invar 36 are discussed in detail in Section A1.2 and A1.3.
Appendices

A1 Material properties

The working material in this project is Invar which belongs to a set of nickel-iron alloys. Based on the proportion of iron and nickel, this set of alloys is broadly categorized into three sub-sets, all of which exhibit uniquely low thermal expansion. They are:

(i) Invar 36 (64% Fe in weight and 36% Ni)
(ii) SuperInvar (63% Fe in weight, 32% Ni and 5% Co)
(iii) Kovar (54% Fe in weight, 29% Ni and 17% Co)

The focus of this thesis is Invar 36, also commonly known as Invar or FeNi 36. The name Invar is derived from the word invariable, referring to its lack of thermal expansion or contraction over a temperature range in the vicinity of 200 °C. The thermal expansion of Invar alloy is indeed far below most kinds of alloys and is close to zero at room temperature, usually less than $2.0 \times 10^{-6} \text{ C}^{-1}$ in the temperature range of 20 - 200 °C [150]. Owing to this unique characteristic and excellent mechanical properties, Invar 36 alloy has been widely used in the fabrication of precision instruments and big molds for aerospace [97].

Although, the major elements of Invar 36 alloy are iron and nickel, several minor elements are used in varied proportions. The composition of the Invar 36 alloys collected from various sources for this study are thus recalled in Section A1.1. The thermophysical and transport properties of interest during melt pool simulation of Invar 36 alloy are mainly the density ($\rho$), the specific heat capacity ($c_p$), the thermal conductivity ($k$), the viscosity ($\mu$), the coefficient of thermal expansion ($\beta$), the latent heat of fusion ($\Delta h_f$) and the solidus ($T_{sol}$) and liquidus ($T_{liq}$) temperatures. These data are collected from various sources such as in-house experimental measurement, research article [94, 96, 97, 151–158], technical datasheet [159], datasheet of commercial companies [160–164], and thermodynamic databases e.g., CompuTherm [165], Thermo-Calc [166]. The temperature dependent properties of Invar 36 are discussed in detail in Section A1.2 and A1.3.
### A1.1 Invar 36 alloy Composition

#### Chemical composition of alloys used in the project

The nominal chemical composition (wt %) of Invar 36 alloy used in this project for the filler metal and workpiece are presented in Table A1.1.

**Table A1.1: Nominal chemical composition of filler metal and workpiece used at University West**

<table>
<thead>
<tr>
<th>Elements</th>
<th>Ni</th>
<th>C</th>
<th>Si</th>
<th>Mn</th>
<th>P</th>
<th>S</th>
<th>Cr</th>
<th>Co</th>
<th>Cu</th>
<th>Fe</th>
</tr>
</thead>
<tbody>
<tr>
<td>Filler metal</td>
<td>35.8</td>
<td>0.027</td>
<td>0.102</td>
<td>0.308</td>
<td>0.003</td>
<td>0.004</td>
<td>-</td>
<td>-</td>
<td>0.005</td>
<td>balance</td>
</tr>
<tr>
<td>Workpiece</td>
<td>36.0</td>
<td>0.01</td>
<td>0.03</td>
<td>0.28</td>
<td>0.004</td>
<td>0.000</td>
<td>0.13</td>
<td>0.01</td>
<td>-</td>
<td>balance</td>
</tr>
</tbody>
</table>

#### Chemical composition of alloys used to obtain thermophysical properties

The chemical composition used for computing thermophysical properties of Invar 36 alloy with CompuTherm [165] can be inferred from Table A1.2. The data reported in this Table come from the Alloy 36 data sheet provided by META-COR, 2018. When computing the thermophysical properties, Ni was set to 36%wt, and the minor elements were set to their maximum possible amount.

**Table A1.2: Chemical composition of Invar 36 alloy used with CompuTherm [165]**

<table>
<thead>
<tr>
<th>Ni</th>
<th>C</th>
<th>Si</th>
<th>Mn</th>
<th>P</th>
<th>S</th>
<th>Cr</th>
<th>Co</th>
<th>Nb</th>
<th>Mo</th>
<th>Fe</th>
</tr>
</thead>
<tbody>
<tr>
<td>35 - 38</td>
<td>≤ 0.1</td>
<td>≤ 0.35</td>
<td>≤ 0.6</td>
<td>≤ 0.025</td>
<td>≤ 0.025</td>
<td>≤ 0.5</td>
<td>≤ 1</td>
<td>-</td>
<td>≤ 0.5</td>
<td>balance</td>
</tr>
</tbody>
</table>

Zhan et al. [97, 151] have worked with experimental and numerical simulation of laser-MIG hybrid welding of Invar 36 alloy with slightly different material composition. The temperature dependent thermo-physical properties used in [97, 151] were derived from [152] and further interpolation. The chemical composition (wt%) of the Invar 36 alloy used in these studies is given in Table A1.3.

**Table A1.3: Chemical composition of Invar 36 alloy used by Zhan et al. [97, 151] and Jiaming [152]**

<table>
<thead>
<tr>
<th>Ni</th>
<th>C</th>
<th>Si</th>
<th>Mn</th>
<th>P</th>
<th>S</th>
<th>Cr</th>
<th>Co</th>
<th>Nb</th>
<th>Mo</th>
<th>Fe</th>
</tr>
</thead>
<tbody>
<tr>
<td>35.5 - 36.5</td>
<td>≤ 0.01</td>
<td>≤ 0.2</td>
<td>0.2-0.4</td>
<td>≤ 0.007</td>
<td>≤ 0.002</td>
<td>≤ 0.15</td>
<td>0.4</td>
<td>-</td>
<td>-</td>
<td>balance</td>
</tr>
</tbody>
</table>
Among commercial companies, Re-steel is a premium provider of nickel alloy plate. They produce Invar 36 alloy in accordance to the Boeing D33028-2 and ASTM-F-1684 specifications. The typical chemical composition (wt%) of Invar 36 produced by Re-steel is given in Table A1.4 [161].

Table A1.4: Chemical composition of Invar 36 alloy produced by Re-Steel

<table>
<thead>
<tr>
<th>Ni</th>
<th>C</th>
<th>Si</th>
<th>Mn</th>
<th>P</th>
<th>S</th>
<th>Cr</th>
<th>Co</th>
<th>Nb</th>
<th>Mo</th>
<th>Fe</th>
</tr>
</thead>
<tbody>
<tr>
<td>36</td>
<td>≤ 0.02</td>
<td>0.2</td>
<td>0.35</td>
<td>0.002</td>
<td>≤ 0.002</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>balance</td>
</tr>
</tbody>
</table>
Similarly, VDM metals is a company producing high-temperature resistance nickel materials and their alloys. Invar 36 alloy is one of their pioneer products which is used by many of today’s key technological companies in aerospace, automotive, oil & gas etc. The chemical composition of Invar 36 alloy obtained from the datasheet of VDM metals is given in Table A1.5 [160].

<table>
<thead>
<tr>
<th>Ni</th>
<th>C</th>
<th>Si</th>
<th>Mn</th>
<th>P</th>
<th>S</th>
<th>Cr</th>
<th>Co</th>
<th>Nb</th>
<th>Mo</th>
<th>Fe</th>
</tr>
</thead>
<tbody>
<tr>
<td>35 - 37</td>
<td>≤ 0.05</td>
<td>≤ 0.4</td>
<td>≤ 0.6</td>
<td>≤ 0.015</td>
<td>≤ 0.015</td>
<td>≤ 0.25</td>
<td>≤ 0.5</td>
<td>-</td>
<td>-</td>
<td>balance</td>
</tr>
</tbody>
</table>

### A1.2 Constant properties

#### Solidus and liquidus temperature

The solidus temperature ($T_{sol}$) and the liquidus temperature ($T_{liq}$) collected from various sources are reported in Table A1.6. The average melting temperature <$T$>and the extend δ$T$ of the melting temperature interval are simply derived from these data according to <$T$>=$0.5(T_{sol}+T_{liq})$ and δ$T$ $= T_{liq} - T_{sol}$

<table>
<thead>
<tr>
<th>$T_{sol}$ [°C]</th>
<th>$T_{liq}$ [°C]</th>
<th>&lt;$T$&gt; [°C]</th>
<th>δ$T$ [°C]</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>1397.8</td>
<td>1436.17</td>
<td>1417</td>
<td>38</td>
<td>Thermo-Calc [166]</td>
</tr>
<tr>
<td>1451.85</td>
<td>1458.85</td>
<td>1455</td>
<td>7</td>
<td>CompuTherm [165]</td>
</tr>
<tr>
<td>1428.96</td>
<td>1449.73</td>
<td>1439</td>
<td>21</td>
<td>Cassel et al. [159]</td>
</tr>
<tr>
<td>1443.85</td>
<td>1453.85</td>
<td>1449</td>
<td>10</td>
<td>Hansen et al. [167]</td>
</tr>
</tbody>
</table>

The solidus and liquidus temperature $T_{sol}$= 1443.85 °C and $T_{liq}$=1453.85 °C reported by Hansen et al. in [167] were obtained from the Fe-Ni equilibrium diagram. These values are used in the literature for modeling of Invar alloy and Fe-Ni alloys [168], and for experimental measurement of the thermophysical properties of liquid Invar made by Seifter et al [158].

The solidus and liquidus temperature $T_{sol}$= 1428.96 °C and $T_{liq}$ =1449.73 °C reported by Cassel et al. in [159] were obtained from experimental measurements with an apparatus designed to give accurate melting characteristics (with an accuracy of 5% or better) over a temperature range from ambient to 1600 °C. The measurements were conducted in controlled argon atmosphere (to avoid oxidation) using sample of Invar 36 (36% nickel) obtained from the PerkinElmer manufacturing group (the composition in minor elements is not provided in [159]).
Similarly, VDM Metals is a company producing high-temperature resistant nickel materials and their alloys. Invar 36 alloy is one of their pioneer products which is used by many of today’s key technological companies in aerospace, automotive, oil & gas etc. The chemical composition of Invar 36 alloy obtained from the datasheet of VDM Metals is given in Table A1.5.

### Table A1.5: Chemical composition of Invar 36 alloy produced by VDM Metals

<table>
<thead>
<tr>
<th>Element</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ni</td>
<td>35 - 37 %</td>
</tr>
<tr>
<td>C</td>
<td>≤ 0.05 %</td>
</tr>
<tr>
<td>Si</td>
<td>≤ 0.4 %</td>
</tr>
<tr>
<td>Mn</td>
<td>≤ 0.6 %</td>
</tr>
<tr>
<td>P</td>
<td>≤ 0.015 %</td>
</tr>
<tr>
<td>S</td>
<td>≤ 0.015 %</td>
</tr>
<tr>
<td>Cr</td>
<td>≤ 0.25 %</td>
</tr>
<tr>
<td>Co</td>
<td>≤ 0.5 %</td>
</tr>
<tr>
<td>Nb</td>
<td>- balance</td>
</tr>
<tr>
<td>Mo</td>
<td>- balance</td>
</tr>
<tr>
<td>Fe</td>
<td>balance</td>
</tr>
</tbody>
</table>

A1.2 Constant properties

Solidus and liquidus temperature

The solidus temperature ($T_{sol}$) and the liquidus temperature ($T_{liq}$) collected from various sources are reported in Table A1.6. The average melting temperature ($T_m$) and the extend $\delta T$ of the melting temperature interval are simply derived from these data according to $T_m = 0.5(T_{sol} + T_{liq})$ and $\delta T = T_{liq} - T_{sol}$.

### Table A1.6: Solidus and liquidus temperature of Invar 36 alloy

<table>
<thead>
<tr>
<th>Source</th>
<th>$T_{sol}$ [°C]</th>
<th>$T_{liq}$ [°C]</th>
<th>$T_m$ [°C]</th>
<th>$\delta T$ [°C]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermo-Calc [166]</td>
<td>1397.8</td>
<td>1436.17</td>
<td>1417</td>
<td>38</td>
</tr>
<tr>
<td>CompuTherm [165]</td>
<td>1451.85</td>
<td>1458.85</td>
<td>1455</td>
<td>7</td>
</tr>
<tr>
<td>Cassel et al. [159]</td>
<td>1428.96</td>
<td>1449.73</td>
<td>1439</td>
<td>21</td>
</tr>
<tr>
<td>Hansen et al. [167]</td>
<td>1443.85</td>
<td>1453.85</td>
<td>1449</td>
<td>10</td>
</tr>
</tbody>
</table>

The solidus and liquidus temperature $T_{sol} = 1443.85$ °C and $T_{liq} = 1453.85$ °C reported by Hansen et al. in [167] were obtained from the Fe-Ni equilibrium diagram. These values are used in the literature for modeling of Invar alloy and Fe-Ni alloys [168], and for experimental measurement of the thermophysical properties of liquid Invar made by Seifter et al. [158].

The solidus and liquidus temperature $T_{sol} = 1428.96$ °C and $T_{liq} = 1449.73$ °C reported by Cassel et al. in [159] were obtained from experimental measurements with an apparatus designed to give accurate melting characteristics (with an accuracy of ±5% or better) over a temperature range from ambient to 1600 °C. The measurements were conducted in controlled argon atmosphere (to avoid oxidation) using sample of Invar 36 (36% nickel) obtained from the PerkinElmer manufacturing group (the composition in minor elements is not provided in [159]).

It can be seen in Table A1.6 that the melting range $[T_{sol}, T_{liq}]$ of reference [159] and [167] do overlap significantly. The melting range computed in [166] shows some overlap with the lower part of the measured melting range obtained in [159]. The melting range computed in [166] and [165] do not overlap. Finally, the melting range computed in [165] shows some overlap with the higher part of the melting range obtained in [167]. Additionally, the melting temperatures $T_{melt}$ collected from various sources are reported in Table A1.7.

### Table A1.7: Melting temperature of Invar 36

<table>
<thead>
<tr>
<th>$T_{melt}$ [°C]</th>
<th>source</th>
</tr>
</thead>
<tbody>
<tr>
<td>1430</td>
<td>[160]</td>
</tr>
<tr>
<td>1427</td>
<td>[161–163, 169]</td>
</tr>
<tr>
<td>1450</td>
<td>[96]*</td>
</tr>
</tbody>
</table>

* $T_{melt}$ = 1450 °C is used in [96] setting the same melting temperature for both INVVAR (36Ni/64Fe), and INVVAR(42Ni/58Fe). In fact, these data were taken from another source (that we do not have). The melting temperature is expected to lie within the melting range so that

$$T_{sol} \leq T_{melt} \geq T_{liq} \text{ or } T_{melt} = <T> \pm 0.5 \delta T.$$

Therefore, the solidus and liquidus temperature $T_{sol} = 1428.96$ °C ≈ 1429 °C (1702 K) and $T_{liq} = 1449.73$ °C ≈ 1450 °C (1723 K) reported by Cassel et al. in [159] are selected for implementation in the thermo fluid simulation model for melt pool.

Latent heat of fusion

The latent heat of fusion per unit mass ($\Delta h_f$) collected from various sources are reported in Table A1.8.

### Table A1.8: Latent heat of fusion of Invar 36

<table>
<thead>
<tr>
<th>$\Delta h_f$ [kJ/(kg·K)]</th>
<th>source</th>
</tr>
</thead>
<tbody>
<tr>
<td>270 - 290</td>
<td>Nickel Iron Alloy [170]</td>
</tr>
<tr>
<td>226</td>
<td>CompuTherm [165]</td>
</tr>
<tr>
<td>267.95</td>
<td>Eagle Alloy [169]</td>
</tr>
<tr>
<td>276</td>
<td>Seifter et al. [158]</td>
</tr>
</tbody>
</table>

The latent heat of fusion $\Delta h_f = 276$ kJ/(kg·K) from the experiments performed by Seifter et al. [158] was measured with an estimated error of ±5%. Taking into account this uncertainty, it implies a range of 262 to 290 kJ/(kg·K). This range

67
shows a good overlap with the range provided in [170]. The latent heat of fusion from the technical datasheet of Invar available in [167] lie within the range estimated from [158]. On the other hand, the latent heat of fusion computed in [165] is significantly lower. The latent heat of fusion $\Delta h_f = 276$ kJ/(kg·K) determined by Seifter et al. [158] is thus selected for implementation in the thermo-fluid simulation model for melt pool in this thesis.

### A1.3 Temperature dependent properties

#### Density

Seifter et al. [158] have presented density data measured for Invar 36 alloy as a function of temperature within the range of 1400K to 2200K with an estimated error of ±4%. Least-squares fit of the measured data give the following linear piecewise functions of temperature:

$$\rho(T) = 8065 - 0.44 T \; \text{for} \; T < T_{sol}$$

$$\rho(T) = 8289 - 0.7083 T \; \text{for} \; T > T_{sol}$$

where $T$ is expressed in Kelvin and $\rho$ in kg/m$^3$.

Zhan et al. [97] have also presented density data measured for Invar 36 alloy as a function of temperature. It should be noticed that these data were taken from another source that is, according to [97] a study by Xu et al. [96]. However, when reading the publication by Xu et al. [96] it turns out that the density is assumed constant (8130 kg/m3). It was not possible to find where the data used in [97] come from and how they were obtained.

Nonetheless, the collected data are compared against the computed data from CompuTherm [165] and Thermo-Calc [166] in Figure 1. The steep decrease in the density value around 1700 K is characteristic of the phase change from solid to liquid. As can be seen, the data computed with CompuTherm [165], Thermo-Calc [166] and by Zhan et al. [97] show very good agreement. The experimental data from Seifter et al. [158] are slightly lower.

Datasheet from commercial companies provide density data at room temperature that are in close proximity such as 8055 kg/m$^3$ [161], 8050 kg/m$^3$ [162], 8130 kg/m$^3$ [164]. The density at 20 °C computed with CompuTherm is about 8350 kg/m$^3$ [165], 8100 kg/m$^3$ with Thermo-Calc [166] and 8200 kg/m$^3$ according to the data reported by Zhan et al. [97], 8000 kg/m$^3$ according to the data reported by Seifter et al. [158]. These data at room temperature thus differ by less than 4.5%. The density data can also be compared against density measurements for
A1. MATERIAL PROPERTIES

pure iron [171] and pure nickel [171]. Since the major composition of Invar is Fe (64%) and Ni (36%), it can be seen in Figure A1.1 that the density data of Invar 36 are between the data for pure iron and pure nickel; as expected they are also closer to the density values of Fe than of Ni.

![Figure A1.1: Density of Invar 36 alloy (Zhan et al. [97], Seifter et al. [158], CompuTherm [165], Thermo-Calc [166]), Pure iron [171] and pure nickel [171] as a function of temperature.](image)

Most studies focusing on weldability of Invar 36 alloy with thermo-mechanical model have considered a constant value of the density (e.g., 8130 kg/m³) in [97, 151, 152]). Concerning thermo-fluid models for the hydrodynamics of the melt pool, the density is needed to determine the force balance in the molten metal. As the molten metal is mechanically incompressible during the process, the density is assumed constant except when modeling the buoyancy force (Boussinesq assumption). In this framework, it is a common practice to set the density at the solidus temperature (from which the melt can begin to flow) as the reference density. The available densities at the solidus temperature are reported in Table A1.9. The density from the measurements performed by Seifter et al. [158] was made with an estimated error of ±4%. Taking into account this uncertainty it implies a range of 6790 to 7355 kg/m³ at the solidus temperature. The discrepancy between the data reported in Table A1.9 is about 8% or less. For consistency, the constant density value of 7275 kg/m³ computed with
APPENDICES

Table A1.9: Density of Invar 36 alloy at solidus temperature

<table>
<thead>
<tr>
<th>$\rho$ [kg/(m$^3$)]</th>
<th>source</th>
</tr>
</thead>
<tbody>
<tr>
<td>7647</td>
<td>Nickel Iron Alloy [170]</td>
</tr>
<tr>
<td>7275</td>
<td>Thermo-Calc [166]</td>
</tr>
<tr>
<td>7600</td>
<td>Eagle Alloy [169]</td>
</tr>
</tbody>
</table>

Thermo-Calc (at 1442 °C) is selected for implementation in the thermo fluid simulation model for melt pool. The temperature 1442 °C is indeed in close proximity to the solidus temperature (1429 °C) selected in Section A1.2.
**Thermal conductivity**

Figure A1.2 shows the thermal conductivity of Invar 36 as a function of temperature from various sources. It can be seen that the thermal conductivity computed using CompuTherm [165] is in good agreement with the experimental data from Seifert et al. [158]. To the best of the author’s knowledge, the thermal conductivity from Seifert et al. [158] is the only available experimental data for Invar 36 in the vicinity of its melting region. It was measured within the range of 1400K to 2200K with an estimated error of ±15%. Least-square fit of the measured data give the following linear piecewise functions of temperature [158]:

\[
\kappa(T) = 4.527 + 1.480 \times 10^{-2} T \text{ for } T < T_{sol}
\]

\[
\kappa(T) = 6.206 + 1.264 \times 10^{-2} T \text{ for } T > T_{sol}
\]

where \( T \) is expressed in Kelvin and \( \kappa \) in \( W/(m \cdot K) \).

At low temperature in the solid state, the thermal conductivity used in [97, 151] and [154] is obtained from experimental measurements reported in [152]. The way the thermal conductivity data used in [97, 151] and [154] were obtained in the liquid range is not specified. Figure A1.2 shows that the thermal conductivity of [158] and [165] are significantly different from the data extracted from Zhan et al. [97, 151] and [154] in the liquid range. At low temperature range up to 600 °C, the thermal conductivity data obtained from the datasheet of VDM metals [160] (see Table A1.10) are slightly higher than the experimental data obtained by Zhang [152]. It is not specified in this datasheet whether the available data are experimental measurements or obtained with different methods. When the thermal conductivity data from VDM metals are linearly extrapolated beyond 600 °C, they are found to agree very well with the data from Seifter et al. [158] at high temperature and with the computed data using CompuTherm [165].

Table A1.10: Thermal conductivity as function of temperature from VDM metals [160]

<table>
<thead>
<tr>
<th>( T[^{\circ}C] )</th>
<th>( \kappa[W/(m \cdot K)] )</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>12.8</td>
</tr>
<tr>
<td>100</td>
<td>14.0</td>
</tr>
<tr>
<td>200</td>
<td>15.1</td>
</tr>
<tr>
<td>300</td>
<td>16.1</td>
</tr>
<tr>
<td>400</td>
<td>17.0</td>
</tr>
<tr>
<td>500</td>
<td>18.1</td>
</tr>
<tr>
<td>600</td>
<td>19.5</td>
</tr>
</tbody>
</table>
Figure A1.2: Thermal conductivity of Invar 36 (Zhan et al. [97, 151], Seifter et al. [158], CompuTherm [165], VDM metals [160]) as a function of temperature.

Handbooks and datasheet from commercial companies provide the thermal conductivity at room temperature. They give similar values such as 10.15 W/(m·K) [162], 10.5 W/(m·K) [161, 163, 164]. The thermal conductivity computed in [165] at room temperature is almost twice large. The thermal conductivity data from VDM metals agree reasonably well with the data in [161–164]. When the thermal conductivity data from Seifter et al. [158] is extrapolated to room temperature it leads to a thermal conductivity of 8.9 W/(m·K), which is within the evaluated error range of ±15% compared to the data provided in [161–164]. Therefore, the thermal conductivity data selected for implementation in the thermo fluid simulation model for melt pool combine:

- the data from VDM metals [160] in the solid state and low temperature range, with

- the data from Seifter et al. [158] in the high temperature range of the solid state and

- the data from Seifter et al. [158] in the liquid state.

The thermal conductivity expressed as linear piecewise functions of temperature is then

\[
\kappa(T) = \begin{cases} 
6.293 + 1.185 \times 10^{-2} T & \text{for } T < T_{\text{sol}} \\
2.755 + 1.264 \times 10^{-2} T & \text{for } T > T_{\text{sol}} 
\end{cases}
\]

where \( T \) is expressed in Kelvin and \( \kappa \) in W/(m·K).

Specific heat capacity

Figure A1.3 shows the specific heat capacity of Invar 36 as a function of temperature obtained from various sources. Zhan et al. did not explain how specific heat capacity data reported in [94, 97, 151, 153] were obtained. The specific heat capacity data from Seifter et al. in [158] is based on enthalpy measurements made in the temperature range of 1400 K to 2200 K with an estimated error of ±4%. The least-square fit of these data in the sub-range \( T_{\text{liq}} < T < 2200 \) K leads to

\[
h(T) = -3.271 \times 10^{-1} + 8.012 \times 10^{-4} T,
\]

with \( T \) expressed in Kelvin and \( h(T) \) in MJ/kg. The inferred specific heat capacity at constant pressure has thus a value of 801 J/(kg·K) in the liquid state [158].

The specific heat capacity at constant pressure derived from the enthalpy measurements in the high temperature range of the solid state are reported in Table A1.11. They are of same order as the data provided by VDM metals [160] at lower temperature and reported in Table A1.12. Datasheet from commercial companies at room temperature give also specific heat capacity value in close proximity such as 515 J/(kg·K) [162–164]. The specific heat capacity of pure iron [171] and pure nickel [171] are also reported in Figure A1.3.
\kappa(T) = 6.293 + 1.185 \times 10^{-2} T \text{ for } T < T_{sol}

\kappa(T) = 2.755 + 1.264 \times 10^{-2} T \text{ for } T > T_{sol}

where \( T \) is expressed in Kelvin and \( \kappa \) in \( W/(m \cdot K) \).

### Specific heat capacity

Figure A1.3 shows the specific heat capacity of Invar 36 as a function of temperature obtained from various sources. Zhan et al. did not explain how specific heat capacity data reported in [94, 97, 151, 153] were obtained. The specific heat capacity data from Seifter et al. in [158] is based on enthalpy measurements made in the temperature range of 1400 K to 2200 K with an estimated error of ±4%. The least-square fit of these data in the sub-range \( T_{liq} < T < 2200K \) leads to

\[ h(T) = -3.271 \times 10^{-1} + 8.012 \times 10^{-4}T, \]

with \( T \) expressed in Kelvin and \( h(T) \) in MJ/kg. The inferred specific heat capacity at constant pressure has thus a value of 801 J/(kg·K) in the liquid state [158]. The specific heat capacity at constant pressure derived from the enthalpy measurements in the high temperature range of the solid state are reported in Table A1.11. They are of same order as the data provided by VDM metals [160] at lower temperature and reported in Table A1.12. Datasheet from commercial companies at room temperature give also specific heat capacity value in close proximity such as 515 J/(kg·K) [162–164]. The specific heat capacity of pure iron [171] and pure nickel [171] are also reported in Figure A1.3.

Table A1.11: Specific heat capacity at constant pressure in the solid state derived from the enthalpy; Seifter et al. [158]

<table>
<thead>
<tr>
<th>( T[\degree C] )</th>
<th>( C_p[J/(kg \cdot K)] )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1177</td>
<td>480</td>
</tr>
<tr>
<td>1277</td>
<td>490</td>
</tr>
<tr>
<td>1377</td>
<td>500</td>
</tr>
</tbody>
</table>

In Figure A1.3, the specific heat capacity data from Zhan et al. [151] are significantly different from the other data throughout the plotted temperature range. In the solid state, the data calculated with CompuTherm [165] and ThermoCalc [166] show strong agreement above 600 °C. Below 600 °C, fair differences can be observed in the plot. The steep rise in specific heat capacity value between 200 and 400 °C is due to magnetic heat of transformation at
Figure A1.3: Specific heat capacity of Invar36 alloy (Zhan et al. [97], Seifter et al. [158], CompuTherm [165], Thermo-Calc [166], VDM metals [160]), pure iron [171], and pure nickel [171] as a function of temperature.

curie temperature [155]. The anomalous maxima at curie temperature is observed to be significantly overestimated by Thermo-Calc [166] in comparison to CompuTherm [165]. Besides, large differences can be observed between the data from Seifter et al. [158] and VDM Metals [160] compared to CompuTherm [165] and Thermo-Calc [166]. In the liquid state, the data obtained with CompuTherm [165] and Thermo-Calc [166] are in good agreement with the specific heat capacity at constant pressure derived from the enthalpy measurements by Seifter et al. [158]. Furthermore, the specific heat in the liquid phase is between the values for pure iron [158] and pure nickel [158] but here closer to the values of iron. For temperature below the solidus temperature the data of VDM metals [160], CompuTherm [165] and Thermo-Calc [166] are thus retained from 600 °C and above and the specific heat capacity is assumed to be a linear function of temperature. Although this assumption is probably questionable for T less than about 400 °C, \( C_p \) is assumed to be a linear function of temperature all over the solid-state temperature range. An analytic expression is indeed more convenient for implementation in the thermo fluid simulation model for melt pool, and the error made is relatively small compared to the data of VDM metals [160] (less than 10%). The resultant expression is set to
Table A1.12: Specific heat capacity at constant pressure as function of temperature; VDM metals [160]

<table>
<thead>
<tr>
<th>$T$ [$^\circ$C]</th>
<th>$C_p$ [J/(kg·K)]</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>486</td>
</tr>
<tr>
<td>100</td>
<td>518</td>
</tr>
<tr>
<td>200</td>
<td>545</td>
</tr>
<tr>
<td>300</td>
<td>523</td>
</tr>
<tr>
<td>400</td>
<td>524</td>
</tr>
<tr>
<td>500</td>
<td>529</td>
</tr>
<tr>
<td>600</td>
<td>545</td>
</tr>
</tbody>
</table>

$C_p(T) = 0.19 \times T + 398$ for $T < T_{liq}$

where $T$ is in Kelvin and $C_p$ in J/(kg·K). Above the liquidus temperature the specific heat capacity value 801 J/(kg·K) obtained by Seifter et al. [158] is selected for implementation.

**Coefficient of thermal expansion**

The coefficient of thermal expansion ($\beta$) as a function of temperature obtained from various sources is shown in Figure A1.4. It is observed that the data provided by Zhan et al. [94] agree fairly well with the data from Re-Steel [161], VDM Metals [160] (reported in Table A1.13), High Temp Metals [163] and experimental measurements. Although, small offset between datapoints is observed below 200 $^\circ$C, strong agreement can be seen above 200 $^\circ$C. On the other hand, the data computed using Thermo-calc [166] is higher than the data provided by Zhan et al. [94] and other sources almost by an order of magnitude up to 200 $^\circ$C. Similarly, significant differences are observed in the temperature range between 200 and 800 $^\circ$C. The CTE data computed using CompuTherm [165] are uniformly low (mostly between $0.1 \times 10^{-6}$ and $0.2 \times 10^{-6}$ C$^{-1}$). Above 100 $^\circ$C they show poor agreement with the other sources. In the temperature range of 20-100 $^\circ$C the coefficient of thermal expansion recorded from the datasheet of commercial companies show closely related values such as $1.2 \times 10^{-6}$ K$^{-1}$ in [162] and [172], $1.4 \times 10^{-6}$ K$^{-1}$ [161], $0.6 - 2.1 \times 10^{-6}$ K$^{-1}$ [160]. Similar values at room temperature are also recorded in literatures.

For implementation in the thermo fluid simulation model for melt pool, the coefficient of thermal expansion is only needed in the liquid state to determine the force balance in the melt, and the resultant flow acceleration. The data of Invar 36 provided by Zhan et al. [94] is selected since it has good agreement with the other sources e.g. VDM Metals [160], Re-Steel [161], High Temp Metals [163].
up to 600°C and also agrees reasonably well with the Thermo-Calc [166] data from 800°C to 2000°C. The coefficient of thermal expansion in the liquid state is then given by the following linear function of temperature:

$$\beta(T) = 12.357 + 1.536 \times 10^{-3} T \text{ if } T > T_{sol},$$

where the temperature $T$ is in K and $\beta \times 10^{-6}$ in °C$^{-1}$.

**Viscosity**

The viscosity of liquid Invar 36 as a function of temperature computed using CompuTherm was provided in [165]. This is the only information we could find for the viscosity of this alloy. These data are also compared with the viscosity for pure iron [171] and pure nickel [171] as shown in Figure A1.5.

From Figure A1.5, it is observed that the viscosity data for Invar 36 is in good range between the data pure iron [171] and for pure nickel [171]. The viscosity data to implement in the thermo fluid simulation model for melt pool is thus the
A1. Material properties

Table A1.13: Coefficient of thermal expansion as function of temperature; VDM metals [160]

<table>
<thead>
<tr>
<th>$T$ [°C]</th>
<th>$\beta$ [$10^{-6}K^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>0.6-2.1</td>
</tr>
<tr>
<td>200</td>
<td>1.6-3.6</td>
</tr>
<tr>
<td>300</td>
<td>4.4-5.5</td>
</tr>
<tr>
<td>400</td>
<td>7.4-8.4</td>
</tr>
<tr>
<td>500</td>
<td>8.9-9.7</td>
</tr>
<tr>
<td>600</td>
<td>10-10.7</td>
</tr>
</tbody>
</table>

Figure A1.5: Viscosity of Invar 36 (CompuTherm [165]), pure iron [171] and pure nickel [171] as a function of temperature

data computed using CompuTherm [165]. It is expressed as an analytic function of temperature similar to [173], leading to

$$\mu(T) = 10^{-0.619+2334T^{-1}} \text{ for } T > T_{sol},$$

where, the temperature $T$ is expressed in K and the dynamic viscosity in mPa.s (i.e. $10^{-3}$ kg/(m.s)).
Surface tension

We have no knowledge of surface tension measurements for Invar 36. Brillo and Egry [157] performed the experimental study of the surface tension of nickel, copper, iron and their binary alloys. Figure A1.6 shows the surface tension measurement data of Brillo and Egry [157] at temperature ranging from about 1100 to 1800 °C for nickel-iron binary alloys in various proportions. For pure iron and pure nickel the data of Figure A1.6 are in good agreement with the measurements reported in [173]. The discrepancy between the data of [157] and the data reported in [173] is indeed 3% or less.

![Figure A1.6: Surface tension data for levitated Fe-Ni alloys as a function of temperature. Adapted from [157]](image)

Interpolating the measurement results (see solid lines in Figure A1.6), Brillo and Egry [157] expressed the surface tension as a linear function of temperature according to

\[
\sigma(T) = \sigma_0 + \left( \frac{\partial \sigma}{\partial T} \right)_0 (T - T_0)
\]

where \(\sigma_0\) is the surface tension at a reference temperature \(T_0\) set to the liquidus temperature. The gradient of surface tension with respect to temperature \(\left( \frac{\partial \sigma}{\partial T} \right)_0\) is also determined at \(T_0\). The coefficients proposed by Brillo and Egry are reported in Table A1.14 and the corresponding plots are the solid black lines in Figure A1.6.
The surface tension of the Invar 36s used in this study is derived from [157].

Table A1.14: Surface tension and surface tension temperature gradient of iron, nickel and their binary alloy [157]

<table>
<thead>
<tr>
<th>% wt Fe</th>
<th>% wt Ni</th>
<th>$T_o$ [°C]</th>
<th>$\sigma_o$ [N/m]</th>
<th>$\left(\frac{\partial \sigma}{\partial T}\right)_0$ [N/(m·K)] × 10^-4</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>0</td>
<td>1538</td>
<td>1.92</td>
<td>-3.97</td>
</tr>
<tr>
<td>75</td>
<td>25</td>
<td>1473</td>
<td>1.93</td>
<td>-1.73</td>
</tr>
<tr>
<td>50</td>
<td>50</td>
<td>1440</td>
<td>1.91</td>
<td>-3.27</td>
</tr>
<tr>
<td>25</td>
<td>75</td>
<td>1440</td>
<td>1.73</td>
<td>-2.76</td>
</tr>
<tr>
<td>0</td>
<td>100</td>
<td>1454</td>
<td>1.77</td>
<td>-3.3</td>
</tr>
</tbody>
</table>

Two assumptions are thus made. It is first assumed that the surface tension of Invar 36 can be simplified to the surface tension of a binary alloy with Nickel and 63.751%wt-Fe (filler metal; see Table A1.1) or 63.536%wt-Fe (workpiece; see Table A1.1). It is also assumed that we can proceed by linear interpolation of the data provided in [157] for 50%wt-Fe and 75%wt-Fe. To proceed, two reference points are set. The first point is defined as the intersection of the lines corresponding to surface tension data at 50%wt-Fe and 75%wt-Fe [157]. These lines are underlined in blue in Figure A1.6. Their intersection is computed to be at $T=1273$ °C and $\sigma = 1.96 \text{ N}\cdot \text{m}^{-1}$. The second reference is determined by linear interpolation at $T=1600$ °C, leading to $\sigma_{\text{Invar36}} = 1.8835 \text{ N}\cdot \text{m}^{-1}$. The surface tension of Invar 36 as function of temperature is then represented by the line passing through these two reference points; its plot corresponds to the dotted red line in Figure A1.6. For Invar 36 the reference temperature $T_o$ is set to 1450 °C according to the liquidus temperature selected in Section A1.2. As a result, the surface tension at the reference temperature $T_o$ is equal to $\sigma_o = 1.92 \text{ N}\cdot \text{m}^{-1}$ and its gradient with respect to temperature is $\left(\frac{\partial \sigma}{\partial T}\right)_0 = -2.48 \times 10^{-4} \text{ N}/(\text{m} \cdot \text{K})$, thus

$$\sigma_{\text{Invar36}}(T) = 1.92 - 2.48 \times 10^{-4}(T - 1450),$$

where T is expressed in °C and $\sigma_{\text{Invar36}}$ in N·m^{-1}.

This expression neglects the presence of surfactant. However, the Invar 36 reported in Table A1.1 contains 40 ppm sulfur. The study of Sahoo et al. [49] shows that in the presence of surfactant the surface tension presents an inflection point and it changes sign depending on the temperature.
**Electrical conductivity**

Seifter et al. [158] have presented electrical resistivity data measured for Invar 36 as a function of temperature within the range of 1400K to 2200K. The estimated error of electrical resistivity with and without the correction of thermal expansion is ± 4% and ± 7% respectively. The electrical resistivity data with correction of thermal expansion is shown in Figure A1.7. Least-squares fit of the measured data give the following linear piecewise functions of temperature [158]:

\[ k_{electrical}(T) = 1.1529 + 0.0001T \text{ for } 1400 < T < 1717 \]

\[ k_{electrical}(T) = 1.2311 + 0.0002T \text{ for } 1727 < T < 2200 \]

where \( T \) is expressed in Kelvin and \( k_{electrical} \) in \( \mu \Omega \cdot m \).

![Figure A1.7: Electrical resistivity of Invar 36 as a function of temperature](image)

At low temperature range up to 600 °C the electrical resistivity data obtained from the datasheet of VDM metals [160] is also shown in Figure A1.7. It is not specified in the datasheet whether the available data are experimental measurements or obtained with different methods. When the electrical resistivity data from VDM metals are extrapolated with logarithmic growth beyond 600 °C, they are found to agree very well with the data from Seifter et al. [158] at high temperature.
Datasheet from commercial companies provide electrical resistivity data for Invar 36 at room temperature that are in close proximity such as 0.75 $\mu\Omega\cdot m$ [164], 0.82 $\mu\Omega\cdot m$ [162,163], 0.84 $\mu\Omega\cdot m$ [174] and agree very well with the data from VDM metals [160].

The constant value of electrical conductivity data to implement in the thermo fluid simulation model for melt pool is thus obtained from the reciprocal of electrical resistivity data from Seifter et al. [158] at solidus temperature.
A2 Preliminary test cases

The multi-physics thermo-fluid model of the melt pool for GMAW application needed to be developed and validated in several stages. Therefore, simulation of standard test cases is performed in the early stage of the project to familiarize with the OpenFOAM library, programming syntax, and to validate the essential aspect of the model before validating the melt pool model at a multi-scale. Two standard test cases are well-documented in literature which are simulated and reported in this chapter. The first test case (Case 1) consists of thermocapillary driven flow with phase change. The thermocapillary force is often a leading order force in welding, therefore it is a relevant test case to simulate and validate an aspect of the physical phenomenon in welding. The second test case (Case 2) is a standard welding test case with a stationary laser beam heat source which has been used for model validation by several authors in the literature. Lastly, the derived polynomial expressions for the thermophysical properties of the studied metal alloy are presented.

Case 1: Thermocapillary driven free surface flow with phase change

The first test case is a 2D free surface flow and phase change problem of pure Bismuth containing argon gas in its atmosphere. The aim of this test case is to ensure that the initial developments atop interfoam solver specifically the integration of energy equation, implementation of thermocapillary force, and phase change are capable of simulating a system of free surface flow with phase change. The schematic of the test case is shown in Figure A2.8. It consists of a 15 mm × 5 mm rectangular cavity with pure Bismuth up to 4 mm height and argon gas in a 1 mm gap on the top. A pseudo-2D mesh (i.e only one cell along the z-axis) is used in OpenFOAM for the simulation of the 2D problem. Thus, a computational domain of size 15 mm × 5 mm × 1 mm with a mesh size of 140 × 60 mm × 1 is used for the simulation. The left wall is maintained at constant temperature $T_{\text{hot}} = 552.55$ K while the right wall is maintained at constant temperature $T_{\text{cold}} = 540.55$ K. A decreasing linear temperature variation between the left wall and right wall is imposed on the top and the bottom surfaces. The boundary conditions of this test case are presented in Table A2.15.

Table A2.15: Boundary condition for the test Case 1.

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Velocity [m/s]</th>
<th>Pressure [Pa]</th>
<th>Alloy volume fraction [-]</th>
<th>Temperature [K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Left</td>
<td>$u = 0$</td>
<td>$\partial p/\partial x = 0$</td>
<td>$\partial \alpha/\partial x = 0$</td>
<td>$T_{\text{hot}} = 552.55$</td>
</tr>
<tr>
<td>Right</td>
<td>$u = 0$</td>
<td>$\partial p/\partial x = 0$</td>
<td>$\partial \alpha/\partial x = 0$</td>
<td>$T_{\text{cold}} = 540.55$</td>
</tr>
<tr>
<td>Top and Bottom</td>
<td>$u = 0$</td>
<td>$\partial p/\partial y = 0$</td>
<td>$\partial \alpha/\partial y = 0$</td>
<td>$-800 \cdot x + 552.55$</td>
</tr>
</tbody>
</table>

In this test case the thermophysical properties of bismuth and argon are assumed
A2. Preliminary test cases

The multi-physics thermo-fluid model of the melt pool for GMAW application needed to be developed and validated in several stages. Therefore, simulation of standard test cases is performed in the early stage of the project to familiarize with the OpenFOAM library, programming syntax, and to validate the essential aspect of the model before validating the melt pool model at a multi-scale. Two standard test cases are well-documented in literature which are simulated and reported in this chapter. The first test case (Case 1) consists of thermocapillary driven flow with phase change. The thermocapillary force is often a leading order force in welding, therefore it is a relevant test case to simulate and validate an aspect of the physical phenomenon in welding. The second test case (Case 2) is a standard welding test case with a stationary laser beam heat source which has been used for model validation by several authors in the literature. Lastly, the derived polynomial expressions for the thermophysical properties of the studied metal alloy are presented.

Case 1: Thermocapillary driven free surface flow with phase change

The first test case is a 2D free surface flow and phase change problem of pure Bismuth containing argon gas in its atmosphere. The aim of this test case is to ensure that the initial developments atop the interfoam solver specifically the integration of energy equation, implementation of thermocapillary force, and phase change are capable of simulating a system of free surface flow with phase change. The schematic of the test case is shown in Figure A2.8. It consists of a 15 mm \( \times \) 5 mm rectangular cavity with pure Bismuth up to 4 mm height and argon gas in a 1 mm gap on the top. A pseudo-2D mesh (i.e only one cell along the z-axis) is used in OpenFOAM for the simulation of the 2D problem. Thus, a computational domain of size 15 mm \( \times \) 5 mm \( \times \) 1 mm with a mesh size of 140 \( \times \) 60 mm \( \times \) 1 is used for the simulation. The left wall is maintained at constant temperature \( T_{\text{hot}} = 552.55 \) K while the right wall is maintained at constant temperature \( T_{\text{cold}} = 540.55 \) K. A decreasing linear temperature variation between the left wall and right wall is imposed on the top and the bottom surfaces. The boundary conditions of this test case are presented in Table A2.15.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Marangoni, ( Ma )</td>
<td>244</td>
</tr>
<tr>
<td>Prandlt, ( Pr )</td>
<td>0.019</td>
</tr>
<tr>
<td>Capillary, ( Ca )</td>
<td>0.0022</td>
</tr>
<tr>
<td>Bond, ( Bo )</td>
<td>0.000188</td>
</tr>
<tr>
<td>Rayleigh, ( Ra )</td>
<td>0.031</td>
</tr>
<tr>
<td>Stefan, ( St )</td>
<td>0.033</td>
</tr>
</tbody>
</table>

Figure A2.8: Schematic for the test Case 1.

An adjustable time stepping with maximum CFL number of 0.02, and maximum time step of \( 10^{-5} \) s was applied. The pressure-velocity coupling was computed with a PISO algorithm. The convergence criteria imposed on the final residuals for each variable was \( 10^{-10} \).

Figure A2.9 shows the temperature distribution and velocity vector field at the steady-state condition. A clockwise recirculating flow can be seen in the region occupied with liquid bismuth whereas the counter-clockwise recirculating flow of the argon gas can be seen on the top of the domain. The linear temperature variation between the left and the right wall leads to the change in surface tension in the bismuth - argon interface. The variation in the surface tension leads to the thermocapillary force which causes the flow of the hot molten bismuth with lower surface tension from the left side towards the cold bismuth with the high constant. The melting temperature is set to \( T_m = 544.55 \) K which lies at \( x_m = 10 \) mm from the left wall as shown in Figure A2.8. The values of the dimensionless numbers associated with this test case are given in Table A2.16. They were defined in Section 2.3, apart from Stefan number that is the ratio of the sensible heat to the latent heat.

Table A2.16: Dimensionless Number for the test Case 1.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Marangoni, ( Ma )</td>
<td>244</td>
</tr>
<tr>
<td>Prandlt, ( Pr )</td>
<td>0.019</td>
</tr>
<tr>
<td>Capillary, ( Ca )</td>
<td>0.0022</td>
</tr>
<tr>
<td>Bond, ( Bo )</td>
<td>0.000188</td>
</tr>
<tr>
<td>Rayleigh, ( Ra )</td>
<td>0.031</td>
</tr>
<tr>
<td>Stefan, ( St )</td>
<td>0.033</td>
</tr>
</tbody>
</table>

Figure A2.9 shows the temperature distribution and velocity vector field at the steady-state condition. A clockwise recirculating flow can be seen in the region occupied with liquid bismuth whereas the counter-clockwise recirculating flow of the argon gas can be seen on the top of the domain. The linear temperature variation between the left and the right wall leads to the change in surface tension in the bismuth - argon interface. The variation in the surface tension leads to the thermocapillary force which causes the flow of the hot molten bismuth with lower surface tension from the left side towards the cold bismuth with the high constant.
surface tension on the right side. The molten bismuth strikes the melt front and creates a recirculating flow of the molten bismuth in the clockwise direction. As the recirculating flow progresses, the melt front starts to deform. The upper half of the melt front deviates more towards the colder side than the lower half.

Figure A2.9: Steady state temperature distribution and velocity field of free surface Marangoni-driven flows with phase change.
The melt front line obtained in the test Case 1 is compared with the reference case of Tan et al. [175]. It can be seen in Figure A2.10 that the melt front line shows good agreement between the test Case 1 and the reference case of Tan et al. [175].

![Melt front comparison](image)

Figure A2.10: Melt front comparison between present test case and the results from Tan et al. [175].

The study of the test Case 1 resulted in the following outcome

a. Familiarizing oneself with the *interfoam* solver source code, a further extension to include other relevant physical phenomena as well as setting up simulation case.

b. The developments made atop native *interfoam* solver worked expectedly and a good agreement was reached with the reference case. It also shows that the extended model is well capable of simulating physical phenomena relevant to welding application.

**Case 2: Simulation of melt pool thermohydrodynamics and free surface deformation with a stationary laser beam**

Additional implementations were made following the computations of test Case 1 which are reported through the simulation performed in the test Case 2. The major new implementations were the heat source term in the form of a laser beam and SSF method [176] for the estimation of the surface forces. The results obtained in the test Case 2 are also compared to the reference cases. This test case is derived from the experimental as well as the numerical study of the melt pool on S705 steel using laser beam heat source conducted by Pitschenede et al. [177]. However, the free surface deformation of the melt pool was not taken
Table A2.17: Material properties of the steel alloy used for the test case 2

<table>
<thead>
<tr>
<th>Parameter (unit)</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg m$^{-3}$)</td>
<td>8100</td>
</tr>
<tr>
<td>Melting temperature (K)</td>
<td>1620</td>
</tr>
<tr>
<td>Dynamic Viscosity (kg m$^{-1}$ s$^{-1}$)</td>
<td>0.006</td>
</tr>
<tr>
<td>Specific heat of solid phase (J kg$^{-1}$ K$^{-1}$)</td>
<td>627</td>
</tr>
<tr>
<td>Specific heat of liquid phase (J kg$^{-1}$ K$^{-1}$)</td>
<td>723</td>
</tr>
<tr>
<td>Thermal conductivity of solid phase (W m$^{-1}$ K$^{-1}$)</td>
<td>22.9</td>
</tr>
<tr>
<td>Thermal conductivity of liquid phase (W m$^{-1}$ K$^{-1}$)</td>
<td>22.9</td>
</tr>
<tr>
<td>Latent heat of fusion (J kg$^{-1}$)</td>
<td>$2.51 \times 10^5$</td>
</tr>
<tr>
<td>Coefficient of thermal expansion (K$^{-1}$)</td>
<td>$1.5 \times 10^{-6}$</td>
</tr>
</tbody>
</table>

into account by Pitschenede et al. [177]. Since then, a number of researchers have simulated this test case and compared it with the reference case of Pitschenede et al. [177], such as Saldi [51], Kidess [178] and Ha and Kim [179]. The underlying differences in the various test studies by different authors were in the selection of the process parameters. Ha and Kim [179] simulated for 20 ppm sulfur concentration and 5200 W laser power including free surface deformation. Kidess [178] simulated with 150 ppm sulfur concentration and 5200 W laser power. Saldi [51] simulated with and without the free surface deformation for 20 ppm and 150 ppm sulfur concentration and 3850 W laser power. Figure A2.11 shows the schematic of the computational domain for the test Case 2 which consists of steel alloy (workpiece sample) on the bottom and argon gas on the top. The steel alloy is also the primary phase in the multi-phase simulation model. The axisymmetric computational domain was chosen for the simulation of this test case since Saldi [51] has already shown significantly small variation in the results obtained between the three-dimensional case and axisymmetric case. The steel sub-domain is discretized with mesh resolution of $160 \times 110 \times 1$ in x, y, and z-direction respectively while the argon sub-domain is discretized with mesh resolution of $160 \times 70 \times 1$ in x, y, and z-direction respectively as shown in Figure A2.11. The grid resolution is uniform and fine in the steel-argon free surface interface. Furthermore, the grid cells within 4 mm radius along the x-axis and 4 mm from the center axis are of uniform. The thermophysical properties of the steel alloy and the argon gas are presented in Table A2.17 and Table A2.18 respectively.

In this test case, the steel alloy with both 20 ppm sulfur and 150 ppm sulfur concentration is simulated. It is well known that the surfactant can alter the surface tension and influence the convective flow in the melt pool. Therefore, the surface tension model for binary alloy proposed by Sahoo et al. [49], where the surface tension is a function of both temperature and surfactant content is
Table A2.17: Material properties of the steel alloy used for the test case 2

<table>
<thead>
<tr>
<th>Parameter (unit)</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg m(^{-3}))</td>
<td>8100</td>
</tr>
<tr>
<td>Melting temperature (K)</td>
<td>1620</td>
</tr>
<tr>
<td>Dynamic Viscosity (kg m(^{-1}) s(^{-1}))</td>
<td>0.006</td>
</tr>
<tr>
<td>Specific heat of solid phase (J kg(^{-1}) K(^{-1}))</td>
<td>627</td>
</tr>
<tr>
<td>Specific heat of liquid phase (J kg(^{-1}) K(^{-1}))</td>
<td>723</td>
</tr>
<tr>
<td>Thermal conductivity of solid phase (W m(^{-1}) K(^{-1}))</td>
<td>22.9</td>
</tr>
<tr>
<td>Thermal conductivity of liquid phase (W m(^{-1}) K(^{-1}))</td>
<td>22.9</td>
</tr>
<tr>
<td>Latent heat of fusion (J kg(^{-1})) (\times 10^5)</td>
<td>2.51</td>
</tr>
<tr>
<td>Coefficient of thermal expansion (K(^{-1})) (\times 10^{-6})</td>
<td>1.5</td>
</tr>
</tbody>
</table>

into account by Pitschenede et al. [177]. Since then, a number of researchers have simulated this test case and compared it with the reference case of Pitschenede et al. [177], such as Saldi [51], Kidess [178] and Ha and Kim [179]. The underlying differences in the various test studies by different authors were in the selection of the process parameters. Ha and Kim [179] simulated for 20 ppm sulfur concentration and 5200 W laser power including free surface deformation. Kidess [178] simulated with 150 ppm sulfur concentration and 5200 W laser power. Saldi [51] simulated with and without the free surface deformation for 20 ppm and 150 ppm sulfur concentration and 3850 W laser power. Figure A2.11 shows the schematic of the computational domain for the test Case 2 which consists of steel alloy (workpiece sample) on the bottom and argon gas on the top. The steel alloy is also the primary phase in the multi-phase simulation model. The axisymmetric computational domain was chosen for the simulation of this test case since Saldi [51] has already shown significantly small variation in the results obtained between the three-dimensional case and axisymmetric case.

The steel sub-domain is discretized with mesh resolution of 160 \(\times\) 110 \(\times\) 1 in x, y, and z-direction respectively while the argon sub-domain is discretized with mesh resolution of 160 \(\times\) 70 \(\times\) 1 in x, y, and z-direction respectively as shown in Figure A2.11. The grid resolution is uniform and fine in the steel-argon free surface interface. Furthermore, the grid cells within 4 mm radius along the x-axis and 4 mm from the center axis are of uniform. The thermophysical properties of the steel alloy and the argon gas are presented in Table A2.17 and Table A2.18 respectively.

In this test case, the steel alloy with both 20 ppm sulfur and 150 ppm sulfur concentration is simulated. It is well known that the surfactant can alter the surface tension and influence the convective flow in the melt pool. Therefore, the surface tension model for binary alloy proposed by Sahoo et al. [49], where the surface tension is a function of both temperature and surfactant content is applied. The resulting expression for the interfacial surface tension is given by:

\[
\sigma = \sigma_0 + \left( \frac{d\sigma}{dT} \right)_0 (T - T_m) - RT \Gamma_s \ln(1 + K_{ai}) \tag{1}
\]

with

\[
\frac{d\sigma}{dT} = \left( \frac{\partial\sigma}{\partial T} \right)_0 - RT \Gamma_s \ln(1 + K_{ai}) - \frac{K_{ai}}{1 + K_{ai}} \frac{\Gamma_s \Delta H^0}{T} \tag{2}
\]

\[
K = k_1 \exp \left[ -\frac{\Delta H^0}{RT} \right] \tag{3}
\]
where $\sigma_0$ and $\left(\frac{\partial \sigma}{\partial T}\right)_0$ are the surface tension and the coefficient of surface tension temperature gradient of pure metal at melting point. $T_m$ is the melting temperature. $R$ is the ideal gas constant, $\Gamma_s$ the surface excess at saturation, $K$ is the equilibrium constant, $k_1$ is the entropy factor, $a_i$ is the percentage weight of surfactant, and $\Delta H^0$ is the standard heat of adsorption. The values of these parameters for a system of Fe-S binary alloy are presented in Table A2.19.

Figure A2.12 shows the variation of surface tension ($\sigma$) and the coefficient of surface tension temperature gradient ($d\sigma/dT$) with respect to temperature. The critical temperature ($T_c$) at which ($d\sigma/dT$) changes from positive to negative is at 1700 K and 1979 K for 20 ppm and 150 ppm sulfur concentration, respectively. It should also be noted that the Marangoni flow which is traditionally outward reverses its direction with the presence of surfactant when the temperature is lower than the critical temperature.

Figure A2.13 shows the boundary condition applied for the test Case 2. The left side is the center axis of the axisymmetric computational domain. The workpiece bottom surface and workpiece right surface remain solid for the simulated duration. Hence the no-slip condition is applied for the velocity while an adiabatic condition is applied for the temperature. On the other hand, the boundary surfaces of the gas subdomain (top and top-right) are open to the atmosphere. The zero-gradient boundary condition is applied for all variables for outflow. For inflow, the flow of only argon gas is allowed at ambient temperature. The inflow velocity is calculated based on the flux in the patch-normal direction whereas the pressure is calculated as a difference of atmospheric pressure and dynamic pressure.

The laser beam heat input with top-hat distribution is imposed at the interface between the argon gas and steel solid/liquid surface as:

Table A2.19: Parameters for calculation of interfacial surface tension of Fe-S binary alloy [49]

<table>
<thead>
<tr>
<th>Parameter (unit)</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_0$ (N m$^{-1}$)</td>
<td>1.943</td>
</tr>
<tr>
<td>$\left(\frac{\partial \sigma}{\partial T}\right)_0$ (N m$^{-1}$ K$^{-1}$)</td>
<td>$-5 \times 10^{-4}$</td>
</tr>
<tr>
<td>$\Gamma_s$ (J/(kg mol m$^2$))</td>
<td>$1.3 \times 10^{-5}$</td>
</tr>
<tr>
<td>$k_1$ (J kg$^{-1}$ K$^{-1}$)</td>
<td>0.00318</td>
</tr>
<tr>
<td>$\Delta H^0$ (J kg$^{-1}$ mol$^{-1}$)</td>
<td>$-1.66 \times 10^5$</td>
</tr>
</tbody>
</table>
where $\sigma_0$ and $(\partial \sigma / \partial T)_0$ are the surface tension and the coefficient of surface tension temperature gradient of pure metal at melting point. $T_m$ is the melting temperature. $R$ is the ideal gas constant, $\Gamma_s$ the surface excess at saturation, $K$ is the equilibrium constant, $a_i$ is the percentage weight of surfactant, and $\Delta H_0$ is the standard heat of adsorption. The values of these parameters for a system of Fe-S binary alloy are presented in Table A2.19.

Figure A2.12 shows the variation of surface tension ($\sigma$) and the coefficient of surface tension temperature gradient ($d\sigma/dT$) with respect to temperature. The critical temperature ($T_c$) at which ($d\sigma/dT$) changes from positive to negative is at 1700 K and 1979 K for 20 ppm and 150 ppm sulfur concentration, respectively. It should also be noted that the Marangoni flow which is traditionally outward reverses its direction with the presence of surfactant when the temperature is lower than the critical temperature.

Figure A2.13 shows the boundary condition applied for the test Case 2. The left side is the center axis of the axisymmetric computational domain. The workpiece bottom surface and workpiece right surface remain solid for the simulated duration. Hence the no-slip condition is applied for the velocity while an adiabatic condition is applied for the temperature. On the other hand, the boundary surfaces of the gas subdomain (top and top-right) are open to the atmosphere. The zero-gradient boundary condition is applied for all variables for outflow. For inflow, the flow of only argon gas is allowed at ambient temperature. The inflow velocity is calculated based on the flux in the patch-normal direction whereas the pressure is calculated as a difference of atmospheric pressure and dynamic pressure.

The laser beam heat input with top-hat distribution is imposed at the interface between the argon gas and steel solid/liquid surface as:

![Figure A2.12](image)

**Figure A2.12:** Variation of surface tension ($\sigma$) and the coefficient of surface tension temperature gradient ($d\sigma/dT$) with respect to temperature for different sulfur concentration; (a) 20 ppm and (b) 150 ppm.
\[ \dot{q}_{laser} = \begin{cases} \eta P \pi r^2, & \text{if } r \leq r_{beam} \\ 0, & \text{if } r > r_{beam} \end{cases} \]  

where \( \eta = 0.13 \) is the laser absorptivity of the workpiece, \( r_{beam} = 1.4 \text{ mm} \) is the radius of the laser beam and \( P = 3850 \text{ W} \) is the laser power. All these values are taken from the reference case by Saldi [51]. The free surface is also subject to heat dissipation by convection and radiation. The convection effect is considered through the inflow of the argon gas from the atmospheric surfaces whereas the heat loss due to radiation is expressed as:

\[ \dot{q}_{rad} = \varepsilon \sigma_B (T^4 - T_{amb}^4) \]  

where \( \varepsilon = 0.5 \) is the emissivity of the workpiece, \( \sigma_B = 5.67 \times 10^{-8} \text{ Wm}^{-2}\text{K}^{-4} \) and \( T_{amb} = 300 \text{ K} \) is the ambient temperature.

The initial time step in the simulation is set to \( 10^{-9} \text{ s} \). An adjustable time step is applied which is controlled by the maximum CFL number 0.1 or the maximum time step \( 10^{-6} \text{ s} \). The coupling of pressure and velocity is achieved by PISO algorithm. The solutions are considered to satisfy convergence criteria when the residuals are below \( 10^{-12} \) for \( \alpha \) and \( 10^{-8} \) for \( p_{rgh}, T, \) and \( U \).
Figure A2.14 shows the comparison of the melt front between the present numerical results and the numerical results by Saldi [51] at $t = 5$ s. The post-solidification fusion profile of the weld bead by Pitschenede et al. [177] is also plotted for comparison with the experimental results. It can be seen that the melt pool width and the penetration depth between the present numerical results and the numerical results by Saldi [51] have a good agreement for both sulfur concentrations. However, both numerical results underestimated the penetration depth and overestimated the melt pool width. The discrepancies between numerical results and experimental results are higher for the case with 150 ppm than with 20 ppm sulfur concentration. Such discrepancies between numerical simulation results and experimental data are commonly reported in the literature. To circumvent the problem and match the simulation results with the experiments, the viscosity and thermal conductivity value were artificially enhanced using an enhancement factor $f$ up to 100 by several authors [63, 180, 181]. For instance, Pitschenede et al. [177] and Saldi [51] both used an enhancement factor $f = 7$ to match the simulation results with the experimental data. However, the use of an enhancement factor has no sound physical basis. Furthermore, the value of the enhancement factor $f$ changes with the change in operating condition as it was evident with the use of a large range of $f$ in literature. The need for the use of an enhancement factor has been motivated to account for the instabilities and turbulent nature of the melt pool. Although Kidess et al. [182] with the use of DNS method did find the melt pool unstable and highly oscillatory leading to the turbulence-like behavior, but it was still insufficient to resolve the observed discrepancies in predicting the melt pool shape between numerical simulation and experimental results. Other likely deficiencies in the numerical model including the mass transport model for surfactant species, the flow of shielding gas are probably needed to advance towards a predictive melt pool model.

The study of the test Case 2 resulted in the following outcomes:

a. Implementation of heat source model with top-hat distribution and surface forces with SSF method [176].

b. Although a good agreement was achieved with the reference numerical case, but both numerical cases under-estimated the melt pool depth and over-estimated the melt pool width in comparison to the experimental results. Further investigation is needed to explore the model deficiencies to advance to a predictive model. However, it is beyond the scope of the present thesis.

c. Model validation with experimental data are still restricted to the post-solidification fusion profile of the weld bead. In process melt pool data such as melt pool width, length, free surface geometry, and free sur-
Figure A2.14: Comparison of melt front between present study and Saldi [51] at $t = 5$ s and post-weld fusion geometry of corresponding experiments by Pitscheneder et al. [177] for different sulfur concentration; (a) 20 ppm and (b) 150 ppm.
face oscillation are invaluable for comparison of the transient and three-dimensional nature of the melt pool.

This thesis deals with the simulation of the melt pool in GMAW process. Additional implementations were needed following the solver development and computations of test Case 2. Additional major developments in the solver to account for GMAW process were the implementations of a moving heat source, arc pressure, electromagnetic force, and metal transfer model. There is a lack of experimental data for the validation of the melt pool model in GMAW process unlike the attractive experimental data by Pitscheneder et al. [177] for laser welding application. Furthermore, the melt pool models for GMAW in literature are known to adjust the arc parameters on an ad-hoc basis to reproduce the simulation results in good agreement with the experimental results. Therefore, the new melt pool solver for the GMAW process was not compared with the available experimental or simulation data from the literature. The data from the experiments performed in-house were used to compare with the simulation results which are reported in the appended Papers.
References


References


REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES


Appended Papers
Paper I

Effect of Substrate Orientation on Melt Pool during Multi-Layer Deposition in V-Groove with Gas Metal Arc

Pradip Aryal, Kjell Hurtig, Fredrik Sikström, Håkan Nilsson, Isabelle Choquet

Published: Proceedings of the 7th World Congress on Mechanical, Chemical, and Material Engineering (MCM’21), Prague, Czech Republic Virtual Conference - August 2021

Paper No. HTFF 130

DOI: 10.11159/htff21.130

Printed with permission
Effect of Substrate Orientation on Melt Pool during Multi-Layer Deposition in V-Groove with Gas Metal Arc

Pradip Aryal\textsuperscript{1}, Kjell Hurtig\textsuperscript{1}, Fredrik Sikström\textsuperscript{1}, Håkan Nilsson\textsuperscript{2}, Isabelle Choquet\textsuperscript{1}

\textsuperscript{1}University West
Department of Engineering Science, 461 86 Trollhättan, Sweden
pradip.aryal@hv.se; kjell.hurtig@hv.se; fredrik.sikstrom@hv.se; isabelle.choquet@hv.se

\textsuperscript{2}Chalmers University of Technology
Mechanics and Maritime Sciences, Fluid Dynamics, SE-412 96 Gothenburg, Sweden
hakan.nilsson@chalmers.se

Abstract – Thermo-fluid dynamic and experimental approaches are used to investigate the influence of 20° uphill, downhill and sideway substrate orientation during metal deposition over a previously deposited bead in a V-groove. The computational fluid dynamic model with free surface deformation and metal transfer gives insight into the melt pool flow and causes of defect formation observed on the solidified beads. The experimental metallographs, high-speed images and computational results show good agreement. It is found that the deposition of a second layer on a smooth first layer cooled down to room temperature leads to large changes in melt pool flow pattern at 20° substrate inclination compared to flat condition. It results in undercut and humps with the uphill orientation and undercut with the side inclination. Therefore, lower angle range is necessary for multilayer gas metal arc deposition for these two last configurations.

Keywords: metal deposition, gas metal arc welding, V-groove, substrate orientation, melt flow, reinforced bead, hump, OpenFOAM

1. Introduction

Metal deposition for multi-pass joining and additive manufacturing with gas metal arc (GMA) processing using non-horizontal substrate orientation would avoid workpiece repositioning necessitating manipulation by large and accurate robots when manufacturing large components. However, the freedom for tilting the arc axis to maintain it normal to a non-horizontal substrate can be limited by defect formation such as overflow, undercut and hump. The effect of the welding position on the molten pool behaviour and resulting bead geometry was studied both experimentally (e.g., Park et al. \cite{1}) and numerically (e.g., Hu et al. \cite{2}, Cho et al. \cite{3}) with GMA processing, single bead deposit, and flat, overhead, and vertical welding position. These authors observed that while the flat position generated continuous bead without noticeable defects, the overhead and vertical up positions were prompt to hump formation. Vertical down position increased bead width, while it reduced height and penetration depth. Besides, it is known that for multi-layer deposition the melt pool can have remarkably different behaviour in the root pass and in the subsequent layers for which it becomes more sensitive to the process parameters. However, the effect of non-flat welding position in GMA multi-layer deposition is to our knowledge poorly documented. This study thus aims at understanding this effect on melt pool thermal flow, free surface deformation, bead geometry, possible defect formation when depositing above the root pass. It is known from earlier studies that overhead and vertical position cannot be an option with GMA heat source. Therefore, in this study the welding position is varied by only 20° uphill, downhill, and sideway to investigate, using both experimental and computational fluid dynamics approaches, whether these conditions could provide an acceptable process window.

2. Experimental setup

Figure 1(left) shows an overview of the experimental setup. A precise movement ABB robot operated a gas metal arc torch with TPS-4000 Fronius power supply. It was used to deposit Invar 36 at the travel speed of 7.5 mm/s from a 1.2 mm diameter electrode wire on Invar 36 plates with same nominal composition. The deposition was shielded by a mixture of 98% Ar and 2% CO\textsubscript{2} flowing at the rate of 15 l/min. The plates (200 mm × 143.5 mm × 10.6 mm) were prepared with a V-groove at 60° with no root gap and mounted on the worktable. This table that can be rotated about its central horizontal axis...
was inclined to position the substrate as illustrated in Fig. 1(right): flat (reference angular position at 0°), downhill (at -20°), uphill (at 20°), and side inclined (at 20°). A data acquisition system was integrated with this setup to measure the arc current and voltage at a sampling frequency of 4 kHz. A vision camera was mounted on the robotic arm and focused behind the nozzle region to capture melt pool images at a frequency of 100 Hz. For each substrate positioning two layers of metal were deposited using the GMA welding system. The torch axis was in each case perpendicular to the substrate, the arc length was approximately 5 mm, and uniform contact-tip-to-work distance was maintained. The first layer deposit (root pass) generated continuous and uniform bead without noticeable defects. It was let to cool down to room temperature and the reinforced bead was 3D scanned before the second layer was deposited. A fifth-degree polynomial that curve fit the profile of the root pass bead reinforcement along the transverse direction was generated.

3. Mathematical model

A transient 3-dimensional melt pool model with metal alloy melting, re-solidification, metal transfer, and free surface deformation was implemented in the open-source software OpenFOAM®. It assumes incompressible and Newtonian fluids (atmosphere and liquid alloy with the Boussinesq approximation) and laminar flow. The alloy-gas interface is tracked with a volume of fluid method and the solid-liquid alloy transition region with a mushy zone approach. The model consists in the following system of equations governing mass, momentum, thermal energy, and metal volume fraction, respectively:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) &= \rho_{\text{drop}} \\
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) &= -\nabla p + \nabla \cdot \left( \mu (\nabla \vec{u} + (\nabla \vec{u})^T) - \frac{2}{3} \mu (\nabla \cdot \vec{u}) I \right) + \rho_m \ddot{g} \left[ 1 - \beta (T - T_m) \right] \\
&- C_D \frac{(1 - f_l)^2}{f_l^3 + \varepsilon_D} \ddot{u} + \left[ \sigma \kappa \ddot{n} + \frac{d \sigma}{dT} \left( \nabla T - \ddot{n} (\nabla \cdot \vec{n}) \right) + p_{\text{arc}} \right] \nabla \alpha \frac{2\rho}{\rho_t + \rho_g} + \dot{\bar{f}}_{\text{arc}} \\
\frac{\partial (\rho C_p T)}{\partial t} + \nabla \cdot (\rho C_p T \vec{u}) &= \nabla \cdot (k \nabla T) + h_{sf} \left[ \frac{\partial (\rho f_l)}{\partial t} + \nabla \cdot (\rho \vec{u} f_l) \right] + \dot{Q}_{\text{arc}} \\
\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \vec{u}) + C_{\alpha} \nabla \cdot [\alpha(1 - \alpha) \vec{u}] &= \dot{\alpha}_{\text{drop}}
\end{align*}
\]

where \( t \) is the time. The variable \( \vec{u} \) is the velocity vector, \( p \) the pressure, \( T \) the temperature and \( \alpha \) is the volume fraction of metal. The one-fluid density is the volume-weighted average \( \rho = \alpha \rho_m + (1 - \alpha) \rho_g \), where \( \rho_m \) and \( \rho_g \) are the metal and the...
atmospheric gas density, respectively. The source terms of metal mass, $\dot{\rho}_{\text{drop}}$, and volume fraction, $\dot{\gamma}_{\text{drop}}$, related to metal transfer in the form of molten droplets are specified hereafter. $I$ denotes the identity matrix. The one-fluid viscosity $\mu$, specific heat capacity $c_p$, and thermal conductivity $k$ are volume-weight averaged using the temperature dependent properties of Invar36 alloy [4]. In the buoyancy force $\vec{g}$ is the gravitational acceleration, $\beta$ the coefficient of volume expansion for the liquid alloy [4], and $\rho_m$ the alloy density at the melting temperature $T_m$. In the second line of Eq. (2) the first term is the Darcy damping. It is active in the mushy zone where the fraction of liquid alloy, $f_l$, is strictly bounded between zero and one. This fraction is a function of temperature, as defined in [5]. The Darcy constants are set to $C_D = 10^7$ and $\varepsilon_D = 10^{-3}$. The surface forces are estimated using the sharp surface force model introduced by Shams et al. [6]. As the densities of the two fluid phases differ by several orders of magnitude, the multiplier $2\rho/(\rho_m + \rho_g)$ introduced by Brackbill et al. is applied [7]. The capillary and thermocapillary forces depend on the surface tension, $\sigma$, the unit vector normal to the free surface, $\vec{n}$, and the surface curvature, $\kappa$. The latent heat of fusion is denoted $h_f$. In equation (4), the third term is the free-surface sharpening term, which is a function of the numerical compression velocity, $u_c$, [8]. The numerical compression factor is set to $C_\alpha = 1$ to satisfy conservation. The effect of the arc is modeled through the arc pressure, $p_{\text{arc}}$, the electromagnetic force $F_{\text{arc}}$, and the heat source, $Q_{\text{arc}}$. These three source terms are respectively estimated using the expression proposed by Tsai and Eagar [9], by Kou and Sun [10], and

$$Q_{\text{arc}} = \frac{\eta_{\text{arc}}VI}{2\pi\sigma_q^2} \exp\left(\frac{-r^2}{2\sigma_q^2}\right)$$  \hspace{1cm} (5)

where $r$ is the radial distance from the center of the arc, $V$ the arc voltage and $I$ the arc current. The arc efficiency, $\eta_{\text{arc}}$, is estimated from the total GMA process efficiency $\eta = 0.8$ [11], and the droplet efficiency according to [12]. The same value of the distribution parameter $\sigma_q$ is assumed for the heat flux, the arc pressure, and the current density according to the relationship proposed in [13]. Based on the experimental measurements, $V = 25.2$ V, $I = 270$ A and $\sigma_q = 1.4$ mm.

Figure 2 shows the computational domain of dimensions $60 \text{ mm} \times 20 \text{ mm} \times 13 \text{ mm}$, which is shorter and narrower than the experimental substrate. For the uphill configuration, a thicker atmosphere layer of up to $z = 23$ mm was used to capture the alloy deposition (see section 4). The results presented below were computed with a mesh size of 0.2 mm uniform in $x, z$, and in $-6 \leq y \leq 6$ mm. A cell-to-cell expansion ratio of 1.2 was applied outside this region. The root pass bead profile scanned during the experiment served to initialise the first layer in the V-groove, as shown in Fig. 2. For the configurations symmetric about $y=0$, only one half of the domain was simulated; this concerns the flat, uphill, and downhill positioning.

Fig. 2: Computational domain after initializing the root pass in the V-groove.
The test cases were computed with an arc torch initially in $x = 10$ mm, so that the alloy remained solid on the domain boundaries. The boundary condition for the gas phase was zero velocity gradient if the flow was outward. Otherwise, the computed pressure was used to determine the magnitude of the normal velocity at the boundary face. The metal alloy had zero-velocity and continuous temperature gradient conditions at the boundaries, making the workpiece semi-infinite for heat conduction. Based on experimental measurements the source terms $\rho_{\text{drop}}$ and $\dot{a}_{\text{drop}}$ reproduced spherical droplets of radius 0.54 mm transferred from the electrode wire at the periodic frequency of 207 s$^{-1}$. The location of the arc and droplet injection was moved at the welding travel speed for a period of 6 s. An adjustable time stepping with maximum CFL number of 0.1, and maximum time step of $10^{-5}$ s was applied. The pressure-velocity coupling was computed with a PISO algorithm. The convergence criteria imposed on the (final) residuals at each physical time step when solving for $a$, $p$, $\vec{u}$ components and $T$ was $10^{-12}$, $10^{-10}$, $10^{-8}$, and $10^{-8}$, respectively.

4. Results and discussion

Figure 3 presents computed results showing the melt pool followed by the resolidified bead and experimental post-process bead for the 20° uphill case (different scales). A non-continuous bead with intermittent humps can be seen in the right. The computational results also show an unstable melt pool with humping bead geometry. As the computational domain was shorter than the experimental substrate, the simulation results did only predict the formation of the first hump. With the other configurations, experimental and computed process and bead surface were all smooth.

![Fig. 3: Bead morphology for the uphill deposit condition. Left: simulation. Right: experiment (different scale).](image)

Figure 4 compares, for each configuration, computational results with experimental macrographs in transverse cross sections. The computed interface between fusion zone (orange/red in Fig. 4) and heat affected zone (yellow in Fig. 4) for the 2nd deposit is plotted at the arc axis location (e.g., section S1 in Fig. 3) when the melt pool has reached quasi-steady dimensions. Superposed on it is the computed bead reinforcement (blue grey in Fig. 4) extracted from the resolidified region (e.g., section S2 in Fig. 3 left). With the flat configuration a) the computed and experimental reinforced bead heights are 0.7 and 0.5 mm above the original workpiece height, respectively. A small depression that can lead to an undercut defect is observed in the metallograph a). To predict it a finer grid size would be required since its length is much lower than 1 mm. With the downhill configuration b) the height at the centre of the reinforced bead reaches the level of the original workpiece surface in the experimental metallographs while it is approximately 0.06 mm lower in the simulations. With the uphill configuration c) and contrary to the other cases, the bead surface is not regular and presents humps as can be seen in Fig. 3. The macrograph image shown in Fig. 4 c) was obtained from a cross section located at 21 mm from the arc start for both experiment and simulation. There, the computed and experimental reinforced bead heights are 0.8 and 0.6 mm above the original workpiece height, respectively. With the side inclined configuration d) the height of the reinforced bead at the centre of the V-groove is at the level of the original workpiece surface in the experimental metallographs. For the numerical simulation it is 0.55 mm above. Furthermore, the computed bead elevation is slightly lower uphill the groove centre and higher downhill. The undercut defect where the deposited metal fails to fill the groove can be seen on the bead edge in the experimental and computational images. Good qualitative agreement is observed in all the computed conditions. The small
differences compared to the experimental bead elevation might be due to the simplified arc physics, uncertainty in arc efficiency, or/and to small differences (≈ 2.5%) in average value of current and voltage between the cases that were not considered in the simulations.

Figure 5 visualises for each case at time $t = 5.0$ s the top view of the fully developed melt pool, its free surface geometry, the temperature field, and the velocity vectors on the free surface. At the rim of the pool crater (corresponding to the red temperature area) the velocity vectors are as expected distributed radially outward due to the thermocapillary force. For the flat deposit a) the maximum velocity outside the pool crater, which also results from the thermocapillary flow, is located in the middle and rear part of the melt where the pool width constricts. A vortex can be seen in the tail end of the melt pool due to the counterflow returning after striking the rear resolidified front. Similar observations can be made for the side inclined position d), but the melt flow is then asymmetric, towards the direction of substrate inclination due to the gravity. The melt pool length is approximately the same in a) and d). Figure 5 shows also that the melt pool is the shortest for the downhill position b) and the longest for the uphill position c). This is due to the gravity force that in the former case supplements the thermocapillary force ahead of the arc to accelerate the flow towards the front part of the melt pool (and decelerate the rear flow). In the latter case it acts on opposite direction, thus accelerates the rear flow (and decelerates the pool front flow) while surface tension is not sufficient to counteract the resultant increased pressure. This can also be seen with the velocity vectors, e.g., the melt flow shows larger velocity vectors towards the forefront in downhill position b) and towards the pool rear in uphill position c). Also, the maximum velocity is the lowest in b) and the largest in c). Due to the weaker flow for the downhill position b) compared to the other cases, no vortex is observed at the rear part of the melt pool in b). Besides, these changes in flow velocity compared to the flat case a) induce pressure changes on the free surface that the surface tension does not sustain. Thus, the pool deformation leading to wider pool front in downhill position b), longer pool rear in uphill position c), and asymmetric pool edge in side inclined position d) compared to the flat case a). The temperature distributions within the melt pools are in close ranges, with a maximum in the vicinity of 2920 K for all cases except the downhill position that is 200 K colder. The melt pool is also wider for the downhill position b) than for the other cases, providing higher degree of cooling rate. The computed melt pool geometries of Fig. 5 are consistent with the top view images of the pool free surface behind the arc acquired during the experiments and shown in Fig 6. These images indeed show the shortest melt pool length for the downhill position b) and an asymmetric pool with more melt towards the downhill direction (indicated by the white arrow in Fig. 6 d)) of the substrate for the side inclined position. For the uphill position c), the melt pool width is significantly
narrower, and gaps indicated with arrows can be seen between the melt pool and the groove wall. They contribute to the undercut defects seen in Fig 4.

Fig. 5: Temperature and velocity vectors on the computed melt pool free surface; a) flat, b) downhill, c) uphill, d) inclined case.

Fig. 6: Melt pool top view captured with a vision camera; a) flat, b) downhill, c) uphill, and d) side inclined (the white arrow points downhill). The red arrows indicate the arc centre travel direction.

Figure 7 shows for each case (at same scale) a longitudinal cross-section passing through the arc axis of the computed melt pool (grey in Fig. 7) and the velocity vectors at time $t = 5.0$ s where pool dimensions are quasi-steady. The horizontal red line indicates the upper surface of the first layer deposit. It should be noticed that the velocity vector plotted at the arc axis location orients differently depending on the dynamic formation/restoration of the pool crater with drop impact. It cannot be compared between the instantaneous images a) to d) since although synchronised with the drop detachment frequency the impact is not exactly at the same time as surface oscillations can differ with the configuration. Two regions recirculating in
opposite directions can be seen in the melt pool in the flat position a). The recirculation flow that is closest to the arc is clockwise, therefore it enhances the heat transfer under the arc and the penetration depth. For the other positions, the clockwise recirculation is absent. For the downhill position b) a significantly shallower melt pool can be observed. The counterclockwise recirculation is then much more extended than in the flat position a) and it flows at a velocity of \( \approx 0.3 \text{ m/s} \), which is about 0.1 m/s larger than in the counterclockwise recirculation of a), indicating a stronger returning flow in the shallower melt pool. For the uphill position c) a significant free surface depression can be seen underneath the arc column since a large volume of melted alloy flows downward, towards the pool rear under the action of the thermocapillary force enhanced by the gravitational force. This fluid accumulates in the trailing region, thus the high alloy thickness visible above the red line indicator in Fig. 7 c), resulting in a hump upon solidification. For the side inclined deposit position d) the melt pool shape at the centerplane is relatively shallow compared to the flat deposit position since some of the liquid metal then flows towards the downhill edge (see Fig. 5d).

Fig. 7: Melt pool and velocity vectors in longitudinal section through the arc axis for a) flat b) downhill c) uphill d) side position.

4. Conclusion

A thermo-fluid model for metal fusion with GMA heat source with tracking of free surface deformation and metal transfer developed in OpenFOAM was applied to study the effect of different substrate orientations on metal layer deposition over a pre-deposited layer in a V-groove. The numerical study was supplemented with experimental observation and the
results were in good qualitative agreement. However, the undercut defects observed in the experimental metallographs were only partially captured by the numerical simulations. A much finer grid size would be needed for a precise prediction of these small undercut defects. Nevertheless, it was found that deposition of a second layer on a smooth first layer that had been cooled down to room temperature leads,
- for flat welding position, to a liquid alloy recirculation pattern that enhances the penetration depth under the arc, and to smooth and continuous reinforced bead,
- for the 20° downhill position, to a large and strong returning flow behind the arc axis towards the melt front, which increases both the melt pool width and its cooling, while it decreases its length and the bead height.
- for the 20° uphill position, to flow acceleration by gravity towards the pool rear, resulting in a narrowing of the pool width, increased pool length, and liquid alloy accumulation at the pool rear resulting in undercuts and bead humps upon solidification.
- for the 20° side inclined position, the trailing part of the melt pool tends to flow downhill resulting in incomplete fusion on the opposite side of the V groove and undercut defects.

Therefore, uphill and side inclined multilayer GMA deposition are not recommended with these process conditions. Further investigations are needed to establish the range of inclination angles where acceptable deposition results are maintained.

Acknowledgements
This research work is supported by grants from the EU project - Horizon 2020: INTEGRADDE, which is gratefully acknowledged. The computations were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at NSC which is gratefully acknowledged.

References
Comparative study of the main electromagnetic models applied to melt pool prediction with gas metal arc: Effect on flow, ripples from drop impact, and geometry

Pradip Aryal, Fredrik Sikström, Håkan Nilsson, Isabelle Choquet


https://doi.org/10.1016/j.ijheatmasstransfer.2022.123068

This is an open access article under the CC BY-NC-ND license
Paper II

Comparative study of the main electromagnetic models applied to melt pool prediction with gas metal arc: Effect on flow, ripples from drop impact, and geometry

Pradip Aryal, Fredrik Sikström, Håkan Nilsson, Isabelle Choquet

Published in International Journal of Heat and Mass Transfer
https://doi.org/10.1016/j.ijheatmasstransfer.2022.123068

This is an open access article under the CC BY-NC-ND license
Comparative study of the main electromagnetic models applied to melt pool prediction with gas metal arc: Effect on flow, ripples from drop impact, and geometry

P. Aryal a, F. Sikström a, H. Nilsson b, I. Choquet a,∗

a Department of Engineering Science, University West, Trollhättan 461 86, Sweden
b Department of Mechanics and Maritime Sciences, Chalmers University of Technology, Gothenburg 412 96, Sweden

A R T I C L E   I N F O

Article history:
Received 30 January 2022
Revised 15 May 2022
Accepted 21 May 2022
Available online 28 May 2022

Keywords:
Maxwell electromagnetic force model
Kou and Sun model
Tsao and Wu model
Metal transfer
Molten pool
Free surface oscillation
Gas metal arc

A B S T R A C T

The present work concerns the electromagnetic force models in computational fluid dynamics simulations of melt pools produced with electric arcs. These are commonly applied to gas metal arcs with metal transfer, in welding and additive manufacturing. Metal drop impact on the melt pool is thus included in this study. The electromagnetic force models applied in literature use either numerical solutions of Poisson equations or one of the two analytical models developed by Kou and Sun, or Tsao and Wu. These models rely on assumptions for which the effect on the melt pool predictions remains to be understood. The present work thoroughly investigates those assumptions and their effects. It has been supported by dedicated experimental tests that did provide estimates of unknown model parameters and validation data. The obtained results show that the assumptions that fundamentally distinguish these three models change the electromagnetic force, including the relation between its components. These changes, which can also be spatially non-uniform, are large. As a result, these models lead to significantly different recirculation flow pattern, thermal convection, melt pool morphology, bead dimensions, and free surface response to the metal transfer. We conclude by proposing conditions in which each of these models is suited or questionable.

© 2022 The Authors. Published by Elsevier Ltd.
This is an open access article under the CC BY-NC-ND license
(http://creativecommons.org/licenses/by-nc-nd/4.0/)

1. Introduction

Gas metal arc (GMA) is widely used in fusion welding with metal transfer because of its high deposition rate and ease of automation. It is also increasingly applied in additive manufacturing (direct energy deposition). The process of metal fusion with a GMA involves heat and mass transfer from an electrode wire through a thermal plasma arc, and coalescence of transferred metal drops with the melt pool. Although the arc and pool are interdependent [1], the unified modelling approach, which consists in computing coupled arc and melt pool models, is seldom used due to the complexity of the physics involved (see [2] and references therein). The decoupled approach, which benefits from a lower computational cost as underlined in [3], is instead more widely applied. This is also the approach used in this study, which focuses on the modelling of the melt pool. Then, the modelling of the effect of the arc on the metal alloy is simplified to source terms or boundary conditions, which need to be set to close the melt pool model. This especially involves determining the electromagnetic force.

Based on dimensional analysis, the main forces driving the fluid flow in GMA melt pools are known to be, in ascending order of importance, the viscous friction force, the buoyancy force, the capillary force and the thermocapillary (or Marangoni) force [4,5]. In comparison, the electromagnetic force is of the same order of magnitude as the thermocapillary force [5], or at a higher order [4], depending on the GMA process conditions. The momentum transferred by the droplets is also important to consider, as demonstrated by Na and Kim [6] and Murphy [7]. These authors used a computational model to compare melt pools predicted with and without the drop effect. In the early study by Na and Kim [6], the authors assumed a Gaussian distribution of the droplet velocity to model the momentum it transfers to the melt pool free surface. In the more recent study by Murphy [7], a self-consistent melt pool model was used, which includes the workpiece, as well the
Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_t$</td>
<td>Activity of species s in solution [wt. %]</td>
</tr>
<tr>
<td>$\bar{A}$</td>
<td>Magnetic potential [T m$^{-1}$]</td>
</tr>
<tr>
<td>$\Lambda$</td>
<td>Mushy zone permeability coefficient [-]</td>
</tr>
<tr>
<td>$\bar{B}$</td>
<td>Magnetic flux density (or magnetic field) [T]</td>
</tr>
<tr>
<td>$c_p$</td>
<td>Specific heat capacity at constant pressure [J kg$^{-1}$ K$^{-1}$]</td>
</tr>
<tr>
<td>$C_{\mu}$</td>
<td>Interface compression factor (numerical) [-]</td>
</tr>
<tr>
<td>$d$</td>
<td>Gaussian distribution factor [-]</td>
</tr>
<tr>
<td>$D$</td>
<td>Diameter [m]</td>
</tr>
<tr>
<td>$\mathcal{E}$</td>
<td>Electric field [V m$^{-1}$]</td>
</tr>
<tr>
<td>$f_{\text{drop}}$</td>
<td>Frequency of drop transfer [s$^{-1}$]</td>
</tr>
<tr>
<td>$f_l$</td>
<td>Liquid fraction [-]</td>
</tr>
<tr>
<td>$\mathcal{F}$</td>
<td>Force applied (per unit volume) [N m$^{-3}$]</td>
</tr>
<tr>
<td>$F_{\text{fr}}$</td>
<td>Electromagnetic force (per unit volume) [N m$^{-3}$]</td>
</tr>
<tr>
<td>$g$</td>
<td>Gravitational acceleration [m s$^{-2}$]</td>
</tr>
<tr>
<td>$\mathcal{h}$</td>
<td>Specific enthalpy [J kg$^{-1}$]</td>
</tr>
<tr>
<td>$h_{fs}$</td>
<td>Latent heat of fusion [J kg$^{-1}$]</td>
</tr>
<tr>
<td>$h_{lv}$</td>
<td>Latent heat of vaporization [J kg$^{-1}$]</td>
</tr>
<tr>
<td>$I$</td>
<td>Electric current [A]</td>
</tr>
<tr>
<td>$\mathcal{I}$</td>
<td>Identity tensor [-]</td>
</tr>
<tr>
<td>$f'$</td>
<td>Current density [A m$^{-2}$]</td>
</tr>
<tr>
<td>$k$</td>
<td>Thermal conductivity [W m$^{-1}$ K$^{-1}$]</td>
</tr>
<tr>
<td>$k_l$</td>
<td>Constant related to the entropy of segregation [J kg$^{-1}$ K$^{-1}$]</td>
</tr>
<tr>
<td>$k_B$</td>
<td>Boltzmann constant [J K$^{-1}$]</td>
</tr>
<tr>
<td>$m$</td>
<td>Atomic weight [kg atom$^{-1}$]</td>
</tr>
<tr>
<td>$m$</td>
<td>Mass per unit time [kg s$^{-1}$]</td>
</tr>
<tr>
<td>$\mathcal{n}$</td>
<td>Unit vector locally normal to the free surface [-]</td>
</tr>
<tr>
<td>$p$</td>
<td>Pressure [Pa]</td>
</tr>
<tr>
<td>$\dot{q}$</td>
<td>Rate of heat transfer per unit area [W m$^{-2}$]</td>
</tr>
<tr>
<td>$q$</td>
<td>Rate of heat transfer per unit volume [W m$^{-3}$]</td>
</tr>
<tr>
<td>$r$</td>
<td>Radial distance [m]</td>
</tr>
<tr>
<td>$(r, \theta, z)$</td>
<td>Cylindrical coordinates</td>
</tr>
<tr>
<td>$R$</td>
<td>Universal gas constant [J mol$^{-1}$ K$^{-1}$]</td>
</tr>
<tr>
<td>$R_w$</td>
<td>Wire radius [m]</td>
</tr>
<tr>
<td>$t$</td>
<td>Time [s]</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature [K]</td>
</tr>
<tr>
<td>$T_l$</td>
<td>Liquidus temperature [K]</td>
</tr>
<tr>
<td>$T_m$</td>
<td>Melting temperature [K]</td>
</tr>
<tr>
<td>$T_s$</td>
<td>Solidus temperature [K]</td>
</tr>
<tr>
<td>$T_v$</td>
<td>Vaporization temperature [K]</td>
</tr>
<tr>
<td>$u$</td>
<td>Fluid velocity [m s$^{-1}$]</td>
</tr>
<tr>
<td>$u_{fr}$</td>
<td>Interface compression velocity (numerical) [m s$^{-1}$]</td>
</tr>
<tr>
<td>$u_{\text{feed}}$</td>
<td>Wire feed rate [m s$^{-1}$]</td>
</tr>
<tr>
<td>$u_{wp}$</td>
<td>Workpiece travel velocity [m s$^{-1}$]</td>
</tr>
<tr>
<td>$V$</td>
<td>Electric potential [V]</td>
</tr>
<tr>
<td>$(x, y, z)$</td>
<td>Cartesian coordinates [m]</td>
</tr>
<tr>
<td>$z$</td>
<td>Vertical elevation [m]</td>
</tr>
</tbody>
</table>

Greek symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>Volume fraction [-]</td>
</tr>
<tr>
<td>$\dot{\alpha}$</td>
<td>Volume fraction per unit time [s$^{-1}$]</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Thermal expansion coefficient of liquid alloy [K$^{-1}$]</td>
</tr>
<tr>
<td>$\beta_r$</td>
<td>Retro-diffusion coefficient [-]</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>Surface tension coefficient [N m$^{-1}$]</td>
</tr>
<tr>
<td>$(\gamma'_0)$</td>
<td>Surface tension at $T_m$ [N m$^{-1}$]</td>
</tr>
<tr>
<td>$(\gamma'_0)$</td>
<td>Surface tension temperature gradient at $T_m$ [N m$^{-1}$ K$^{-1}$]</td>
</tr>
<tr>
<td>$\Gamma_s$</td>
<td>Surface excess at saturation [kg mol$^{-1}$ m$^{-2}$]</td>
</tr>
<tr>
<td>$\Delta H^a$</td>
<td>Standard heat of adsorption [J kg$^{-1}$ mol$^{-1}$]</td>
</tr>
</tbody>
</table>

Subscripts

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\epsilon$</td>
<td>Radiative emissivity [-]</td>
</tr>
<tr>
<td>$\epsilon_0$</td>
<td>Small constant [-]</td>
</tr>
<tr>
<td>$\eta$</td>
<td>Thermal efficiency [-]</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Polar angle [-]</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>Free surface curvature [m$^{-1}$]</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Dynamic viscosity [Pa s]</td>
</tr>
<tr>
<td>$\mu_0$</td>
<td>Permeability of free space [N A$^{-2}$]</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density [kg m$^{-3}$]</td>
</tr>
<tr>
<td>$\rho_\text{per}$</td>
<td>Density per unit time [kg m$^{-3}$ s$^{-1}$]</td>
</tr>
<tr>
<td>$\sigma_{\text{arc.f}}$</td>
<td>Effective radius of the arc current density distribution [m]</td>
</tr>
<tr>
<td>$\sigma_{\text{arc.p}}$</td>
<td>Effective radius of the arc pressure distribution [m]</td>
</tr>
<tr>
<td>$\sigma_{\text{arc.q}}$</td>
<td>Effective radius of the arc heat flux distribution [m]</td>
</tr>
<tr>
<td>$\sigma_t$</td>
<td>Electrical conductivity [$\Omega^{-1}$ m$^{-1}$]</td>
</tr>
<tr>
<td>$\sigma_{\text{SB}}$</td>
<td>Stefan Boltzmann constant [W m$^{-2}$ K$^{-4}$]</td>
</tr>
</tbody>
</table>

Subscripts

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>amb</td>
<td>Ambient condition</td>
</tr>
<tr>
<td>arc</td>
<td>Electric arc</td>
</tr>
<tr>
<td>conv</td>
<td>Convection</td>
</tr>
<tr>
<td>drop</td>
<td>Metal drop</td>
</tr>
<tr>
<td>l</td>
<td>Liquid state</td>
</tr>
<tr>
<td>m</td>
<td>Melting condition</td>
</tr>
<tr>
<td>pool</td>
<td>Melt pool</td>
</tr>
<tr>
<td>rad</td>
<td>Radiation</td>
</tr>
<tr>
<td>sat</td>
<td>Saturation</td>
</tr>
<tr>
<td>vap</td>
<td>Vaporization</td>
</tr>
<tr>
<td>s</td>
<td>Solid state</td>
</tr>
<tr>
<td>0</td>
<td>Arc centre location at the workpiece surface</td>
</tr>
<tr>
<td>1</td>
<td>Primary VOIPH-phase (metal alloy)</td>
</tr>
<tr>
<td>2</td>
<td>Secondary VOIPH-phase (shielding gas)</td>
</tr>
</tbody>
</table>

arc with the metal vapour and the electrode. The effects observed by these authors indicate that the force applied by the falling drop on the melt pool is of the same order of magnitude as the electromagnetic force. The electromagnetic force is thus among the leading order forces in GMA melt pools. However, the literature shows that there is not yet unanimity on how to model it when studying such melt pools with computational fluid dynamics.

Three different electromagnetic force models (EMF models) are being widely used in the literature. The first one is a numerical model that consists in solving partial differential equations governing the electromagnetic field. This model has two main variants. Both compute the electric potential and the current density in the same way. They differ through the computation of the magnetic field. In the first variant, which is the more general of the two, the magnetic vector field is derived from Ampère’s law supplemented with Ohm’s law, either directly or through the magnetic potential vector [8]. This variant is hereafter called the numerical EMF model. It is commonly applied when the arc and melt pool are simulated with a unified approach, as in [2]). However, it is less frequently used in the context of melt pools modelled with a decoupled approach. Nevertheless, Hashimoto et al. [9] used this numerical EMF model to supplement their decoupled melt pool model with drop detachment prediction. In the second variant, the Biot-Savart law is applied to compute the magnetic field [10]. A simplification is then made, which consists in assuming that the radial component of the current density has a negligible contribution to the magnetic field [11]. This EMF model was applied to GMA welding (GMAW) to understand the mechanisms leading to the formation of ripples on the melt pool and the re-solidified bead [12]. It was also used to study the effect on the melt pool of surface active elements at different concentrations in the wire and the workpiece [13], varied process parameters (e.g., current, volt-
age) [14], and operating the arc with and without pulsing of the electric current [15].

We also consider two analytical models which were introduced by Kou and Sun [16] in 1985, and by Tsao and Wu [17] in 1988. Their main advantage is to reduce the computational time through replacing partial differential equations by an integral function for the former and an algebraic expression for the latter. These analytical models were originally introduced for gas tungsten arc assuming a flat workpiece and an axisymmetric configuration. Several developments were made since then. For instance, the Kou and Sun model was adapted by Cho et al. [18] to a V-groove joint shape introducing coordinate mapping and an elliptically symmetric arc. Wu et al. [19] proposed coordinate rotation of the arc to adapt the Kou and Sun model to conditions where the arc axis is not orthogonal to the workpiece surface, as when welding horizontal fillet joints. Zhang and Wu [20] proposed an enhancement factor applied to each component of the Tsao and Wu EMF. More recently, Hamed Zargari et al. [21] who applied the Tsao and Wu model in double-ellipse mode to study tandem-pulsed GMA introduced a new factor in the vertical component of the EMF to increase the model accuracy. To study the effect of a V-groove angle in GMA welding, Chen et al. [22] extended the Tsao and Wu EMF model to V-groove joint shapes by using a body-fitted coordinate system. Ebrahimi et al. [23] applied a similar approach to investigate various groove shapes in GMA welding. The Tsao and Wu EMF model was also applied in additive manufacturing. For instance, Bai et al. [3] used it to analyse the thermal flow in multi-layer deposition with a plasma arc heat source.

The analytical EMF models seem to be the most commonly used today to study melt pools produced by an electric arc heat source with computational fluid dynamics. The model of Kou and Sun was applied to understand the effect of the melt flow on the formation of defects such as lack-of-fusion and porosity when welding narrow gap with a GMA linearly translated or moved following a circular motion trajectory (swing-arc) [24]. It was also used to study the effect of GMA process parameters (e.g., current, voltage) on the melt pool flow and geometry when the arc is electrically pulsed to transfer one drop metal per pulse [25], when the welding torch is tilted to investigate the forces driving the flow [26], or when the weld is covered with slag to study its interaction with the melt pool thermal flow [27]. It was also applied to understand how the convective pattern is modified when a GMA is supplemented with a second heat source operated in keyhole mode such as a laser beam [28] or a plasma arc [29]. The model of Tsao and Wu was as well highly employed to understand the melt pool thermal flow in GMAW and its effect on defect formation such as undercut andaturaing [30], and of the influence of various process conditions on the melt pool flow such as arc swing compared to no swing [31], and the presence of an additional heat source like a laser beam for hybrid welding of aluminium alloy [32], or a second GMA for tandem welding with steady or vibrated workpiece [33]. The EMF model of Tsao and Wu was also applied to analyse the thermal flow in wire-based direct energy deposition with plasma-arc [3] and with GMA [34].

To permit an analytic approximation of the electromagnetic field, simplifying assumptions were introduced by Kou and Sun [16] and by Tsao and Wu [17]. Simplifying assumptions are also used with the numerical EMF model applied to melt pool computational fluid dynamics simulations. The effect of these assumptions on the melt pool predictions is still poorly understood. Kumar and DebRoy [35] compared the components of the electromagnetic forces resulting from the Tsao and Wu and from the Kou and Sun models. However, to our knowledge, a comparative investigation of these electromagnetic force models, in particular with regards to their effect on the melt pool, has not yet been made. This is the subject matter of the present paper. The numerical and the two analytical electromagnetic force models, as well as the assumptions on which they are based, are first recalled in Section 2. Each of these force models was combined with a thermo-fluid model that is presented in Section 3. They were applied to simulate a GMA test case, which has also been conducted experimentally. This test case is introduced in Section 4. The computational results showing the effect of the modelling assumptions on the predicted melt pool are then compared and analysed.

2. Models for the electromagnetic force

The electric arc induces an electromagnetic force

\[ \mathbf{F}_{E,B} = j \times B, \]

that depends on the electric current, \( j \) and the magnetic flux density \( B \) (simply called the magnetic field from now). The \( j \) and \( B \) fields should be determined in the melt pool and in the thermal plasma arc, at least to set the boundary conditions for the melt pool sub-region at the metal-arc interface. These vector fields obey the set of Maxwell equations supplemented by two closure relations, namely the equation governing charge conservation and the generalized Ohm's law. As this study is conducted with a fluid approach, the magnetohydrodynamics approximation can be made in both the melt pool and the thermal plasma arc (see e.g., [11] for more details) since the following assumptions are valid:

(i) The Debye length is much smaller than the characteristic length, so that there is local electro-neutrality.

(ii) The diffusion and thermodiffusion currents due to electrons are small compared to the drift current.

(iii) The characteristic time and length allow neglecting the displacement current compared to the current density (in Ampère's law).

(iv) The Larmor frequency is much smaller than the average collision frequency of electrons, implying a negligible Hall current compared to the drift current.

(v) The magnetic Reynolds number is much smaller than unity, leading to a negligible induction current compared to the drift current.

Assumptions (i)–(v) imply that the electromagnetic phenomena are quasi-steady, the electric field \( \mathbf{E} \) is irrotational, and the magnetic field has constant zero divergence. Therefore \( \mathbf{E} \) and \( \mathbf{B} \) can respectively be derived from a scalar electric potential \( \psi \) and a vector magnetic potential \( \Phi \) that are uniquely defined imposing the Lorentz gauge (i.e., \( \nabla \Phi = 0 \)). Then, the closed system of the Maxwell equations reduces to

\[ \nabla \cdot (\sigma_\epsilon \nabla \psi) = 0, \]

\[ \nabla \times (\mu_\epsilon \nabla \psi) = \nabla \times \mathbf{B}, \]

where the electric conductivity \( \sigma_\epsilon \) depends on e.g., the temperature, \( \mu_\epsilon \) is the permeability of vacuum, and \( \nabla \) denotes the Laplace operator. The current density and magnetic field are then derived from the solutions of these equations according to

\[ j = \sigma_\epsilon \mathbf{E} = -\sigma_\epsilon \nabla \psi, \]

\[ \mathbf{B} = \nabla \times \Phi. \]

A difficulty is the coupling between the thermal plasma arc and the metal sub-regions. The coupling of these two sub-regions, which takes place through the sheath layers, is still an open problem when the interface region deforms in time and space as is the case at the melt pool free surface [36]. Additional simplifications are thus commonly introduced to circumvent this difficulty.
2.1. Numerical EMF model

To simplify the problem and evaluate the electromagnetic force in the melt pool without modelling the thermal plasma arc, it is also commonly assumed that

(vi) The electromagnetic part of the problem can be modelled as if the melt pool free surface was frozen (while the thermal model can predict free-surface deformation).

In addition, in this study

(vii) The current density distribution at the workpiece upper surface located at \( z_0 \), \( J(x, y, z_0) = 0 \), obeys a pseudo-Gaussian distribution such that

\[
\frac{\partial V}{\partial z} = -\frac{1}{\pi \sigma_r \sigma_z} \exp\left(\frac{-d^2 r^2}{\sigma_r \sigma_z}\right) \frac{d}{dz}
\]

with

\[
r^2 = (x-x_0)^2 + (y-y_0)^2.
\]

where \( z \) is the arc axis, \( d \) the factor of the pseudo-Gaussian, \( \sigma_{r,z} \) the effective radius of the arc with respect to the current density field, and \( x_0 \) and \( y_0 \) are the coordinates of the arc centre.

(viii) The electrical conductivity \( \sigma_e \) is constant.

Concerning assumption (vi), the surface is treated differently depending on the application. In electric arc welding the melt pool free surface is generally set flat (all the time along the simulated process) to compute the electromagnetic force. In direct energy deposition with a GMA, some authors set the contour of the frozen surface from scans of experimental beads [8]. The contour of the frozen surface can then be updated each time a new metal layer begins to be deposited. Assumption (vii) is valid if the surface is flat, but other current density distribution on flat surface could be used in Eq. (6), such as a double ellipsoid for instance. Besides, the restrictions (vii) and (viii) are not needed to proceed to a numerical solution of this EMF model. They are only required when looking for an analytic solution as in Sections 2.2 and 2.3. In the test cases of this study, the numerical EMF model uses a flat shape for the frozen surface of (vi) as well as the assumptions (vii)-(viii). This is for consistency purpose when comparing the different EMF models.

2.2. Kou and Sun EMF model

Kou and Sun [16] used a cylindrical coordinate system \( (r, \theta, z) \) and supplemented (i)-(viii) with the following assumptions:

(ix) (a) The lower surface of the workpiece is electrically insulated, and

(b) the workpiece extends far away enough from the arc centre so that \( V \) can be set to zero on all the lateral boundaries of the workpiece (i.e. \( r_{\text{boundary}} \to \infty \)).

(x) The problem is axisymmetric, implying that the axial \( B_z \) and radial \( B_r \) components of the \( B \) field are everywhere equal to zero, as well as the azimuthal component, \( J_\theta \), of the current density field.

(xi) The azimuthal component, \( B_\theta(r, z) \), of the magnetic field is defined from Ampère’s law (formulated in integral form in [16]), given by

\[
\frac{1}{r} \frac{\partial}{\partial r} \left(r B_\theta(r, z)\right) = \mu_0 J_\theta(r, z).
\]

Note that, by construction, the EMF model of Kou and Sun satisfies the basic principle of current (or charge) conservation, and therefore assumption (ix) means that

(ix*) (a) The electric current cannot pass through the lower surface of the workpiece, so \( J_\theta = 0 \) at \( z = 0 \).

(b) The electric current passes through the lateral faces of the workpiece.

The constraint (ix*) is only a sub-part of (ix). Nevertheless, it might be problematic since experimental set-ups do not always permit to satisfy it. The workpiece is indeed often connected to the electrical ground through its lower surface lying on the welding table. Besides, it should be noticed that assumption (xi) is not contained in (vii), and Eq. (7) is not based on axisymmetry alone. When using axisymmetry alone, as shown in [11], the complete expression of Ampère’s law indeed involves a second contribution to \( B_\theta \) through

\[
\frac{\partial B_\theta(r, z)}{\partial z} = -\mu_0 J_\theta(r, z).
\]

If the problem is effectively axisymmetric and (ix) holds, the main difference between the numerical EMF model of Section 2.1 and the model of Kou and Sun therefore lies in neglecting the contribution of \( J_\theta \) to \( B_\theta \) (assumption (xi)). Hence, if the above assumptions are valid, the simplified variant of the numerical EMF model with magnetic field defined from the Biot-Savart law (see Section 1) is equivalent to the model of Kou and Sun.

Assumptions (i)-(xii) allow deriving an analytic solution of Eqs. (2)-(3). The derivation steps were explained in detail by Kumar and DebRoy [35] and are not repeated here. With the convention of axis orientation and origin indicated in Fig. 1 they lead to

\[
J_r = \frac{1}{2\pi} \int_0^\infty \lambda J_1(\lambda r) \exp\left(-\frac{\lambda^2 \sigma_\text{arc}^2}{4d}\right) \frac{\cosh(\lambda z_0 - z)}{\sinh(\lambda z_0)} d\lambda,
\]

\[
J_0 = \frac{1}{2\pi} \int_0^\infty \lambda J_0(\lambda r) \exp\left(-\frac{\lambda^2 \sigma_\text{arc}^2}{4d}\right) \frac{\sinh(\lambda z_0 - z)}{\sinh(\lambda z_0)} d\lambda,
\]

\[
B_\theta = -\mu_0 d \int_0^\infty \lambda J_1(\lambda r) \exp\left(-\frac{\lambda^2 \sigma_\text{arc}^2}{4d}\right) \frac{\sin(\lambda z_0 - z)}{\sinh(\lambda z_0)} d\lambda,
\]

where \( J_0 \) is the Bessel function of zero order and first kind, \( J_1 \) is the Bessel function of first order and first kind, and \( z_0 \) is the workpiece thickness (see Section 4.1, Table 1). The electromagnetic force field
in cartesian coordinates is then
\begin{align}
(F_r, g)_r &= \frac{x - x_0}{r} j_0 B_0, \\
(F_r, g)_y &= \frac{y - y_0}{r} j_0 B_0, \\
(F_r, g)_z &= j_0 B_0.
\end{align}

2.3. Tsao and Wu EMF model

Tsao and Wu [17] also used the above assumptions (i)–(viii) and (x)–(xii) but not assumption (ix) to develop their EMF model. Instead they made the two following additional simplifications:

(xii) The radial component \( j_r \) of the current density in the workpiece is the average value through the workpiece thickness.

(xiii) The vertical component of the current density \( j_z \) in the angular component of the magnetic field \( B_0 \) decrease linearly with \( z \) down to zero at the lower surface of the workpiece [at \( z = 0 \)].

It can be seen that, although (xii)–(xiii) and (ix*) are not equivalent, the assumptions (xii)–(xiii) satisfy the constraints listed in (ix*). It implies that (ix*) is common to the two analytical EMF models. The simplifications (xii)–(xiii) imply that the scalar Poisson equation governing the electric potential, Eq. (2), is no longer used. The simplified Eq. (7) governing the magnetic field is only solved at the workpiece upper surface and no longer within its volume. In this framework the electromagnetic force depends on \( j \) and \( B \) as already expressed in Eqs. (12)–(14), but the components of the current density and the magnetic field now write

\begin{align}
J_r &= \frac{1}{2\pi r r_0} \left[ 1 - \exp \left( \frac{-dr^2}{\sigma_{arc,j}} \right) \right], \\
J_z &= -\frac{ld}{\pi \sigma_{arc,j}} \frac{z}{z_0} \exp \left( \frac{-dr^2}{\sigma_{arc,j}} \right), \\
B_0 &= \frac{\mu_0 l d}{2\pi r} \frac{z}{z_0} \left[ 1 - \exp \left( \frac{-dr^2}{\sigma_{arc,j}} \right) \right].
\end{align}

3. Thermo-fluid model

Each of the above EMF models was combined with the thermo-fluid model described in this section to simulate the melt pool produced by a GMA. A one-fluid, unsteady and three-dimensional approach with free-surface capturing was used. It includes the shielding atmosphere and the metal in both solid and liquid states, with melting, re-solidification, and vaporization. The fluid flow equations were expressed in a fixed reference frame. In the model, the arc was at a fixed position and the workpiece was translated at the uniform velocity \( U_{\text{arc}} = -U_T \) (where \( U_T \) is the travel speed) imposing appropriate boundary conditions on the velocity field. The thermal plasma arc and the metal transfer were simplified using closure models. The governing equations are first presented, followed by the closure models.

3.1. Governing equations

The fluids are treated as immiscible, mechanically incompressible and Newtonian. The flow is assumed to be laminar, so that no turbulence model is used. The deformation of the liquid metal free surface is tracked with a volume of fluid approach. The system of governing equations includes mass, momentum, and energy conservation, supplemented with a transport equation for the volume fraction of metal alloy. These equations respectively are

\begin{align}
\partial_t \rho + \nabla \cdot (\rho \vec{u}) &= \rho_{\text{drop}}, \\
\partial_t \left( \rho \vec{u} \right) + \nabla \cdot \left( \rho \vec{u} \vec{u} \right) &= \rho_{\text{drop}}. \\
\end{align}

where \( \vec{u} \) is the velocity vector, \( p \) the pressure, \( T \) the temperature and \( \alpha \) the volume fraction of metal alloy. In the metal \( \alpha = 1 \), in the atmosphere \( \alpha = 0 \), and at the interface region \( 0 < \alpha < 1 \). The one-fluid density, \( \rho \), dynamic viscosity, \( \mu \), specific heat capacity, \( c_p \), and thermal conductivity, \( k \), are defined by a mixture model based on the distribution of volume fraction according to

\begin{align}
\phi &= \alpha \phi_1 + (1 - \alpha) \phi_2, \quad \text{if} \quad \phi = \rho \text{ or } \mu, \\
\phi &= \alpha \phi_1 + (1 - \alpha) \phi_2, \quad \text{if} \quad \phi = k \text{ or } c_p.
\end{align}

where \( t \) denotes the time, \( \vec{u} \) the velocity vector, \( r \) the pressure, \( T \) the temperature and \( \alpha \) the volume fraction of metal alloy. In the metal \( \alpha = 1 \), in the atmosphere \( \alpha = 0 \), and at the interface region \( 0 < \alpha < 1 \). The one-fluid density, \( \rho \), dynamic viscosity, \( \mu \), specific heat capacity, \( c_p \), and thermal conductivity, \( k \), are defined by a mixture model based on the distribution of volume fraction according to

\begin{align}
\phi &= \alpha \phi_1 + (1 - \alpha) \phi_2, \quad \text{if} \quad \phi = \rho \text{ or } \mu, \\
\phi &= \alpha \phi_1 + (1 - \alpha) \phi_2, \quad \text{if} \quad \phi = k \text{ or } c_p.
\end{align}

Subscripts 1 and 2 refer to the primary VOF-phase (the metal alloy) and the secondary one (the shielding gas), respectively. Index \( s \) holds for the solid phase and \( l \) for the liquid one. The properties of the metal alloy and shielding gas are given in Section 4.2, Tables 2, 3 and 4, respectively. The mass fraction of liquid metal \( f_l \) ranges from zero in the solid region to one in the liquid region. It is defined by a continuous function with continuous derivative [37], given by

\begin{equation}
f_l = \frac{1}{2} \left( \text{erf} \left( \frac{4(T - T_m)}{\delta_T - T_l} \right) + 1 \right),
\end{equation}

where \( T_s \) is the solidus temperature, \( T_l \) is the liquidus temperature, and \( T_m = 0.5(T_s + T_l) \) is the arithmetic averaged melting temperature.

Considering the right-hand side of these equations, in Eq. (18), the mass source term due to metal transfer in the form of drops is defined with the closure model of Section 3.2. In the momentum conservation equation, Eq. (19), the forces are, from left to right, the pressure force, the viscous friction force, the weight, the buoyancy force applied on the liquid alloy (Boussinesq approximation), the Darcy damping term active in the mushy zone, the capillary and the thermodiffusion forces acting at the melt pool free surface, the electromagnetic force, the arc pressure force, \( \vec{F}_{\text{arc}} \), and the
force caused by the momentum of the injected drops, \( F_{\text{drop}} \). The two last forces are defined in Section 3.2. For the electromagnetic force, \( F_{\text{EM}} \), three alternatives are treated using the three EMF models of Section 2. The other forces are defined here. In the viscous friction force, \( I \) denotes the identity tensor. Next, \( g \) is the gravitational acceleration, \( \beta \) the thermal expansion coefficient of the liquid alloy, \( \rho_0 \) the alloy density at the melting temperature \( T_0 \). \( A \) is the permeability coefficient and \( \varepsilon_0 = 10^{-3} \) (dimensionless) is a small constant to prevent from division by zero. The Peclét number adjacent to the solid-liquid interface calculated as introduced by Ebrahimi et al. [38], leads to \( \text{Pe}^* = 2 \) for the GMAW test case of this study. It was shown in [38] that at this order, \( \text{Pe}^* = \gamma(1) \), the numerical results have only a low sensitivity to the value of \( \gamma \). Besides, a too large \( \gamma \)-value may lead to numerical oscillations, the recommended upper-bound being 10. In this work \( \gamma \) was set to 10^6 (dimensionless).

The surface tension coefficient, \( \gamma \), is a function of both the temperature and the fraction of surfactant present in the alloy, according to [39]

\[
\gamma = \gamma_0 + \left( \frac{\partial \gamma}{\partial \alpha} \right) \left[ T_0 - RT \right] \ln \left[ 1 + k_\text{a} \alpha \exp \left( -\Delta H^\text{f}/RT \right) \right],
\]

where \( \gamma_0 \) and \( \left( \partial \gamma/\partial \alpha \right)_0 \) are the surface tension and the surface temperature gradient of the dominant metal alloy element (here Fe) at temperature \( T_0 \). The last term at the right-hand side of the Eq. (25) is the influence of the alloying element. \( R \) is the universal gas constant, \( \Gamma \), the surface excess at saturation, \( k_\text{a} \), a constant related to the entropy of segregation, \( a_\text{i} \), the weight percentage of surface active element, and \( \Delta H^\text{f} \) the standard heat of adsorption. The free surface curvature, \( \kappa \), and the unit vector locally normal to the free surface, \( \vec{n} \), are given by

\[
\kappa = -\left( \nabla \cdot \vec{n} \right), \quad \text{and} \quad \vec{n} = \frac{\nabla \alpha}{|\nabla \alpha|}.
\]

As the density of the atmosphere and liquid alloy differ by several orders of magnitudes, the last factor in the capillary and thermocapillary forces is introduced so that surface tension acceleration remains independent of density [40].

In the energy conservation equation, Eq. (20), \( h_{ij} \) is the latent heat of fusion and \( h_v \) is the latent heat of vaporisation. The second term at the right-hand side of Eq. (25) is the effect of the melting of the alloy. It includes a convective contribution as phase change in an alloy is non-isothermal. The third term describes evaporation of alloy constituents. It is modelled for the two major constituents alone assuming that they have a uniform \% weight in the alloy. As element diffusion is neglected. Condensation is ignored. The mass flux of evaporation of an element is given by (see e.g. [41])

\[
\dot{m}_{\text{ap}} = p_\text{ap} \sqrt{\frac{m}{2\pi k_b T}} (1 - \beta_i),
\]

where \( m \) is the element atomic weight, and \( k_b \) the Boltzmann constant. In the alloy, the mass flux \( \dot{m}_{\text{ap}} \) of a constituent \( i \) is weighted by its mass fraction, leading to the term \( (\dot{m}_{\text{ap}}) \) in Eq. (20). The retro-diffusion coefficient, \( \beta_i \), is assumed to be zero. The saturated vapor pressure of the constituent writes

\[
\dot{p}_{\text{sat}} = \dot{p}_{\text{amb}} \exp \left[ \frac{\mu_{\text{sat}} T_0}{k_b T_0} \left( \frac{T}{T_0} - 1 \right) \right],
\]

where \( \dot{p}_{\text{amb}} \) is the ambient pressure at standard condition (=101325 Pa), and \( T_0 \) the vapourisation temperature at standard condition. The third term at the right-hand side of Eq. (20) is the radiative cooling at the metal surface according to the grey body model. \( \epsilon_{\text{rad}} \) is the radiative emissivity of the metal, and \( \sigma_T \) the Stefan-Boltzmann constant. The energy source term due to the electric arc, \( q_{\text{arc}} \), and the transferred metal drops, \( \dot{q}_{\text{drop}} \), are defined by closure relations presented in Section 3.2.

The transport Eq. (21) is a modified VOF formulation introduced by Weller [42]. The third term of Eq. (21), which is only active at the interface, aims at enhancing the interface sharpening by reducing the numerical smearing of \( \alpha, \vec{u} \) is the compression velocity and \( C_\alpha \) the compression factor [42]. In this study \( C_\alpha \) is set to 1 to satisfy conservation. The source term \( \dot{q}_{\text{drop}} \) due to metal transfer is defined in Section 3.2.

### 3.2. Arc and metal transfer closure source terms

As electrode melting and thermal plasma arc are not predicted by the model, their effect on the melt pool is included through closure relations. The periodic metal transfer from the electrode is modelled injecting in the computational domain drops of molten alloy that are initially assumed to be identical, uniform, and spherical. At injection the diameter of a drop is defined according to (see e.g., [27])

\[
D_{\text{drop}} = \left( \frac{6\pi^2 U_{\text{wire}}}{\dot{m}_{\text{drop}}} \right)^{1/3},
\]

where \( R_\text{w} \) is the wire radius, \( U_{\text{wire}} \) is the wire feed rate, and \( \dot{m}_{\text{drop}} \) the frequency of the drop transfer. The drop velocity, \( \vec{u}_{\text{drop}} \), temperature, \( T_{\text{drop}} \), and centre location \( (x_{\text{drop}}, y_{\text{drop}}, z_{\text{drop}}) \) at injection are set based on experimental observation. At these conditions drop injection creates locally a periodic source term of mass \( \dot{m}_{\text{drop}} = \dot{m}_{\text{drop}} \rho_{\text{drop}} \), momentum \( F_{\text{drop}} = \rho_{\text{drop}} \vec{u}_{\text{drop}} \), thermal energy \( q_{\text{arc} \rightarrow \text{drop}} = \dot{q}_{\text{arc} \rightarrow \text{drop}} \) and metal volume fraction \( \alpha_{\text{drop}} = \dot{q}_{\text{drop}}/\dot{q}_{\text{arc} \rightarrow \text{drop}} \).

The electric arc acts on the melt pool through pressure and drag force, as well as heat transfer that is mainly due to temperature gradient and free electron enthalpy. In studies opting for a decoupled approach, the heat transfer from the arc is described as an overall phenomenon without distinguishing the different types of contributions. The drag force applied by the arc on the melt pool surface is often omitted, as in [12,14,25,26,32–34] concerning the examples discussed in Section 1. This is also the approach used in this study.

The arc pressure force is applied at the free surface. It is therefore modelled in a similar way as the surface tension force (see Section 3.1), as

\[
f_{\text{arc}} = p_{\text{arc}} |\nabla \alpha| \frac{2\rho}{\rho_1 + \rho_2},
\]

where \( p_{\text{arc}} \) is the pressure exerted by the arc. It is calculated using the empirical relation proposed by Lin and Edgar [43] given by

\[
p_{\text{arc}} = \frac{\mu_{\text{al}}}{4\pi^2 \sigma_{\text{arc}}} \exp \left( \frac{-r^2}{2\sigma_{\text{arc}}^2} \right),
\]

where \( \sigma_{\text{arc}} \) is the arc pressure distribution parameter.

The rate of heat input from the arc per unit area of the workpiece surface is assumed to obey a Gaussian distribution as in several previous studies e.g., [12,25]. This choice is supported by the side view images of the arc, which were acquired during the experiments (see Section 4.1). It is thus expressed as

\[
q_{\text{arc}} = \frac{\eta_{\text{arc} \rightarrow \text{pool}} V I}{2\pi \sigma_{\text{arc}}} \exp \left( \frac{-r^2}{2\sigma_{\text{arc}}^2} \right),
\]

where \( \sigma_{\text{arc}} \) is the arc heat flux distribution parameter, and \( \eta_{\text{arc} \rightarrow \text{pool}} \) the fraction of the process electric power that is transferred from the arc to the melt pool. It is defined from the arc thermal efficiency,

\[
\eta_{\text{arc}} = \eta_{\text{arc} \rightarrow \text{pool}} + \eta_{\text{arc} \rightarrow \text{drop}}.
\]
and requires determining the fraction of the process electric power transferred from the arc to permit metal transfer

$$\eta_{\text{arc-drop}} = \frac{Q_{\text{arc-drop}}}{VI}. \quad (34)$$

The rate of heat transferred from the arc to the metal wire to form drops includes solid metal heating, fusion, and liquid metal heating up to $T_{\text{drop}}$ according to

$$\dot{Q}_{\text{arc-drop}} = \frac{\pi D^2}{6} f_{\text{drop}}$$

$$\times \left[ \rho_{l,M} (C_p)_{l,M} (T_{\text{fus}} - T_{\text{amb}}) + \frac{\rho_{l,M} \sigma_{l,M}}{2} h_l + \rho_{l,M} (C_p)_{l,M} (T_{\text{drop}} - T_{\text{fus}}) \right]. \quad (35)$$

To complete the above closure relations and Eq. (6), the parameters $\eta_{\text{arc}}, d, \sigma_{\text{arc}}, \sigma_{\text{arc},f}, \sigma_{\text{arc},p}$ and $T_{\text{drop}}$ were estimated for the test case of this study, as reported in Section 4.2.

4. Test case

The GMA test case of this study was investigated both experimentally and numerically. The experiments were conducted to collect data that permit closing the model and to provide validation data. The experimental set-up is therefore presented first, in Section 4.1. Then, the parameters entering the source terms and boundary conditions for the arc and drop are specified in Section 4.2, as well as the material data. Next, the computational domain as well as boundary and initial conditions are presented in Section 4.3. Finally, the main characteristics of the solution method are given in Section 4.4.

4.1. Experimental set-up for data collection

Bead-on-plate GMAW experiments were carried out in pulsed mode with one drop of metal transferred per pulse. Figure 2 shows a picture of the experimental set-up. It consisted of a power source, an ABB robot, a wire feeding system, a gas shielding system, and a computer controlled measurements system. The workpiece with dimensions 150 mm × 20 mm × 60 mm (length × width × thickness) and the 12 mm diameter filler wire were both made of Invar 36, although some of the minor elements differed slightly. The lower third of the workpiece was clamped in a fixture connected to the ground. The welding torch was maintained perpendicular to the workpiece and the contact-tip-to-workpiece distance was 16 mm.

Pure argon gas was flowing through the welding torch at a constant flow rate of 15 l/min to shield the molten metal from the atmosphere. A single bead was deposited along the centreline of the workpiece using the process parameters reported in Table 1. This operation was repeated three times. The electrical signals were recorded using a computer data acquisition system at a sampling frequency of 4kHz. Figure 3a shows a sample of their waveforms. The value of the electric current and arc voltage ranged approximately from 90 to 400 A and 22 to 30 V, respectively. These time-variations are not considered in the simulations.

High speed imaging with an acquisition rate at 10,000 frames per second was used to capture drop size and motion, specifically drop velocity towards impingement into the melt pool. A collimated high power LED emitting 10 W optical power at a center wavelength of 450 nm was positioned on one side of the workpiece to provide backlighting during imaging. On the other side, a camera (IDT CCM-1540) was positioned to capture side view im-

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Notation</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Workpiece thickness</td>
<td>$s_i$</td>
<td>60</td>
<td>mm</td>
</tr>
<tr>
<td>Welding current (average)</td>
<td>$I$</td>
<td>225</td>
<td>A</td>
</tr>
<tr>
<td>Arc voltage (average)</td>
<td>$V$</td>
<td>25.6</td>
<td>V</td>
</tr>
<tr>
<td>Pulse frequency</td>
<td>$f_{\text{pul}}$</td>
<td>156</td>
<td>Hz</td>
</tr>
<tr>
<td>Filler wire radius</td>
<td>$R_W$</td>
<td>0.6</td>
<td>mm</td>
</tr>
<tr>
<td>Wire feed rate</td>
<td>$U_w$</td>
<td>8</td>
<td>m min$^{-1}$</td>
</tr>
<tr>
<td>Welding travel speed</td>
<td>$U_t$</td>
<td>8</td>
<td>mm s$^{-1}$</td>
</tr>
</tbody>
</table>

Fig. 2. Picture of the welding set-up.

Fig. 3. (a) Sample of the electrical signal waveform recorded during the experiments. (b) Side view images of the one pulse one drop GMAW before and after drop detachment.

Table 1
Parameters used in both simulations and experiments made with Invar 36 workpiece and filler wire.
ages of the process interaction zone. A dielectric-coated spectral filter with a center wavelength of 450 nm and a full width half max of 40 nm was mounted in the optical path of the camera matching the spectral distribution of the LED output power. The setup, shown in Fig. 2, was optimized to make the metal transfer visible through the arc attenuating partially the light entering the camera. However, the arc could still be distinguished in most of the captured images. An example of images can be seen in Fig. 3b. The captured images were used to extract data for the effective radius of the arc, drop size, and impingement drop speed. Besides, cross-sections of the weld beads were made at 55 mm, 65 mm, and 75 mm from the start of the weld. The sectioned specimens were mounted in epoxy resin, polished and etched using Marble’s reagent. The samples subjected to this standard metallographic procedure were then analysed in a light optical microscope.

### 4.2. Closure parameters and material data

The closure parameters for arc and metal drop modelling were collected from the literature and the experiments of Section 4.1. The total arc efficiency was set to $\eta_{arc} = 0.85$, based on a trial-and-error approach applied to reproduce numerically the dimensions of the bead cross sections obtained in the experiments. This value is at the high end of the range experimentally evaluated for GMW (from about 0.68 to 0.85, see [44] and references therein). The pseudo-Gaussian distribution factor was set to the standard value $d = 3$, as proposed by e.g., Kou and Sun [16]. The arc heat flux distribution parameter, $\eta_{arc,q}$, is known to be governed by several process parameters including the arc current and the arc length, as shown in e.g., [45] within the frame of gas tungsten arcs (GTA). Compared to GTA, a difficulty appears when the electrode is non-refractory, or when the elevation of the melt pool free surface varies with time as the arc length then changes with time. When modelling the melt pool with a decoupled approach, this variation with time uses to be neglected. The distribution parameter $\eta_{arc,q}$ can then be approximated from spectral analysis or from measured irradiation using Abel inversion [46]. In the absence of such means, it is also commonly approximated either from arc simulation, or from empirical equations derived for gas tungsten arc welding, or from imaging of the thermal plasma arc. For instance, Wu et al. [47] did simulate a plasma arc assuming a flat workpiece surface to determine $\eta_{arc,q}$ and then used this parameter to model a melt pool with keyhole. Ebrahimi et al. [48] applied a fitted function of the arc length and arc current based on experimental measurements made by Edgar and Tsai [45] for GTA on water cooled workpiece. Estimation from images was used in this study by manually defining a reasonable pixel intensity threshold to define the arc distribution and then measure the diameter at a reference level in $z$-direction using image tool software as described by Zhu et al. [49]. A set of such images can be seen in the supplementary material, S1. Measurements from captured arc images for two complete pulsation cycles (120 images) were used and the average value of the diameters resulted in $\eta_{arc,q} = 1.4$ mm as estimate. The arc pressure was assumed to have the same distribution as the arc heat flux. The current distribution parameter was adjusted by trial-and-error to $\eta_{arc,f} = 1$ mm to reproduce the penetration depth obtained experimentally from the macrograph images. The adjustment was performed using the most general of the three EMF models, that is the numerical model of Section 2.1. Concerning drop conditions at detachment from the electrode wire, the vertical position $z_{\text{drop}}$ was estimated to 2.1 mm above the workpiece upper surface from the high-speed camera observation. The frequency of the drop transfer was obtained from the welding data logger. In the studied process, the metal drops impact the melt pool with a high velocity. The drop speed was estimated before the impact from the high-speed images leading to 1.3 m s$^{-1}$.

### Table 2

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho_s$</td>
<td>8130</td>
<td>kg m$^{-3}$</td>
</tr>
<tr>
<td>$L$</td>
<td>7225</td>
<td>kg m$^{-3}$</td>
</tr>
<tr>
<td>$T_s$</td>
<td>1702</td>
<td>K</td>
</tr>
<tr>
<td>$T_c$</td>
<td>1723</td>
<td>K</td>
</tr>
<tr>
<td>$\rho_s$</td>
<td>$10^{4} \text{ Jm}^{-3} $</td>
<td>$10^{-1} $</td>
</tr>
<tr>
<td>$c_{p}$</td>
<td>389</td>
<td>J kg$^{-1}$ K$^{-1}$</td>
</tr>
<tr>
<td>$c_{v}$</td>
<td>301</td>
<td>J kg$^{-1}$ K$^{-1}$</td>
</tr>
<tr>
<td>$k_s$</td>
<td>6.293</td>
<td>W m$^{-1}$ K$^{-1}$</td>
</tr>
<tr>
<td>$k_l$</td>
<td>2.755</td>
<td>W m$^{-1}$ K$^{-1}$</td>
</tr>
<tr>
<td>$\gamma_0$</td>
<td>1.92</td>
<td>N m$^{-1}$</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>$-3.97 \times 10^{-4}$</td>
<td>N m$^{-2}$</td>
</tr>
<tr>
<td>$\eta_0$</td>
<td>$1.3 \times 10^{-5}$</td>
<td>kg mol$^{-1}$ m$^{-3}$</td>
</tr>
<tr>
<td>$k_b$</td>
<td>0.00318</td>
<td>-</td>
</tr>
<tr>
<td>$\sigma_b$</td>
<td>0.004</td>
<td>wt. %</td>
</tr>
<tr>
<td>$\Delta H_{\text{f}}$</td>
<td>$-1.66 \times 10^{6}$</td>
<td>J kg$^{-1}$ mol$^{-1}$</td>
</tr>
<tr>
<td>$\beta$</td>
<td>$2.76 \times 10^{3}$</td>
<td>J kg$^{-1}$</td>
</tr>
<tr>
<td>$s_{\text{ref}}$</td>
<td>0.7</td>
<td>[52]</td>
</tr>
</tbody>
</table>

### Table 3

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Property</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe (64 Wt.%)</td>
<td>m</td>
<td>9.273280 $\times 10^{-26}$</td>
<td>kg atom$^{-1}$</td>
</tr>
<tr>
<td></td>
<td>$T_s$</td>
<td>3135</td>
<td>K</td>
</tr>
<tr>
<td></td>
<td>$h_r$</td>
<td>6.280</td>
<td>$10^{3}$</td>
</tr>
<tr>
<td>Ni (36 Wt.%)</td>
<td>m</td>
<td>9.746268 $\times 10^{-26}$</td>
<td>kg atom$^{-1}$</td>
</tr>
<tr>
<td></td>
<td>$T_c$</td>
<td>3186</td>
<td>K</td>
</tr>
<tr>
<td></td>
<td>$h_r$</td>
<td>6.787</td>
<td>$10^{3}$</td>
</tr>
</tbody>
</table>

This value is also in good agreement with the experimental results of Lin et al. [50] for GMW with 1.2 mm wire. To maintain consistency, all the model parameters were kept the same in all the simulated cases.

The material properties used in the simulations are reported in Tables 2–4. Constant values were assumed for the argon gas properties. The cases computed resulted in a maximum temperature less than 3000 K. The thermal conductivity and specific heat capacity of argon show insignificant variations with $T$ when $300 \leq T \leq 3000$ K [51]. However, in this temperature range the argon density decreases with $T$ while its viscosity increases $T$ [51]. Nevertheless, in the arc area the effect of these variations is negligible compared to the intensity of the arc source terms. Outside the arc area, the effect of this simplification on the computed alloy fields remains to be evaluated. During the experiments, a thin oxide layer was observed floating on the melt pool free surface. The radiative emissivity was thus set based on the experimental measurements of Barka et al. [52] for Invar 36 at high temperature in the presence of a thin oxide layer.

### 4.3. Computational domain, boundary and initial conditions

A 10 mm wide cuboid domain corresponding to half of the workpiece along the y-direction (see Fig. 2) was used for all the
simulations. This is equivalent to assuming symmetry although flow instability might occur in the melt pool due to e.g., the Marangoni recirculation induced by the presence of surfactant [60]. A symmetry boundary condition was thus applied to all the variables at \( y = 0 \), which coincides with the face BCGF in the computational domain of Fig. 4. Dimensions and conditions along the other directions were model dependent, and will be described later. In all the computations of this study the corner B (see Fig. 4) defines the origin of the domain.

Concerning the numerical EMF model, the computational domain used to solve Eqs. (2)-(3) includes only the metal subdomain of Fig. 4 since the atmosphere does not need to be considered at this stage. It was designed long enough along the travel direction to contain the domain needed for the thermo-fluid model. In a preliminary study, the influence of the thickness and length of the simulated workpiece on the EMF-fields was investigated. It was concluded that it is important that the electromagnetic boundary conditions can satisfy symmetry with the modelling assumption (\( x \)) made by the analytical EMF models. The domain length along \( x \) was thus set identical on both sides of the arc. The arc axis was positioned at the centre (\( x_0 = 50 \) mm) of a domain that spanned 100 mm along the \( x \)-direction. The current density distribution defined in Eq. (6) was applied as boundary condition for the electric potential, Eq. (2), at the upper surface of the workpiece (EFGH at \( z_0 \)) with the parameters specified in Section 4.2. To investigate the solution (in)dependence with respect to the position of the lower boundary surface (ABCD in \( z = 0 \)), domains of various thicknesses were used. Two cases are reported below with \( z_0 = 4 \) mm and \( 15 \) mm thick workpiece. The results obtained with the experimental configuration and with a 10 mm thick workpiece whose lower face was set to \( V = 0 \) while the lateral faces were electrically insulated. Results obtained with lateral grounding are also discussed later. The boundary conditions for the magnetic potential, Eq. (3), were set to zero gradient at \( z_0 \) and \( z = 0 \), and to zero on all the other metal boundaries.

The computational domain used to solve the thermo-fluid model, Eqs. (18)-(21), is shown in Fig. 4. It spans \( 60 \times 10 \times 15 \) mm in the \( x, y \), and \( z \) directions, respectively. Its lower part was initialized with a 10 mm thick solid workpiece at 300 K and \( \alpha = 1 \), and the upper part with a 5 mm thick layer of argon gas at rest, at atmospheric pressure, 300 K, and \( \alpha = 0 \). The boundary conditions applied to Eqs. (18)-(21) are summarized in Table 5.

In Table 5, the rate of heat transfer by convection is \( q_{conv} = \rho c_{p} \rho \frac{dT}{dx} \) with the constant \( \rho c_{p} \rho = 100 \) W m\(^{-2}\) K\(^{-1}\). The ambient conditions are \( \rho_{amb} = 300 \) K, and \( \rho_{amb} = 101325 \) Pa. At the workpiece boundaries AEFB, ABCD, and EIJF the temperature gradient was extrapolated along the direction normal to the boundary.

At injection, the drop center was aligned with the arc axis thus \( x_{drop} = x_0 = 50 \) mm, and \( y_{drop} = y_0 = 0 \) mm. The vertical position \( z_{drop} \) was obtained from experimental observation (see Section 4.2). The fluid velocity (\( u_{drop} \)) and temperature (\( T_{drop} = 2100 \) K) were assumed uniform throughout the drop. Contrary to \( u_{drop} \) \( T_{drop} \) could not be measured in the experiments of this study. It was therefore set from a CMA study by Zhou et al. [8], which was selected because of its similar range of process conditions. To initialize the drops, the quantity \( a_{drop} \) was set at each injection patching on the computational mesh a sphere of diameter \( d_{drop} \) centred in \( (x_{drop}, y_{drop}, z_{drop}) \).

As the numerical EMF model was solved using a large domain, the computed electromagnetic force fields were mapped cell to cell about the centre of the arc to the smaller thermo-fluid domain shown in Fig. 4. These mapped fields were used as body force source term in the momentum equation. It was ensured that the electromagnetic force fields in the vicinity of the arc axis remained identical before and after mapping.

### 4.4. Solution method

The EMF and thermo-fluid models were implemented in the OpenFOAM open-source software. The numerical EMF model was solved with a fluid model, setting the convergence criteria to \( 10^{-8} \) for both \( V \) and \( \alpha \). Concerning the thermo-fluid model, the pressure-velocity coupling was solved using the Pressure-Implicit with Splitting of Operators (PISO) algorithm. The discretization of the convective term in the VOF equation was achieved by Van Leer scheme, which is a second-order scheme that ensures boundedness of the scalar field \( \alpha \) between 0 and 1. The Limited Linear scheme was used for the remaining convective terms in the governing equations. The Limited Linear scheme is a blended 1st/2nd order scheme that returns a first-order upwind differencing scheme in regions with a rapidly changing gradient and the second-order central differencing scheme elsewhere. The diffusion term in the governing equations was discretized using the central differencing scheme. The highly coupled governing equations were solved iteratively for each time step until the pre-defined criteria for convergence were satisfied before advancing to the next time step. The convergence criteria on the residual value was set to \( 10^{-12} \) for volume fraction, \( 10^{-8} \) for pressure and velocity, and \( 10^{-10} \) for temperature. The time step for advancing the solution was adjusted automatically imposing a maximum Courant number of 0.1 and a maximum allowed time step of \( 10^{-5} \) s.

A first grid study was conducted with the EMF model and a second with the thermo-fluid model, using in each study 4, 5 and 6 cells per millimetre. When performing the second grid study with the thermo-fluid model, the coarse, medium and fine mesh had 375 360, 660 000 and 2 054 250 cells, respectively. It led to a fully developed melt pool with variation in penetration depth,

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Variable</th>
<th>( u )</th>
<th>( p )</th>
<th>( T )</th>
<th>( u )</th>
</tr>
</thead>
<tbody>
<tr>
<td>AEFB</td>
<td>( \dot{U}_{in} )</td>
<td>( \dot{p} = 0 )</td>
<td>( -k_{T} )</td>
<td>const</td>
<td>1</td>
</tr>
<tr>
<td>AEDH</td>
<td>( \dot{U}_{in} )</td>
<td>( \dot{p} = 0 )</td>
<td>( -k_{T} )</td>
<td>( q_{amb} )</td>
<td>1</td>
</tr>
<tr>
<td>HGCD</td>
<td>( \dot{U}_{in} )</td>
<td>( \dot{p} = 0 )</td>
<td>( T = T_{amb} )</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>ABCD</td>
<td>( \dot{U}_{in} )</td>
<td>( \dot{p} = 0 )</td>
<td>( -k_{T} )</td>
<td>const</td>
<td>1</td>
</tr>
<tr>
<td>BFCG</td>
<td>( \dot{U}_{in} )</td>
<td>( \dot{p} = 0 )</td>
<td>( \dot{p} = 0 )</td>
<td>const</td>
<td>0</td>
</tr>
<tr>
<td>EIJF</td>
<td>( \dot{U}_{in} )</td>
<td>( \dot{p} = 0 )</td>
<td>( -k_{T} )</td>
<td>const</td>
<td>0</td>
</tr>
<tr>
<td>ELII</td>
<td>( \dot{U}_{in} )</td>
<td>( \dot{p} = 0 )</td>
<td>( p = p_{amb} )</td>
<td>( -k_{T} )</td>
<td>( q_{amb} )</td>
</tr>
<tr>
<td>LGKH</td>
<td>( \dot{U}_{in} )</td>
<td>( \dot{p} = 0 )</td>
<td>( -k_{T} )</td>
<td>( q_{amb} )</td>
<td></td>
</tr>
<tr>
<td>IJCF</td>
<td>( \dot{U}_{in} )</td>
<td>( \dot{p} = 0 )</td>
<td>( \dot{p} = 0 )</td>
<td>( \dot{p} = 0 )</td>
<td>( \dot{p} = 0 )</td>
</tr>
<tr>
<td>IJLJ</td>
<td>( \dot{U}_{in} )</td>
<td>( \dot{p} = 0 )</td>
<td>( -k_{T} )</td>
<td>( q_{amb} )</td>
<td></td>
</tr>
</tbody>
</table>

* The gradient is extrapolated.
half-width and length below 6% for the medium compared to the coarse mesh, and 1% for the fine compared to the medium mesh. The medium-sized mesh provided a good compromise between quality of the solution and computational time. The mesh used for all the calculations presented hereafter thus has a uniform grid size of 0.2 mm in x, 0 ≥ y ≥ 6 mm, and 0 ≥ z = zp ≥ −6 mm to ensure that the electromagnetic force variations are captured and that the melt pool is within the region of uniform cell size. Outside that region a cell to cell expansion ratio of 1.14 was applied. Besides, this mesh implies that 6 cells are used to discretize the droplet along its diameter, which is more than the minimum of 4 mesh cells usually recommended, as in [27] and references therein. Each simulation was executed in parallel using 20 cores Intel Xeon Gold 6130 CPU @ 2.90 GHz × 32 on a computing cluster provided by the Swedish National Infrastructure for Computing (SNIC). The computational time per simulation with the thermo-fluid model and the medium-sized mesh took about 168 h of physical time (≈ 3360 Core hours) to simulate 12 s of GMAW.

5. Results and discussion

Experimental set-ups do not always comply with assumption (ix’). For instance, the electric potential (V) is often grounded under the workpiece through the working table, or as in this study through a fixture that covers only the lower part of lateral faces of the workpiece. Besides, it can be seen in the literature that the analytical EMF models were applied to a variety of workpiece thicknesses ranging from thin (e.g., 2.3 mm [62], 4 mm [34]) to thick (e.g., 10 mm [26], 20 mm [31]). The influence of the location of the electric potential ground on the electromagnetic force is thus investigated in this study for various workpiece thicknesses. The results are reported for both thin (4 mm) and thick (10 mm) workpieces in Section 5.1. Next, the GMAW conditions of Section 4 are applied. The effect of the assumptions that fundamentally differentiate the three EMF models is examined. Their impact on the current density, magnetic field and resultant electromagnetic force are analysed in Section 5.2. Finally, the effect of these modelling assumptions on the melt pool flow and temperature field (Section 5.3), melt pool geometry (Section 5.4), as well as on the free surface ripples resulting from the impact of the transferred metal drops (Section 5.5), are successively analysed.

5.1. Effect of V-ground location for thin and thick workpiece

The test cases of this section apply to the workpiece alone (no atmosphere and no metal transfer) and the numerical EMF model alone (without thermo-fluid model). The boundary conditions that are not discussed in this section are set as described in Section 4. Figure 5 shows the computed current density vectors, electric potential and electromagnetic force distributions. The plots are presented for two different metal thicknesses: 10 mm in Fig. 5a, b and 4 mm in Fig. 5c–h. Each thickness is combined with two different boundaries for grounding the electric potential: a lateral grounding in Fig. 5a, c, e (left side), and a lower surface grounding in Fig. 5b, d, f (right side). Comparing Fig. 5a and b, it can be seen that for the thick workpiece the ground potential can be at the two studied locations without significantly changing the V-isolines or the vector distribution in the area where the melt pool is expected to form (i.e., |z| ≤ 5 mm, z ≥ −3 mm). On the contrary, Fig. 5c, d show that for the thinner workpiece these two conditions do not give equivalent fields in the region of interest. A comparison between the V-isolines in Fig. 5e (lateral ground) and Fig. 5f (lower surface ground) shows clear differences. Their significant effect on the electromagnetic force can be seen in Fig. 5g and h, plotted along the radial direction at x = 2 and 1 mm below the workpiece upper surface (i.e., where liquid alloy could be present). Let us consider for instance the extrema of the electromagnetic field components, which are reached at x ≈ 2 mm. For the vertical component (Fz), the absolute value of its extremum at 1 mm (resp. 2 mm) below the surface of the workpiece is about 15% (resp. 70%) larger when setting the electric potential ground at the lateral surface rather than at the lower surface. For the radial component (in these plots (Fx, Ey)) the difference is more significant, as the absolute value of its extremum at 1 mm (resp. 2 mm) below the surface is about 30% (resp. 170%) larger when setting the electric potential ground at the lower surface rather than at the lateral surface. These results imply that assumption (ix’−a)) is particularly important to respect when applying the analytical EMF models to thin workpieces, while it could be neglected for thick workpieces when the arc is operated in conduction mode as in this study. Besides, for an electric arc operated in keyhole mode (plasma arc) it is anticipated that this assumption might not be reasonable to circumvent when applying one of the analytical EMF models to a 10 mm thick workpiece, especially when burn-through occurs, since then the region of influence of the EMF force extends deeper into the workpiece.

5.2. Effect of the EMF models on the electromagnetic force

This section focuses on the different EMF models (without thermo-fluid model). The test cases apply to the workpiece alone (no atmosphere and no metal transfer). The computational results presented in the sequel were all obtained for a 10 mm thick workpiece, with the setting of the GMAW test case of Section 4. It was checked in Section 5.1 that the boundary condition V = 0 can be set at the lower or at the lateral surface of the 10 mm-thick workpiece without affecting the results, when computing the numerical EMF. It implies that the constraint (ix’) can also be satisfied by the numerical EMF model in the studied test case. Then, the Kou and Sun model differs from the numerical EMF model through (xi) alone, and from the Tsao and Wu model through (ix’)/(xii)–(xiii). Figure 6 shows the current density calculated with each of the three EMF models, plotted along the x direction at y = 0. In these plots Jx is equivalent to Jx and z = 0 to r. The results are reported at elevations that would be in the melt pool (close to its surface (upper figures at z = 9.9 mm) or deeper (lower figures at z = 8.1 mm). The plots at the left side show the x-component of the current density while those at the right side show the y-component. It can be seen that the numerical model and the model of Kou and Sun lead to the same results for both Jx and Jy. This is as expected since these two models are based on the same assumptions for determining the electric potential (provided that the boundary conditions are treated consistently). On the other hand, the additional simplifications of the Tsao and Wu model lead everywhere to clear differences in both Jx and Jy. It can be seen that these differences are not systematic. Jx is indeed more than one order of magnitude smaller with the model of Tsao and Wu than with the two other models when z = 9.9 mm. On the contrary, it is larger in the vicinity of the arc centre (x − x0 = 0) when z = 8.1 mm. The maximum value of Jy is about 30% larger at z = 9.9 mm with the model of Tsao and Wu than with the two other models, and it is more than one order of magnitude larger at z = 8.1 mm. It implies that the components Jx and Jy do not change with the same proportions when changing from the Tsao and Wu model to any of the two other models. Furthermore, the proportionality factor varies with the position. As a result the simplifications made when predicting Jx and Jy with the model of Tsao and Wu cannot be simply compensated by a constant multiplying factor to recover the more general results of the two other models. Figure 7 shows the component Bz of the magnetic field along the x direction at y = 0 and the elevations z = 9.9 mm and z =
Fig. 5. Solution of the numerical EMF model for (a)-(b): 10 mm and (c)-(h): 4 mm thick workpiece. (a)-(d): current density vectors; (e)-(f): electric potential isolines from -0.08 to 0 V with intervals of 0.01 V; with V grounded at lateral (left plots) and at the lower surface (right plots). Electromagnetic force along x at (g): 2 mm and (h): 1 mm below the upper surface; with solid and dashed lines for ground at lateral and at lower surface, respectively.
Fig. 6. Current density components at $y = 0$ as functions of the position along $x$ (arc center in $x - x_0 = 0$). Top (a), (b): at $z = 9.9$ mm. Bottom (c), (d): at $z = 8.1$ mm. Left (a), (c): $J_x$ (or here $J_r$ for the analytical EMF models). Right (b), (d): $J_z$.

Fig. 7. Magnetic field component $B_y$ as function of the position along $x$ (arc center in $x - x_0 = 0$). (a): at $z = 9.9$ mm. (b): at $z = 8.1$ mm. For the analytical EMF models $B_y$ here corresponds to $B_θ$.

8.1 mm. In these plots $B_y$ is equivalent to $B_θ$ and $x - x_0$ to $r$. It can be seen that the model of Tsao and Wu overestimates the magnetic field everywhere compared to the two other models. This overestimation changes amplitude depending on the spatial location. For instance, close to the arc center ($x - x_0 = 0$) it is much larger at $z = 8.1$ mm than at $z = 9.9$ mm. This is a consequence of assumption (xiii) which implies that $B$ decreases linearly with $z$ rather than exponentially. Therefore, here too the simplification made cannot be compensated by a constant multiplying factor to recover the more general results of the two other models. Besides, the mag-
netic fields computed using the numerical model and the analytical model of Kou and Sun now differ to a significant extent. This is due to the contribution of $\mathbf{J}_c$ (as in Fig. 6) to $\mathbf{B}_s$ that is ignored in the model of Kou and Sun (see assumption (xi) and the following discussion). The results show that locally this contribution can reach up to 90% of the value of the magnetic field (see Fig. 7(a) at $|x-x_0| \approx 1$ mm). Recall that in this case the model of Kou and Sun is equivalent to the simplified version of the numerical EMF model that computes the magnetic field from the Biot-Savart law. Therefore, the two variants of the numerical EMF model (see Section 1) cannot be considered as equivalent in the context of GMA (nord gas tungsten arc [11]).

Figure 8 shows for each of the three EMF models the $x$ and $z$ components of the electromagnetic force plotted as functions of $x$ relative to the arc centre (in $x_0$) at $y = 0$ and at the elevations $z = 9.9$ mm and $z = 8.1$ mm. As expected, the results reflect the differences in current density and magnetic field previously observed. It can be seen that the difference in assumptions made in the models of Kou and Sun and Tsao and Wu lead to significant differences for both $(F_{x,y})_x$ and $(F_{x,y})_z$. While in the studied example the model of Kou and Sun overestimates the components of the electromagnetic force by a factor of about two compared to the numerical model, no clear proportionality is seen between the model of Tsao and Wu and the two others. For instance, let us compare the absolute extrema reached with the model of Tsao and Wu compared to the numerical model. For the component $(F_{x,y})_z$ the extrema are almost three times larger at $z = 9.9$ mm, and more than two orders of magnitude larger at $z = 8.1$ mm. While for the component $(F_{x,y})_x$ they are about five times smaller at $z = 9.9$ mm, and one order of magnitude larger at $z = 8.1$ mm. In other words, the modelling assumptions (xii)-(xiii) (Section 2.2) change not only the amplitude of the electromagnetic force but also the proportion of its components, furthermore in a space-dependent way.

5.3. Effect of the EMF models on the melt pool flow and temperature field

The calculation results presented in the following were computed for the complete GMW test case with workpiece, atmosphere and transferred metal drops. They were obtained combining the thermo-fluid model with each of the EMF models. The EMF model is the only element varied in the next comparisons. The simulation results are from now time-dependent. Time $t = 0$ s is the time when the arc heat source is switched on. The metal transfer starts at $t = 0.03$ s and continues with the drop frequency $f_{\text{drop}} = 156$ Hz. It was checked that at time $t = 8$ s the melt pool was already fully developed with each of the models (see Section 5.4). The computations were conducted up to the time $t = 12$ s. Look-
ing at the simulation results over several cycles of metal transfer while the melt pool is fully developed, it can be observed that in a large part of the liquid alloy the computed fields present almost no variation with time (see supplementary material, movies S2-S5c). However, this observation does not apply to the drop impact area or to the free surface area due to the propagation of ripples issuing from drop impact. In these two last areas the flow, in particular its velocity, shows some periodicity related to the metal transfer periodicity (see also Sections 5.3, 5.5). However, possible random fluctuation of the mean flow is not investigated in the scope of this study.

Figure 9 presents, at time $t = 12$ s, velocity vectors computed in the liquid alloy with each of the three EMF models. Figure 9a shows top-view images with the melt pool free surface in grey color, and Fig. 9b presents side view images in a longitudinal section at $y = 0$ (symmetry plane). The arc axis is aligned with the 2-axis and passes through $x = 50$ mm, and $y = 0$ mm. At this location it can be seen in both Fig. 9a and b that the velocity vectors have different orientations with the different EMF models. This is related to the dynamics of the flow during the drop impact cycle, which is discussed in Section 5.5. Figure 9a shows that at the free surface, in a radius of approximately 3 mm about the arc axis, the velocity vectors are oriented radially outward due to the combined effect of the thermocapillary force (outward), the $\gamma$-components of the electromagnetic force (inward radial contribution), and the dynamics of the flow related to the ripples caused by the drops (outward). The black line plotted at the melt pool surface in Fig. 9a represents the temperature isoline $T = 1850$ K, across which the thermocapillary force of an iron alloy containing 40 ppm sulfur changes sign. It can be seen that at the free surface the flow changes direction across that line, and that recirculation vortices form at the rear part of the melt pool. When observed over a time period while the melt pool is fully developed, this isoline is quasi-steady with negligible oscillation (see supplementary material S2). It is also observed in Fig. 9a that the shape of this isoline is different with the different EMF models, in particular the transition shoulder in the vicinity of $x = 40$ mm. Its shape is smoother with the Kou and Sun model than with the numerical EMF model, while it is more abrupt with the Tsao and Wu model. It is important to note here that the EMF models have also different effects on the thermocapillary flow.

Figure 9b shows that under the free surface the melt pool flow is very different depending on the EMF model, as highlighted by the white arrows indicating recirculation regions. Examining the fully developed melt pool as time evolves, it can be observed (see supplementary movies S3) that the recirculation regions remain the same in all models, except near the arc axis where the flow pattern shows dynamic evolution related to the periodic drop impact. Behind the arc axis ($x < 50$ mm) a very large recirculation is observed with the Kou and Sun model. It is associated with a downward melt pool flow at the arc center that is characteristic of a leading order electromagnetic force. With the numerical EMF model this recirculation region is smaller, while with the Tsao and Wu model it is not observed. On the contrary, a recirculation rotating in the other direction (seen counterclockwise in Fig. 9b), which is characteristic of a leading order thermocapillary force, is observed with the model of Tsao and Wu, as well as with the two other models but then further behind the arc. It is largest with the Tsao and Wu model, and extends from the arc region to far downstream up to about $x = 40$ mm (or P2), where the thermocapillary force changes direction. It has a smaller size with the numerical EMF model as it faces the first recirculation in the vicinity of $x = 45$ mm (or P1). The smallest size is given by the Kou and Sun model. In that case the reverse direction swirls confront at $x ≈ 47.5$ mm (or P2). The assumptions (xi) and (ix)/(xii)-(xiii) that differentiate the three EMF models thus introduce simplifications with significant consequences on the melt pool flow. It was seen in Fig. 8a that the electromagnetic force components have an amplitude that depends on the EMF model close to the arc axis $|x - x_0| < 4$ mm. The electromagnetic force component $(F_{Em2})$, which is oriented downward, has the largest amplitude with the Kou and Sun model and the smallest amplitude with the Tsao and Wu model (Fig. 8b). These differences are consistent with the differences in recirculation flow observed under the free surface in Fig. 9b in the arc axis area $|x - x_0| \leq 4$ mm. In that same region the amplitude of the radial component (oriented inward) of the electromagnetic force about the arc axis is smallest with the numerical EMF model (resp. largest with the Tsao and Wu model; see Fig. 8a). Thus, it decelerates the less (resp. the most) the thermocapillary flow. However, this seems to be in contradiction with the radial extent of the melt pool that is wider with the Tsao and Wu model than with the numerical EMF model (Fig. 9a, and 14 d). Moreover, Fig. 8 shows that for each of the EMF models the electromagnetic force is negligible at more than 5 mm from the arc centre. Thus the differences in flow pattern in the region of P1 and P2 are not simply direct effects of the electromagnetic force. The problem becomes more complex by the presence of both solid/liquid and liquid/gas interfaces that interact with the thermal convection. Free-surface oscillations are also known to influence the thermocapillary flow [63]. The indirect effect of the electromagnetic force on the flow dynamic due to differences in melt pool morphology (Section 5.4) and the oscillation during drop impact and coalescence (Section 5.5) need also to be considered.

Figure 10 shows the evolution over time of the maximum fluid velocity, $u_{max}$, computed at the melt pool free surface (isosurface $\phi_{fl} = 0.5$) for the different EMF models. The time interval reported, 11.95 ≤ $t$ ≤ 12 s, includes 8 cycles of metal transfer. It can be seen that that $u_{max}$ follows a periodic pattern with a frequency corresponding to the metal transfer frequency. The extrema reached by $u_{max}$ are almost the same for the different EMF models. During each cycle of metal transfer, $u_{max}$ varies between about 1.6 to 0.4 m s$^{-1}$. Figure 10 shows that the time $t = 12$ s corresponds to the end of a cycle, thus the maximum velocity of about 0.4 m s$^{-1}$ in Fig. 9. The minimum value of $u_{max}$ is thus 50 times larger than the welding travel speed $U_w = 0.008$ m s$^{-1}$, and the maximum value is about 20% above the initial drop velocity $|U_{drop}| = 1.3$ m s$^{-1}$. The root mean square of $u_{max}$ was calculated over the reported time interval, leading to the values indicated in Fig. 10 for each EMF model. The RMS value obtained with the numerical and the Kou and Sun models are very similar, while with the Tsao and Wu model it is about 20% lower. A possible reason for this difference is proposed below examining the temperature field. Besides, the evolution of $u_{max}$ over a metal transfer cycle follows different patterns depending on the EMF model, as can be observed in Fig. 10. With the numerical and Kou and Sun models it goes up and down two times, while with the model of Tsao and Wu there is only one peak per cycle. This might be related to the primary and secondary ripples discussed in Section 5.5.

Figure 11 visualizes the computed temperature distribution at the symmetry plane $y = 0$ and at time $t = 12$ s. It can be seen that the three EMF models result in different convection of the heat transferred to the workpiece by the arc and the metal drops. The heat is convected deeper into the material and over a wider extent with the Kou and Sun model compared to the numerical EMF model. It shows that the overestimation of the amplitude of $(F_{Em2})$ made by the Kou and Sun model due to assumption (xi) through neglecting the contribution of $J_x$ to $B_x$ enhances the thermal convection towards the melt pool depth. With the model of Tsao and Wu the heat transferred to the material is instead confined to the close vicinity of the free surface. It shows that for this EMF model the underestimation of $(F_{Em2})$ in the upper part of the melt pool.
The maximum temperature of the metal is also affected by the EMF model used. Its value is about 2800 K with the numerical EMF model and the Kou and Sun model, and about 2500 K with the Tsao and Wu model. These values, that are at the free surface, are at least 300 K lower than the vaporization temperature of the main constituents of the studied alloy. The computed effect of vaporization is insignificant for the melt pool in terms of both energy and mass loss. It confirms that material loss can be neglected, as done in the model (Section 3.1). Besides, a higher maximum temperature is known to strengthen the thermocapillary force, and is expected to result in a larger fluid velocity. Thus, it could explain
why the RMS value of \( u_{\text{max}} \) obtained with the Tsao and Wu model is lower than with the two other models.

5.4. Effect of the EMF models on the melt pool geometry

Figure 12 presents the time evolution of the melt pool half-width, penetration depth and half-volume computed with the three EMF models. The results from the different models share in common that at the start of the process the melt pool width and volume increase almost linearly for about 1 s until the trailing edge of the initially circular melt pool begins to develop. The melt pool half-width and penetration depth reach a stable condition after approximately 4 s. However, the melt pool length and volume require longer time to stabilize. The increase in melt pool volume is followed by a decrease at \( t \approx 6 \) s due to the rapid cooling when the re-solidification of the trailing edge starts. The length and volume expand over a longer time before reaching a quasi-steady condition at \( t \approx 8 \) s. The results reached at fully-developed melt pool show that the three EMF models lead to different melt pool dimensions. The model of Tsao and Wu leads to a wider and shallower melt pool with smaller volume than the two other EMF models. The model of Kou and Sun instead produces a narrower and deeper melt pool with a volume slightly larger than the numerical EMF model. These geometrical differences result from the distinct effect on the thermal flow of the different simplifying assumptions underlying the EMF models studied. For instance, the most shallow melt pool observed with the model of Tsao and Wu is a consequence of the quasi-absence of convective recirculation of alloy under the arc as a result of the underestimation of \( (F_p g)_y \) in the upper part of the melt pool. It can also be seen that with the model of Tsao and Wu (resp. Kou and Sun) the reduced (resp. increased) melt pool depth is not balanced by the increased (resp. reduced) width since the melt pool volume is smaller (resp. larger) than with the numerical EMF model while the total amount of heat input and its space-distribution (Eq. (32)) is the same for all the cases. The change in force balance due to the simplifying assumptions on the tail region therefore changes also the fraction of heat transferred to the workpiece that is used to melt the alloy.

Figure 13 compares the melt pool geometry computed with each of the three electromagnetic models, at time \( t = 12 \) s. The top-view images of Fig. 13a show that the largest melt pool width (at section AA') is reached downstream the arc center (located at \( x = 50 \) mm) at rather similar locations with the numerical EMF model and with the Kou and Sun model, while it is further away with the model of Tsao and Wu. The transition to the tail region is closer to section AA' with the Kou and Sun model than with the two other ones as the front area is then not only narrower.
but also shorter. The side view images in Fig. 13b show that the model of Tsao and Wu leads to a very different melt pool shape, compared to that of the other models. The largest melt pool depth (at section CC) is indeed reached much further downstream the arc center with this model than with the other ones. As noticed in Section 5.3, with this model the largest penetration depth is not governed by the same effects as for the other models. For the two other EMF models the deepest melt pool depth is reached under the arc at $x_0 = 50$ mm. According to the recirculation pattern it is believed to be mainly governed by the electromagnetic force (combined with the metal transfer). With the Tsao and Wu model the largest depth is reached at $x = 35$ mm. There, the electromagnetic force is known to be negligible. Thus, these results show that the change in proportion of the force components ($f_{\text{EMF}}^x$, $f_{\text{EMF}}^{z}$) observed in Fig. 8 when changing from e.g., the numerical EMF model to the Tsao and Wu model turn out to be large enough to induce drastic changes in the predicted melt pool morphology.

Figure 14 (a)-(b) present macrograph images of the bead along the longitudinal and transverse directions. Figure 14a shows the uniformity of the penetration depth and the reinforced bead height. Figure 14b visualizes the fusion boundary used for comparison with the computational results obtained at time $t = 12$ s with the different EMF models. Experimental measurements are also reported in Table 6 for three different samples. The accuracy of the measurements was evaluated to be ±0.1 mm due to the uncertainty in positioning the fusion boundary. The values computed with the different EMF models are also reported in this table. Their uncertainty is evaluated based on the mesh cell-size to be equal to ±0.1 mm. The computed boundaries of the reinforced bead plotted in Fig. 14c were extracted from the re-solidified surface (defined by the isosurface $\alpha = 0.5$) at the section BB' (shown in Fig. 13a).

The numerical EMF model and the Tsao and Wu model are in good agreement with the experimental data, the relative error being less than 4% compared to the average experimental value. With the Kou and Sun model the relative error is larger, reaching approximately 16%. Since the added mass (and thus volume) from the wire feed is the same for all the simulated cases, the increased reinforced height with the Kou and Sun model is correlated to the reduced melt pool width. The melt pool depth and width reach the maximum values at different distances from the arc center. The computed edge of the fusion zone is defined by the solidus isotherm. The melt pool width compared to the experimental data in Fig. 14d is plotted in section AA, and the penetration depth compared in Fig. 14e is plotted in section CC (see Fig. 13). It can be seen that the (maximum) width predicted with the numerical EMF model is in good agreement with the experimental results. With the Tsao and Wu model it is overestimated whereas with the Kou and Sun model it is underestimated. The maximum relative error between the numerical simulations and the experimental results is about 15%. Figure 14e shows that the maximum penetration depth obtained with the numerical EMF model is in very good agreement with the experimental results, with a difference of less than 3%. This is simply a direct consequence of the adjustment of the closure parameter $\sigma_{\text{arc}}$, as explained in Section 3.2. Nevertheless, the morphology of the fusion zone simulated using the numerical EMF model slightly differs from the experimental data. Besides, it can be seen that the penetration depth is overestimated by approximately 30% with the Kou and Sun model and underestimated by approximately 30% with the Tsao and Wu model. These differences are significant. Furthermore, while the depth to width ratio is correctly reproduced by the numerical EMF model, it is not by the two other models. The GMAW example of this study therefore shows that assumptions (ix)|(xii)–(xiii) as well as (xi) alter the leading order physics predicted in the melt pool.

### 5.5. Effects of the EMF models on the ripples from drop impact

The general dynamics of the surface is first discussed before going into detailed comparisons with the three EMF models. Figure 15 presents symmetry plane views of the melt pool computed with the numerical EMF model. The plots show the drop impact area at different instances in time chosen to highlight particular features within a period of metal transfer when the melt pool is fully developed. When a metal drop is transferred (see A) and enters the melt pool (B) a depression forms (C) until reaching

<table>
<thead>
<tr>
<th>Height [mm]</th>
<th>Width [mm]</th>
<th>Depth [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experimental Sample 1</td>
<td>2.5±0.1</td>
<td>10.2±0.1</td>
</tr>
<tr>
<td>Sample 2</td>
<td>2.45±0.1</td>
<td>10.3±0.1</td>
</tr>
<tr>
<td>Sample 3</td>
<td>2.6±0.1</td>
<td>10.4±0.1</td>
</tr>
<tr>
<td>Average exp. value:</td>
<td>2.5±0.1</td>
<td>10.3±0.1</td>
</tr>
<tr>
<td>Numerical</td>
<td>2.6±0.1</td>
<td>10.1±0.1</td>
</tr>
<tr>
<td>Computed Kou &amp; Sun</td>
<td>2.9±0.1</td>
<td>8.8±0.1</td>
</tr>
<tr>
<td>Tsao &amp; Wu</td>
<td>2.5±0.1</td>
<td>10.8±0.1</td>
</tr>
</tbody>
</table>

Fig. 13. Melt pool geometry computed with each EMF model; $t = 12$ s.
the maximum depression (D). The metal pushed away causes the formation of a primary ripple that moves away from the point of drop impact as time evolves (see supplementary movie S4). Next, the free surface starts restoring (E) with a central jet formation (F) resulting in a secondary ripple (G) that is still partially present when the next drop is transferred (H).

Figure 16 compares the evolution over time of the liquid alloy top-most surface, which includes both the free surface and the drop. It is computed with the different EMF models and is reported at the arc centre. This location coincides with the location of the drop impact. The figure shows two cycles of metal transfer taking place when the melt pool is fully developed. The plots start when
The drop is injected into the computational domain (in A, as in Fig. 15). A sudden increase in top-most surface elevation can be seen when a new drop is injected since at this instant the height reported in Fig. 16 includes the diameter of the drop (1.2 mm) and the space between the drop and the free surface. In B the drop has partially entered the free surface (similar to B in Fig. 15), and in C it is totally immersed and has initiated a depression at the melt pool free surface. Figure 16 shows that the depression (in D, as in Fig. 15) is the deepest with the Kou and Sun model, with a free surface lowering reaching about 1.3 mm, whereas the Tsao and Wu model leads to the shallowest lowering of only 0.5 mm. Compared to the numerical EMF model the restored height (in R) is 0.5 mm higher with the Tsao and Wu model, while it is 0.2 mm lower with the Kou and Sun model. Furthermore, the time needed to reach the deepest depression after the drop impact is the longest with the Kou and Sun model, while it is almost the same with the two other models. On the contrary, the time needed to restore the elevation as prior to impact (e.g., from D to R) is the shortest with the Kou and Sun model while it is the longest with the Tsao and Wu model. These variations are caused by the force balance at the free surface and the thickness of liquid alloy under the impact point, which are different for each of the three EMF models (see previous sections). The effect on the amplitudes and propagation of the ripples is now examined as they move away from the point of drop impact.

The primary ripple that moves towards the front side of the melt pool is reflected as it reaches the liquid/solid transition region (see S4). Along this back and forth travel, the amplitude of the ripple progressively attenuates. Towards the rear side of the melt pool, the propagation is more complex. It is now examined in more details. In the computations with the numerical and the Kou and Sun EMF models, primary and secondary ripples are observed to travel away from the point of drop impact (see S5A-B). With the model of Tsao and Wu, no secondary ripple is seen to travel away (S5C). The speed of the crests of the ripples computed with each of the models was evaluated along the travel direction, after the arc centre, from the time $t = 11.95$ s to $t = 12$ s. This time interval includes 8 cycles of metal transfer. The evaluation was made by sampling the times of passage of the crests, first at $x = 46$ mm and next at $x = 45$ mm. For the cases with secondary ripples, as the primary and the secondary ripples alternate, the crests successively detected were alternately distributed in a set $A$ and a set $B$. However, as it was difficult to determine whether the ripples passing at $x = 46$ mm were primary or secondary, the correspondence between set ($A$ or $B$) and ripple type (primary or secondary) could not be established. Nevertheless, the minimum, maximum and mean crest velocities were calculated for each set over the time interval above mentioned. The results are reported in Table 7. It can be seen that in all the cases the ripples move much faster than the welding travel speed, $V_F = 8$ mm s$^{-1}$. They also show that the primary ripples predicted by the model of Tsao and Wu are on average slightly slower (about 10%) than the slowest set ($A$) of ripples predicted by the two other models. Finally, it can be seen that when both primary and secondary ripples are present, they have different average velocities. It implies that a $B$-ripple might catch up with the $A$-ripple ahead of it.

Figure 17 presents the free surface elevation computed with the different EMF models and plotted at three locations along the travel direction over a period of 0.05 s. These locations are positioned at increasing distances after the arc center, as shown in Fig. 17a: 5 mm (point P1), 7.5 mm (P2) and 10 mm (P3). It can

**Table 7**

<table>
<thead>
<tr>
<th>Model</th>
<th>Set $A$</th>
<th>Set $B$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>mean</td>
<td>max.</td>
</tr>
<tr>
<td>Numerical</td>
<td>856.6</td>
<td>909.1</td>
</tr>
<tr>
<td>Kou &amp; Sun</td>
<td>836.7</td>
<td>1000.0</td>
</tr>
<tr>
<td>Tsao &amp; Wu</td>
<td>761.2</td>
<td>909.1</td>
</tr>
</tbody>
</table>

The velocity along the x-direction of the crest of the ripples moving towards the rear part of the melt pool, for each EMF model.


be seen in Fig. 17b that with the Tsao and Wu model a ripple passes in P1 at the frequency of 156 Hz (i.e., the drop transfer frequency). When using the numerical EMF model and the Kou and Sun model the number of ripples passing P1 at that frequency is doubled. Two ripples can clearly be distinguished with the numerical EMF model while partial overlap is observed with the Kou and Sun model. These differences are related to the location of drop impact on the secondary ripple (see S5a-c). It occurs on the crest of the secondary ripple with the model of Tsao and Wu (therefore the primary and secondary ripples are merged). With the two other models, the drop falls over a longer distance before reaching the free surface whose elevation is then lower just prior to impact (see Fig. 17). This delay permits the secondary ripple to travel, so that the drop impact takes place at some distance after the passage of the secondary crest. In the computations with the Kou and Sun model the delay is even larger than with the numerical EMF model. The delayed impact generates a surface elevation with two crests that move away from the point of impact. These two crests are more or less differentiated depending on the delay and on the point of observation (as they travel at different speeds). Figure 17c shows that when reaching further away to point P2, the primary and secondary ripples are merged for these two last models. The remaining differences are a small phase shift and the slightly larger crest elevation with the Kou and Sun model compared to the numerical one. The amplitude of the ripples predicted by the Tsao and Wu model is still clearly the smallest at P2 while it becomes the largest at P3. Ripples could be expected to lower their amplitude along their travel away from the arc center due to energy dissipation. But this is not the case here. With the numerical EMF model the ripple amplitude increases between P1 and P2, and further between P2 and P3. With the Kou and Sun model no noticeable change in ripple amplitude is seen between P2 and P3. Also, the predicted amplitude in P3 is almost the same with the Kou and Sun model as with the numerical EMF model while it is clearly overestimated by the Tsao and Wu model. Several factors can affect the ripple amplitude. Among them are the thickness of the liquid layer beneath the ripple, and the current (or flow field) within this layer. According to Fig. 13b the thickness of the liquid layer beneath the ripple is rather uniform between P1 and P3. On the other hand the recirculation flow patterns are clearly different between P1 and P3 for the three EMF models, Fig. 9b. They could contribute to the differences in the space-evolution of the ripple amplitude obtained with the three EMF models.

6. Conclusions

The three electromagnetic force models most commonly applied to fluid dynamics simulation of melt pools formed with an electric arc were investigated. One was numerical and the two others analytical (Kou and Sun [16], and Tsao and Wu [17]). The underlying assumptions were first recalled and their impact on the computed electromagnetic force studied. These models were then applied combined with a thermo-fluid model to compare their effect on the melt pool flow, geometry and ripples from drop impact during metal transfer with a gas metal arc. From the obtained results and their analysis, the following conclusions and recommendations are drawn:

1. When an electric arc is operated in conduction mode on a workpiece with local thickness $\geq$ 10 mm, it has negligible effect on the electromagnetic force acting in the melt pool area to ground the electric potential (V) at the lower surface of the workpiece rather than at the lateral ones. In these specific conditions, the analytical EMF models can therefore be applied to study a problem with V grounded at the lower surface although assumption \((\approx)-(a))\) is not satisfied, since then the electromagnetic force predicted in the melt pool is not undermined by the inappropriate grounding.

2. It should not be presumed that conclusion 1 holds also for an electric arc operated in keyhole mode. Further investigation is recommended in such case.

3. For small workpiece thickness, e.g., 4 mm, the electromagnetic force in the melt pool area is very different when changing the electric potential ground from the lower to the lateral faces. It is therefore advised to avoid using any of the analytic EMF models when the metal thickness under the arc is less than $\approx$ 10 mm and an underside electric potential ground is applied in the experiments to be simulated. The numerical EMF model (either the complete or the simplified variant) is then strongly
recommended, as it gives the freedom to set the true boundary conditions for $V$. It is stressed that if the arc is positioned above a groove e.g., a Y-groove, the thickness to consider is the root face height rather than the workpiece thickness.

4. The assumption of axisymmetric electromagnetic field (assumption (xi)) does not imply that the contribution of the radial current density ($j_r$) to the azimuthal magnetic field ($B_\theta$) is negligible in the melt pool.

5. The two analytical models and the simplified variant (based on Biot-Savart law) of the numerical EMF model do all neglect the contribution of $j_r$ to $B_\theta$ (assumption (xi)). The complete variant of the numerical EMF model (Section 2.1) is the only one among the studied EMF models that does not neglect this contribution.

6. Neglecting the contribution of $j_r$ to $B_\theta$ leads to an overestimation (in absolute value) of the components of the electromagnetic force in the melt pool area. In the studied GMAW problem this overestimation reached locally above.

7. The simplifying assumptions (xii)–(xiii), which are specific to the Tsao and Wu model, significantly change the components of the electromagnetic force in the melt pool area compared to any of the other models. These changes are in different proportions depending on the force component as well as the distance from the free surface. The discrepancy with the other (less simplified) models locally reached more than one order of magnitude in the studied GMAW application.

8. The assumptions that fundamentally distinguish each of the studied EMF models result in the prediction of different recirculation flow patterns in the GMA melt pool while using the same closure parameters (Section 4.2), as observed in the test case of this study. In turn, they result in clear differences in the computed maximum velocity amplitude, thermal convection, melt pool morphology, head dimensions and proportions, and free surface response to the metal transfer, depending on the EMF model selected.

9. Although the model of Kou and Sun (and the simplified variant of the numerical model) overestimates the electromagnetic force, it led to a satisfactory qualitative prediction of the flow recirculation, free surface response to drop impact, ripple propagation, and melt pool morphology compared to the more complete numerical EMF model (Section 2.1). These computational outputs were on the contrary significantly distorted with the model of Tsao and Wu in the investigated GMA problem while using the same closure parameters as with the other EMF models.

10. Above listed deficiencies of the electromagnetic forces predicted by the analytical models (and the simplified numerical model) can be compensated by tuning the amplitude of other forces applied by the arc on the melt pool to recover satisfying agreement with measured bead width and penetration depth (specifically under the arc). For instance, strategies already in use in the literature consist in adjusting the arc pressure (resp. the arc shear stress) to counterbalance the underestimation of the electromagnetic force along the vertical (resp. radial) direction by the Tsao and Wu (resp. Kou and Sun) model. Therefore, if the aim is to evaluate the effect of the different forces acting on the melt pool flow individually, this approach can be inappropriate since it can be biased by construction. Then, the complete variant of the numerical EMF model (Section 2.1) is instead strongly recommended.

11. As the assumptions specific to the analytical EMF models (and the simplified variant of the numerical EMF model) alter the predicted thermal flow compared to the more general numerical EMF model, this last one is recommended when seeking for a quantitative prediction of the melt pool. Yet, also this last one is based on assumptions (see Section 2.1) that may require further consideration in a future study.

Declaration of Competing Interest

The authors declare that they have no competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Credit authorship contribution statement

P. Aryal: Methodology, Software, Validation, Investigation, Visualization, Writing – original draft. F. Sikström: Conceptualization, Validation, Investigation, Writing – review & editing. H. Nilsson: Methodology, Writing – review & editing. I. Choquet: Conceptualization, Methodology, Validation, Investigation, Visualization, Writing – review & editing, Supervision.

Acknowledgments

This research work is supported by grants from the EU project - Horizon 2020: INTEGRADDE, which is gratefully acknowledged. The computations were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at NSC which is gratefully acknowledged. The authors would also like to thank Kjell Hurtig for his technical support during experiments.

Supplementary material


References


H. Hamed Zargari, K. Ito, M. Kumar, A. Sharma, Visualizing the vibration effect on the tandem-pulsed gas metal arc welding in the presence of surface tension active elements, Int. J. Heat Mass Transf. 161 (2020) 120310.


H. Hamed Zargari, K. Ito, M. Kumar, A. Sharma, Visualizing the vibration effect on the tandem-pulsed gas metal arc welding in the presence of surface tension active elements, Int. J. Heat Mass Transf. 161 (2020) 120310.


M. Benslov, Modeling the physics of interaction of high-pressure arcs with their electrodes: advances and challenges, J. Phys D 53 (2020) 013002.

Comparative study of the main electromagnetic models applied to melt pool prediction with gas metal arc: Effect on flow, ripples from drop impact, and geometry

Pradip Aryal, Fredrik Sikström, Håkan Nilsson, Isabelle Choquet


https://doi.org/10.1016/j.ijheatmasstransfer.2022.123068

This is an open access article under the CC BY-NC-ND license.
Systematic analysis of the effect on the simulated melt pool of different approaches for modelling arc pulsation

Pradip Aryal, Isabelle Choquet

Submitted to International Journal of Heat and Mass Transfer

Elsevier

Printed with permission
Tidigare avhandlingar – Produktionsteknik

PEIGANG LI Cold Lap Formation in Gas Metal Arc Welding of Steel An Experimental Study of Micro-lack of Fusion Defects, 2013:2.

NICHOLAS CURRY Design of Thermal Barrier Coatings, 2014:3.


MOHIT KUMAR GUPTA Design of Thermal Barrier Coatings A modelling approach, 2014:5.


EBRAHIM HARATI Improving fatigue properties of welded high strength steels, 2017:11.


MORGAN NILSEN Monitoring and control of laser beam butt joint welding, 2019:27.

ARBAB REHAN Effect of heat treatment on microstructure and mechanical properties of a 5 wt.% Cr cold work tool steel, 2019:28.

KARL FAHLSTRÖM Laser welding of ultra-high strength steel and a cast magnesium alloy for light-weight design, 2019:29.

EDVARD SVENMAN An inductive gap measurement method for square butt joints, 2019:30.

NAGESWARAN TAMIL ALAGAN Enhanced heat transfer and tool wear in high-pressure coolant assisted turning of alloy 718, 2019:31.

ADNAN AGIC Edge Geometry Effects on Entry Phase by Forces and Vibrations, 2020:32.

ASHWIN DEVOTTA Improved finite element modeling for chip morphology prediction in machining of C45E steel, 2020:34.


ARUN RAMANATHAN BALACHANDRANURTHI Towards understanding the fatigue behaviour of Alloy 718 manufactured by Powder Bed Fusion processes, 2020:42


ANDERS JOHANSSON Challenging the traditional manufacturing objectives: Designing manufacturing systems for both product manufacturing and value production, 2022:48.

WELLINGTON UCZAK DE GOES Thermal barrier coatings for diesel engines, 2022:49.

SEYYED MOHAMMAD ALI NOORI RAHIM ABADI Laser metal fusion and deposition using wire feedstock: Process modelling and CFD simulation, 2022:52.
Metal fusion using pulsed Gas Metal Arc: Melt pool modelling and CFD simulation

Gas metal arc (GMA) has revolutionized metal processing and production technology for several decades with its remarkable efficiency and versatility. In recent years, this technology has been increasingly applied in Additive Manufacturing (AM) due to its ability to fabricate large and complex parts. However, there are concerns associated with process-related defects and the predictive capability of the numerical models used to understand the underlying process. Thus, in-depth process understanding, and improved modelling is needed for overcoming these challenges and unlocking the full capabilities of this technology. To address this issue, numerical modelling using Computational Fluid Dynamics (CFD) was developed and applied in this work besides physical experiments to supplement the modelling work.

Based on the modelling work, it was possible to explain how the flow pattern in the melt pool and its geometry resulted in defect formations when changing the orientation of a workpiece by as little as 20° compared to the flat position. Furthermore, the state-of-the-art numerical models of the melt pool physics use distinct sub-models to compute the electromagnetic force and time-dependent behavior of a pulsed arc. These sub-models were thus comparatively analyzed to explain their significant differences when predicting the melt flow pattern, thermal convection, free surface oscillation, melt pool shape, and solidified bead geometry. The proposed improvements in modelling based on this analysis have provided more accurate prediction of the process fusion zone, signifying a promising step toward developing a more reliable and predictive simulation model.

Pradip Aryal

Pradip comes from the enchanting lands of Syangja, Nepal. He received his B. Eng degree in Aircraft Design and Engineering and his M.Sc. in Mechanical Engineering. Following his master’s, Pradip worked as a Product Design Engineer for two years. He embraced fresh challenges as he stepped into the role of a Ph.D. candidate at University West in 2019, embarking on a journey into the captivating realm of Computational Fluid Dynamics (CFD). His research delved into the intricacies of modelling the metal fusion process. His research interests include CFD, and multi-scale multi-physics simulation approach to understanding metal additive manufacturing processes.