

Influence of Oxygen Content upon Molten Pool Dynamics in Submerged Arc Welding

Insights from dynamic oxygen transport and region-specific surface tension

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Abstract

In submerged arc welding, complex oxygen transport from the flux critically governs molten-pool dynamics by altering surface tension, yet the underlying mechanisms remain poorly understood. This study addresses this critical gap by developing a comprehensive numerical framework that, for the first time, couples a multi-pathway oxygen transport model with dynamic, region-specific surface tension calculations. Analysis of simulation results across varying oxygen levels reveals that the specific oxygen level dictates the competition between centrifugal spreading and centripetal return flows. Under low oxygen conditions, spreading flow dominates, resulting in a wider molten pool. Conversely, as oxygen content increases, Marangoni convection reverses: outward spreading flow diminishes while centripetal flow intensifies, leading to a significant contraction in the molten pool width. Furthermore, higher oxygen content induces an internal vortex that drives deeper penetration and delays solidification at the rear. This work elucidates the mechanism governing the transition in flow patterns driven by oxygen content and provides a physical basis for controlling weld formation by regulating the flux oxygen supply.

Keywords

- Submerged Arc Welding
- Oxygen Transport
- Surface Tension
- Marangoni Convection
- Molten Pool Dynamics

Introduction

Submerged arc welding (SAW) serves as a cornerstone of shipbuilding and pipeline construction, renowned for its high efficiency (Refs. 1, 2). Fluxes play a pivotal role in this process by forming molten slags that shield the molten pool and govern weld quality (Refs. 3–5). While fluxes transfer various elements (e.g., O, Ti, Mn, Si) into the molten pool (Refs. 6–10), the influence of oxygen is particularly critical. Specifically, oxygen exerts profound effects on the welding process, significantly influencing both molten pool flow behavior and the mechanical properties of the weld metal (Refs. 11–14).

Extensive studies have established that oxygen, as a surface-active element, is the dominant factor governing surface flow, far outweighing the influence of other alloying elements (Refs. 15, 16). Variations in oxygen content can reverse the direction of Marangoni convection within the molten pool (from centrifugal to centripetal flow), thereby fundamentally altering the molten pool geometry and thermal distribution (Refs. 17–20). This mechanism of oxygen-induced flow reversal has been validated and leveraged across various welding techniques, such as laser and activated gas tungsten arc welding, underscoring the critical role of oxygen in determining weld formation (Refs. 19, 21).

However, molten pool flow in SAW differs significantly from that in other techniques due to two unique characteristics. First, flux decomposition (Refs. 22–24) generates an intense, localized oxygen supply via multiple pathways (Refs. 24–26), resulting in steep surface concentration gradients and a high bulk oxygen content (200–1400 ppm) (Refs. 9, 22). Second, the existence of spatially distinct surface domains introduces a level of complexity absent in other processes (Refs. 27, 28). Consequently, the molten pool dynamics are governed by region-specific surface tensions, where the gas/liquid metal surface tension, γ_{g-l} , and the slag/liquid metal surface tension, γ_{s-l} , exert distinct hydrodynamic influences in their respective zones. These factors make the characterization of oxygen transport and distribution essential for elucidating the unique dynamics of the molten pool in SAW.

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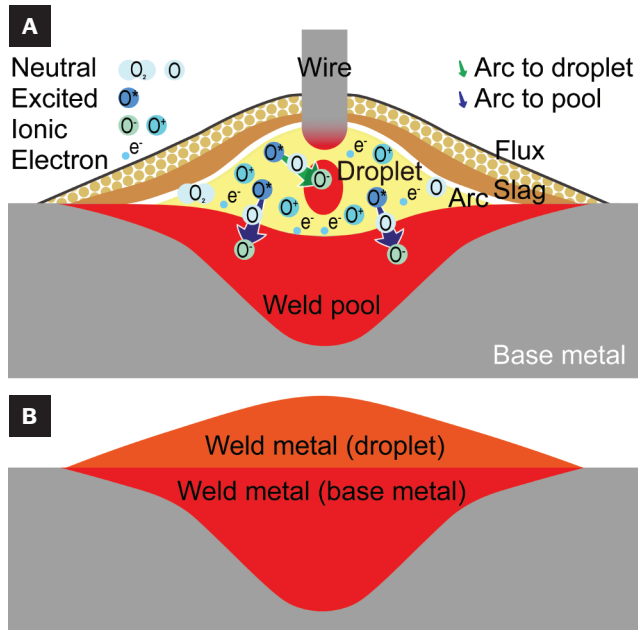


Fig. 1 – A – Schematic diagram of the oxygen state in the SAW arc cavity region; B – schematics of the weld bead transverse section.

Direct observation of oxygen distribution and internal flow fields remain challenging due to the inherent opacity and complexity of the SAW process (Refs. 29, 30). Moreover, isolating oxygen as a single variable is complicated by the fact that flux composition simultaneously influences slag characteristics and arc behavior (Refs. 31–35). Nevertheless, numerical simulation has emerged as a powerful alternative, particularly for quantitatively analyzing molten pool dynamics under well-controlled variable conditions. In other welding processes, numerical approaches have been successfully employed to reveal how oxygen content dictates Marangoni convection and molten-pool formation (Refs. 36, 37).

However, most existing models fail to adequately capture the complex conditions characteristic of SAW, specifically higher oxygen contents, multi-pathway supply mechanisms, and steeper concentration gradients. While experimental investigations into oxygen transfer between the slag and the weld metal have been conducted (Refs. 9, 24, 25), the coupled effects of oxygen transport, composition-dependent γ_{g-l} and γ_{s-l} , and the molten pool flow remains insufficiently clarified. This knowledge gap has hindered flux design strategies aimed at controllable oxygen delivery and optimized molten pool behavior.

Our group has conducted a series of interrelated studies on the effects of slag viscosity in SAW, laying the foundation for modeling the SAW molten pool (Refs. 38, 39). This study builds on our prior modeling work by establishing a comprehensive computational framework that addresses these limitations by capturing complex oxygen transport behaviors and typical oxygen content levels in the SAW pool. A salient feature of the proposed framework is a dedicated oxygen-transport model tailored for SAW, which incorporates an internal oxygen-concentration field within the molten

pool. Crucially, γ_{g-l} and γ_{s-l} are continuously updated as functions of oxygen concentration.

Subsequently, the framework is applied to simulate SAW molten pool behavior across a representative range of oxygen concentrations. The results elucidate how variations in oxygen levels alter γ_{g-l} and γ_{s-l} distributions and reshaping molten-pool flow patterns in SAW. This enhanced understanding provides a solid foundation for rational flux design and process control aimed at improving weld formation.

Computational Methods

Numerical simulations were conducted using ANSYS Fluent based on CFD theory to solve the fundamental conservation laws. As this work builds on our previous framework (Refs. 38, 39), the standard governing equations (including heat and driving force models) are provided in Appendix A for brevity. Nomenclature and material properties are listed in Appendix B (Table B1) and Appendix C (Fig. C1, Table C1), respectively. Specifically, physical models and variable properties were implemented via C-based User-Defined Functions.

In terms of modeling scope, this study focuses primarily on the continuum dynamics of the molten pool. Given the inherent complexity of the SAW process, characterized by multiphase interactions, dynamic interfaces, and the discrete-to-continuum transition of the flux, establishing a unified model that simultaneously resolves the entire physico-chemical evolution remains a significant challenge. Therefore, the complex phase transition from discrete granular flux to liquid slag and the magnetohydrodynamics of the arc plasma are not explicitly resolved as separate phases. Instead, a secondary fluid phase is introduced in the upper domain, primarily to facilitate the volume of fluid (VOF) method in capturing free surface fluctuations. Accordingly, the thermal and mechanical effects of the arc and slag are mathematically incorporated as volumetric source terms and boundary conditions acting on the metal interface. The following sections detail the simulation setup, with a specific focus on the coupled oxygen transport and region-specific surface tension model, which serves as the primary innovation.

Oxygen Transport and Region-Specific Surface Tension Model

In earlier simulations of arc-welding molten pools, oxygen concentration was often assumed to be uniformly distributed throughout the entire molten region, with a fixed value prescribed as an input (Refs. 12, 28, 36, 37). Consequently, γ_{g-l} was treated solely as a function of temperature in these studies, even though the Belton relationship (Ref. 40), expressed in Eq. 1, was introduced to account for the effect of active elements such as oxygen and sulfur.

$$\begin{aligned} \gamma_{g-l} &= \gamma^0 - A(T - T_m) \\ &- RT\Gamma_{s1} \ln \left(1 + k_O a_O e^{\frac{-\Delta H^0}{RT}} \right) \\ &- RT\Gamma_{s2} \ln \left(1 + k_S a_S e^{\frac{-\Delta H^0}{RT}} \right) \end{aligned} \quad (1)$$

While the uniform assumption applies to most arc welding scenarios, it is ill-suited for SAW due to the intense, localized oxygen supply from the flux, particularly in the arc center area (Refs. 9, 24, 25, 41). Consequently, spatially resolving the oxygen distribution is imperative to capture the resultant non-uniform driving forces.

The high Péclet number of the system ($Pe \approx 2 \times 10^5$) indicates that advection significantly dominates diffusion (Refs. 42, 43); therefore, oxygen transport within the molten pool is modeled as a purely convective process:

$$\frac{\partial a_o}{\partial t} + \nabla \cdot (\mathbf{v}a_o) = S_o \quad (2)$$

The primary challenge in applying Eq. 2 to SAW lies in the formulation of the oxygen source term, S_o . To address this, the complex physicochemical pathways (illustrated in Fig. 1A) were simplified into two dominant modes of oxygen transfer: (I) droplet transfer (arc-droplet-pool), and (II) direct surface absorption (arc-pool) (Refs. 41–45). Specifically, the oxygen content in droplets (Path I) was measured using the water-cooled copper-plate collection technique described in our previous work (Refs. 25, 45, 46). As illustrated in Fig. 1B, the weld metal consists of droplets and a portion of the base material. After determining the oxygen contents of the weld bead, droplet, and base metal, the oxygen increment per unit time $\dot{m}_o$ in Path II can be directly calculated as:

$$\dot{m}_o = v_w \rho \left[\frac{(\psi_{W_BM} + \psi_{W_d})a_{W_o}}{-\psi_{W_BM}a_{BM_o} - \psi_{W_d}a_{d_o}} \right] \quad (3)$$

Due to the absence of direct data on the spatial oxygen distribution above the molten pool, this study models oxygen transport in Path II as a uniform surface flux over the plasma arc region:

$$q_o(x, y, K_o) = K_o \frac{\dot{m}_o}{6\pi\sigma_q^2} \quad (4)$$

$$K_o = \frac{\dot{m}_o}{\iint \frac{\dot{m}_o}{6\pi\sigma_q^2} ds} \quad (5)$$

A distinguishing characteristic of the SAW process is that the molten pool surface comprises both a slag-covered region and an arc cavity region (Refs. 30, 47, 48). Consequently, distinct governing surface tension terms apply to these zones, as defined in Eq. 6 and illustrated in Fig. 2.

$$\gamma = \begin{cases} \gamma_{s-l} & \in C_\Omega[(x - v_w t)^2 + y^2 \leq L_w^2] \\ \gamma_{g-l} & \in (x - v_w t)^2 + y^2 \leq L_w^2 \end{cases} \quad (6)$$

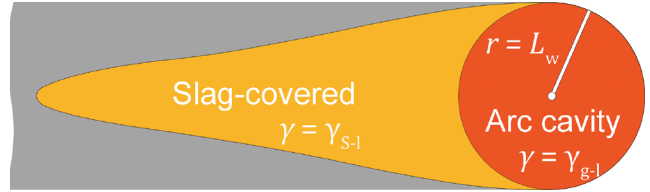


Fig. 2 — Schematic of the region-specific surface tension definition.

In this formulation, L_w denotes the effective radius of the arc cavity, defined herein as the half-width of the slag shell. This parameter delineates the surface boundary conditions: the region (arc cavity region) within this radius ($r \leq L_w$) is subject to γ_{g-l} , whereas the region (slag-covered region) beyond ($r > L_w$) is governed by γ_{s-l} . Although the arc cavity is inherently dynamic, driven by arc plasma pressure and gas expansion from flux decomposition until constrained by the slag shell (Refs. 30, 47), a static approximation is adopted because explicitly resolving such transient fluctuations remains computationally prohibitive. Consequently, γ_{g-l} and γ_{s-l} , though spatially distinct, are implemented mathematically as a unified volumetric source term acting on the continuous molten pool surface.

Moreover, although the molten pool surface is mostly slag-covered and thus governed by γ_{s-l} , oxygen remains the dominant factor controlling this term, significantly surpassing the impact of other alloying elements (Refs. 15, 16, 28, 49). Therefore, the Girifalco-Good relationship is used to determine γ_{s-l} by relating γ_{g-l} and the gas/slag surface tension γ_{g-s} (Refs. 50–52):

$$\gamma_{s-l} = \gamma_{g-s} + \gamma_{g-l} - 2\zeta_{s-l}\sqrt{\gamma_{g-s}\gamma_{g-l}} \quad (7)$$

Here, γ_{g-s} is experimentally measured as a function of temperature, while γ_{g-l} was calculated using Equation 1. ζ_{s-l} represents the interaction coefficient derived from the flux composition. It is calculated using the full mixing rule, incorporating both linear contributions from pure oxides and binary interaction effects between components:

$$\zeta_{s-l} = \sum_{i=1}^n N_i \zeta_i + \sum_{i=1}^{n-1} \sum_{j=i+1}^n N_i N_j \zeta_{ij} \quad (8)$$

In this expression, N_i and N_j denote the mole fractions of components i and j , respectively. The term ζ_i is the surface tension coefficient for the pure oxide i with the liquid metal, while ζ_{ij} represents the binary interaction parameter between components i and j , adopted from Ref. 52. Specifically, based on the molar fractions derived from the flux composition (detailed in the Experimental Procedures), ζ_{s-l} was calculated to be 0.425.

Table 1 — Experimental Baseline and Simulation Configurations for Model Validation						
Scheme Type	$a_{w,O}$ (ppm)	$a_{BM,O}$ (ppm)	$a_{d,O}$ (ppm)	$\dot{m}_O$ (kg s ⁻¹)	Oxygen Transport Model	Surface Tension Mode
Experimental Measurement	640	7	1002	N/A	N/A	N/A
Constant O Model	640	N/A	N/A	N/A	N/A	Eq. 7
O Transport Model	640	7	1002	2.22×10^{-4} (Eq. 3)	Eq. 2	Eq. 6

Table 2 — Parametric Study Cases of Oxygen Effects Using the O Transport Model				
No.	Target Condition		Calculated Model Inputs	
			$\alpha_{d,O}$ (ppm)	$\dot{m}_O$ (kg s ⁻¹)
Case 1	200	7	313	0.67×10^{-4}
Case 2	400	7	626	1.36×10^{-4}
Case 3	600	7	939	2.08×10^{-4}
Case 4	800	7	1252	2.78×10^{-4}
Case 5	1000	7	1565	3.49×10^{-4}
Case 6	1200	7	1878	4.19×10^{-4}
Case 7	1400	7	2191	4.89×10^{-4}

Simulation Strategy and Setup

The simulation strategy comprised two distinct phases: (1) model comparison and validation to confirm the successful implementation of the coupled oxygen transport and region-specific surface tension model, and (2) parametric study to investigate the influence of oxygen content systematically.

Phase I: Model comparison and validation. Input parameters for the numerical simulations were obtained following the protocols described in the Experimental Procedures section. As detailed in Table 1, simulations were conducted and compared using two distinct approaches to highlight the importance of O transport on Y_{g-I} and Y_{s-I} .

Constant O Model: This model represents a simplified approach, assuming a uniform oxygen distribution fixed at 640 ppm. Critically, it applies the Y_{s-I} defined by Eq. 7 across the entire molten pool surface.

O Transport Model: This model incorporates two key physical advancements to capture realistic SAW dynamics. First,

it implements dynamic oxygen transport, as described by Equation 2. To ensure consistency with experimental benchmarks, oxygen inputs are defined by directly assigning molten droplet (1002 ppm) and base metal (7 ppm) contents, supplemented by $\dot{m}_O$ (2.22×10^{-4} kg s⁻¹) inversely calculated via Equation 3. Second, it employs a region-specific surface tension assignment, as defined by Equation 6.

Phase II: Parametric study. Following the validation, the O Transport Model was employed to investigate the influence of oxygen content on molten pool dynamics. As listed in Table 2, seven representative cases (Cases 1–7) were designed to cover the typical oxygen range in SAW (200–1400 ppm). To ensure physical consistency, input parameters were scaled from the experimental baseline, maintaining a constant droplet-to-flux oxygen ratio.

The governing equations were solved using the pressure-based solver in ANSYS Fluent. Pressure-velocity coupling was achieved via the Pressure-Implicit with Splitting of Operators algorithm, while spatial discretization employed a Second-Order Upwind Scheme to maintain accuracy. To

explicitly resolve the transient interface of the molten pool, the VOF model was implemented using the Geometric Reconstruction Scheme. Each simulation covered a physical time of 16.0 s with a time step of 2×10^{-4} s. Performed on a dual-CPU workstation (Intel® Xeon® Gold 5215, 2.5 GHz), each case required approximately 261 hours.

Experimental Procedures

A single-electrode SAW experiment (MZS-1250, Aotai Electric Co., Ltd., China) was performed using EH36 shipbuilding steel. Welding parameters were maintained at a current of 650 A (DC), a voltage of 35 V, and a travel speed of 7.5 mm s^{-1} . Consumables consisted of a 4 mm wire (CHW-S3, Atlantic China Welding Consumables, Inc., China) and a $30\text{CaO}-10\text{Al}_2\text{O}_3-45\text{SiO}_2-15\text{CaF}_2$ (wt-%) flux. This flux composition was modified from our prior work, which employed a high-viscosity $\text{CaO}-\text{Al}_2\text{O}_3-\text{SiO}_2$ system to investigate viscous effects (Refs. 38, 39). In the present study, CaF_2 was specifically introduced to reduce slag viscosity, thereby ensuring that the influence of oxygen on γ_{s-l} was not obscured by dominant viscous forces (Ref. 54).

The physicochemical properties of the molten slag were measured using a high-temperature tester (VDR-16000, Chongqing University, China). The slag viscosity was determined to be $0.221 \text{ Pa}\cdot\text{s}$ via the rotating cylinder method, and the γ_{g-s} was measured using the immersion cylinder method. The γ_{g-s} data were subsequently fitted and extrapolated as a function of temperature (Refs. 32, 58), providing the necessary data to calculate the γ_{s-l} via Equation 7. During the welding process, molten droplets were acquired by employing the specialized water-cooled copper plate technique, as detailed in our previous study (Refs. 25, 45, 46).

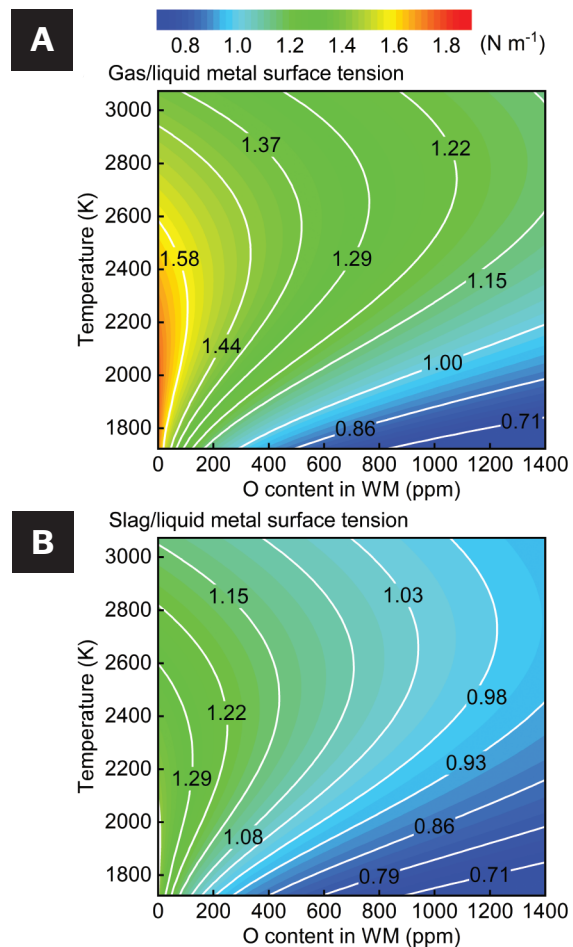


Fig. 3 — Calculated thermophysical properties used as model inputs: A — γ_{g-l} ; B — γ_{s-l}

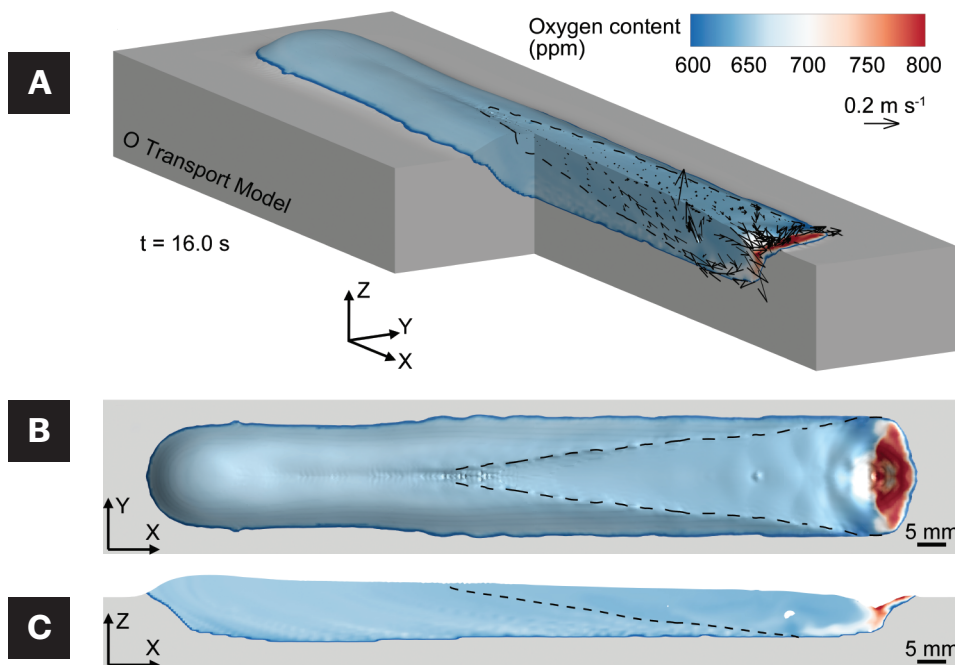


Fig. 4 — Oxygen distribution in the weld metal at $t = 16.0 \text{ s}$ by the O Transport Model: A — Three-dimensional view; B — top view; C — cross-sectional view along the symmetrical plane.

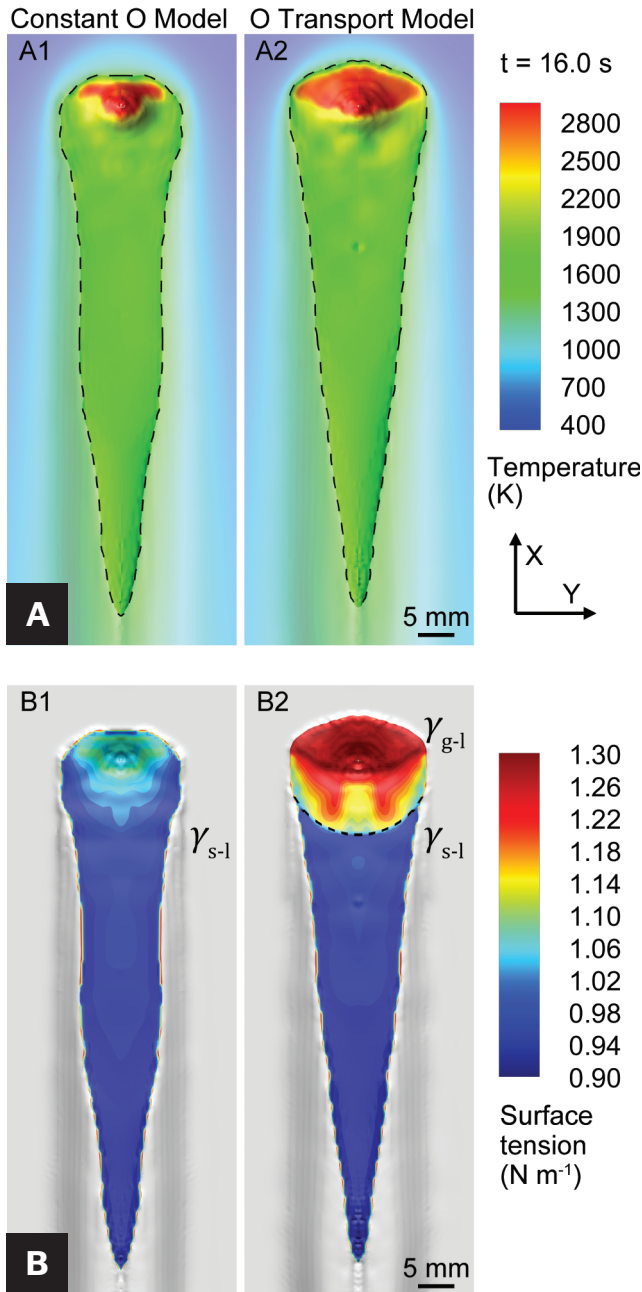


Fig. 5 — Molten pool surface: A — Temperature; B — γ_{g-l} & γ_{s-l} at $t = 16.0$ s; A1 and B1 — Constant O Model; A2 and B2 — O Transport Model.

Post-welding measurements indicated slag and wire consumption rates of 2.5 g s^{-1} and 1.9 g s^{-1} , respectively. These data were used to calculate thermal efficiency. The calculated η_a , η_s , and η_d were approximately 0.465, 0.163, and 0.192, respectively. To quantify the geometric contributions of the base metal and filler wire to the weld bead, high-resolution cross-sectional macrographs were processed using ImageJ software to measure the respective areas. The measured area of the fused base metal ($\psi_{w_{BM}}$) was 84.87 mm^2 , and the area of the deposited droplet of metal (ψ_{w_d}) was 36.00 mm^2 . These geometric parameters provide the necessary inputs for calculating the direct oxygen flux in Eq. 3. Additionally,

the solidified slag shell half-width in the quasi-steady welding stage was measured to be 0.011 m , serving as L_w .

The oxygen content was quantified using the inert gas fusion-infrared absorption method (ONH Analyzer, ONH-3000, NCS Testing Technology Co., Ltd., China) (Ref. 45). The base metal and weld metal were machined into $\Phi 3 \times 6 \text{ mm}$ cylinders using Electrical Discharge Machining, while the collected droplets were used directly. Crucially, all specimens were ground sequentially with 240 grit and 400 grit sandpapers to remove surface oxides and contaminants prior to analysis. Quantitative measurements revealed an average oxygen content of 640 ppm in the quasi-steady state region of the weld metal. Correspondingly, the oxygen concentrations in the base metal and molten droplets were determined to be 7 ppm and 1002 ppm, respectively. Additionally, to characterize the longitudinal oxygen distribution, measurements were conducted at the arc-ignition and arc-extinction zones, yielding values of 654 ppm and 788 ppm, respectively.

Results

The calculated γ_{g-l} and γ_{s-l} profiles are visualized in Fig. 3 as functions of temperature and oxygen concentration. These nonlinear curves serve as the constitutive relations that drive the Marangoni flow in the simulations.

Phase I: Model Comparison and Validation

Figure 4 illustrates the simulated oxygen distribution within the weld bead at $t = 16.0$ s using the O Transport Model. Results for the Constant O Model are excluded because it assumes a uniform oxygen field. The figure comprises a three-dimensional view (Fig. 4A), a top view (Fig. 4B), and a longitudinal cross-section along the symmetry plane (Fig. 4C). The calculated results demonstrate that the oxygen concentration exhibits a pronounced peak near the arc center, reaching a calculated maximum of 853 ppm. Conversely, beyond this localized enrichment zone, the distribution across the bulk molten pool and the solidified weld metal remains macroscopically homogeneous, approximating the baseline level of 640 ppm, with only a minor elevation to approximately 650 ppm observed in the arc ignition zone.

Figures 5A1 and 5A2 compare the surface temperature distributions at $t = 16.0$ s calculated by the Constant O and O Transport models, respectively. While both models exhibit a high-temperature zone concentrated at the front end, the O Transport Model (Fig. 5A2) yields a noticeably expanded high-temperature region and a wider pool front compared to the Constant O Model.

Figures 5B1 and 5B2 illustrate the distinct γ_{g-l} and γ_{s-l} distributions. As these stresses collectively form a unified physical field acting on the molten pool, it is physically appropriate to visualize them within a single combined contour plot to reflect the continuous nature of the driving force. To aid interpretation, a dashed line is superimposed to demarcate the distinct regimes; this graphical convention is consistently applied hereafter. In the O Transport model (Fig. 5B2), high γ_{g-l} values are localized at the leading edge, while the remain-

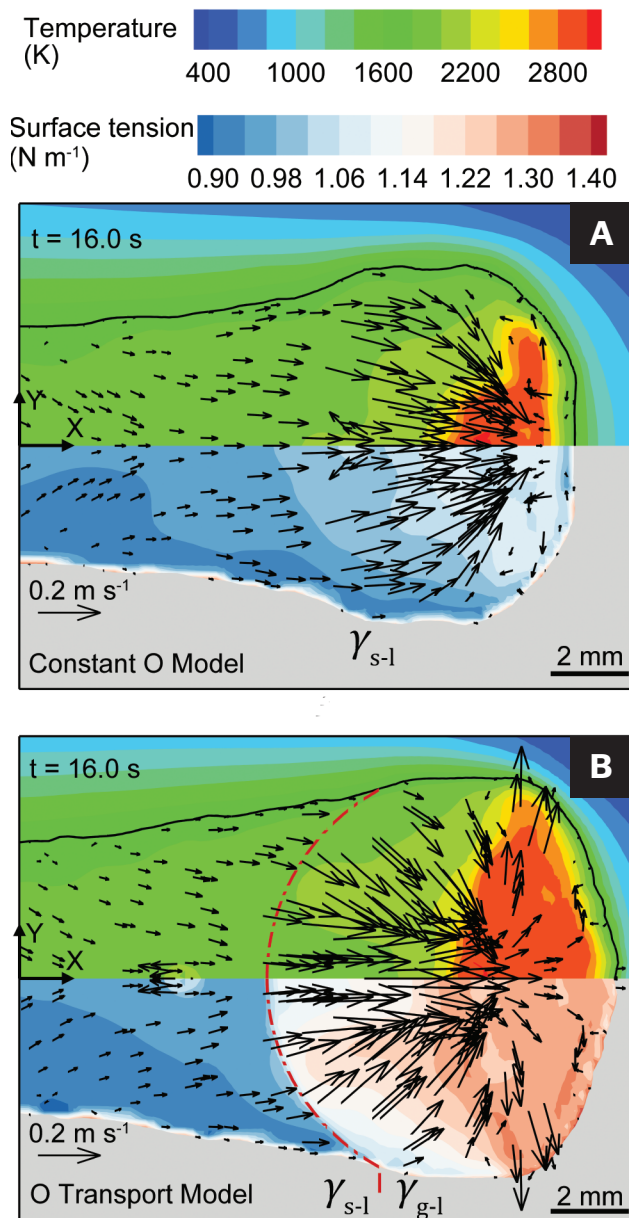


Fig. 6 — Flow conditions at the center of the molten pool surface at $t = 16.0$ s: A — Constant O Model; B — O Transport Model.

der of the pool exhibits significantly lower and uniform γ_{s-l} , establishing a sharp gradient at the boundary between the arc cavity and the slag-covered region. In contrast, the Constant O model (Fig. 5B1) presents a flatter and more uniform distribution comprising solely of γ_{s-l} . Furthermore, in the O Transport Model, distinct gradients also exist within the effective range of γ_{g-l} .

Figure 6 contrasts the surface flow dynamics at the molten pool center for the Constant O Model and the O Transport Model. In both cases, a dominant rear-to-front flow pattern is established; however, distinct differences in velocity magnitude and trajectory are evident. In the O Transport Model (Fig. 6B), flow vectors indicate significantly higher velocities. Notably, upon reaching the arc center, the high-speed

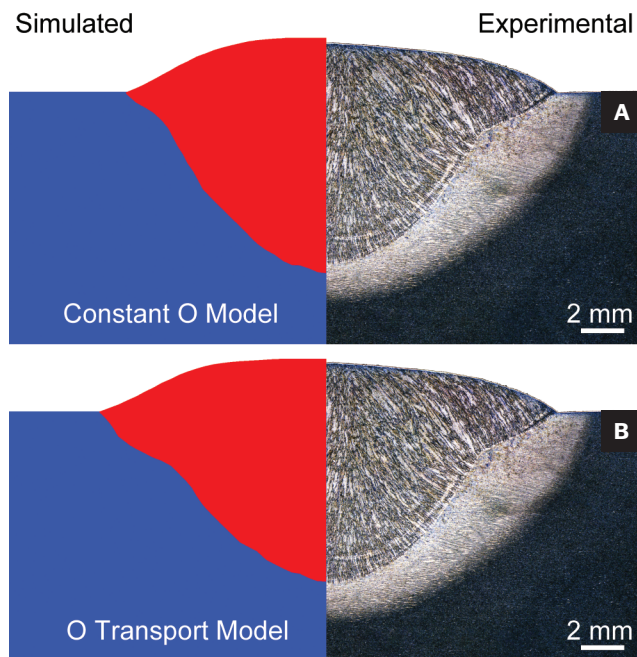


Fig. 7 — Comparison of cross-sectional weld bead profiles after experiment and simulation: A — Constant O Model; B — O Transport Model.

molten metal does not stagnate but continues to spread outward towards the pool periphery. In contrast, this outward spreading motion is absent in the Constant O Model (Fig. 6A), where flow vectors indicate a slower, more centralized recirculation pattern.

Figure 7 compares simulated weld bead profiles with a representative cross section extracted from the quasi-steady state region of the experimental weld bead. Quantitatively, the measured dimensions of this representative profile are a half-width of 10.76 mm and a penetration depth of 7.92 mm. The Constant O Model (Fig. 7A) exhibits significant deviation from this benchmark, yielding a half-width of 9.34 mm and a penetration depth of 8.53 mm. These values correspond to relative errors of -13.2% in width (underestimation) and $+7.7\%$ in penetration (overestimation). In contrast, the O transport model (Fig. 7B) produces a profile that closely matches the experimental fusion line. The calculated half-width is 10.72 mm, and the penetration depth is 7.92 mm, limiting dimensional deviations in both width and penetration to less than 0.5%.

Phase II: Parametric Study of Oxygen Effects

Figure 8 presents comparative distributions of γ_{g-l} and γ_{s-l} , temperature, and flow fields for representative oxygen levels selected from the full parametric range (200–1400 ppm). Regarding surface tension (top row), although a consistent color map is used, legend bounds are dynamically scaled to highlight gradients. A clear global trend is evident that increasing oxygen content progressively attenuates the magnitude of both γ_{g-l} and γ_{s-l} .

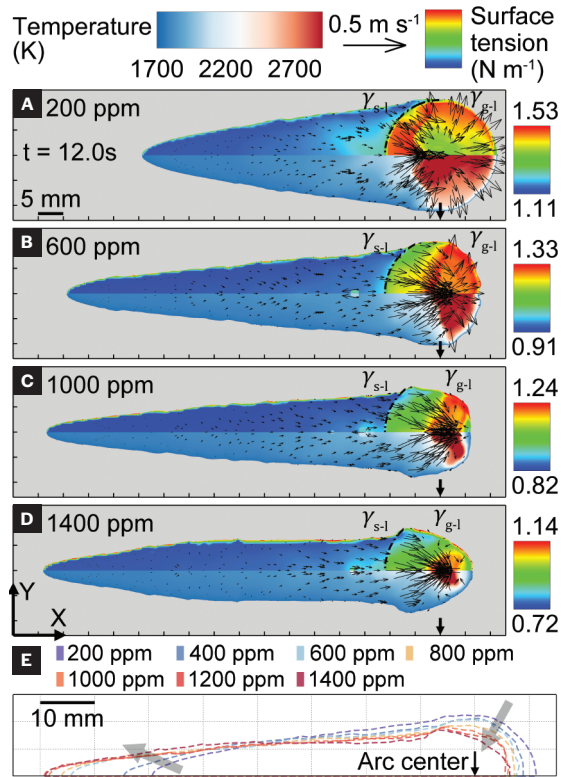


Fig. 8 — Comparison of γ_{g-l} & γ_{s-l} (top half), temperature (bottom half), and flow field on the upper surface of the molten pools using the O Transport Model with varying oxygen contents at $t = 12.0 \text{ s}$: A — Case 1 (200 ppm); B — case 3 (600 ppm); C — case 5 (1000 ppm); D — case 7 (1400 ppm); E — comparison of molten pool boundary profiles for all simulated cases (Cases 1–7). Note: Intermediate cases are omitted for brevity.

Velocity vectors reveal the evolution of the surface flow patterns. Specifically, the inward return flow originating from the molten pool rear persists across all cases. In contrast, the hydrodynamic behavior around the arc center undergoes a fundamental transition, shifting from outward spreading to inward converging. At 200 ppm (Fig. 8A), a high γ_{g-l} region near the cavity boundary drives strong outward spreading, coinciding with a broad high-temperature zone. As oxygen increases to 600 ppm (Fig. 8B), this high γ_{g-l} region shifts to the leading edge; outward flow weakens as return flow encroaches upon the cavity. At 1000–1400 ppm (Figs. 8C–D), both the high γ_{g-l} and high-temperature zones contract significantly toward the center. The spreading flow is effectively suppressed, yielding a dominant centripetal mode. This hydrodynamic shift correlates with the geometric evolution in Fig. 8E, where higher oxygen levels narrow the pool front while elongating the tail.

Figure 9 compares temperature distributions and flow fields on the longitudinal symmetry plane. Across all simulated oxygen levels, a clockwise vortex characterizes the bulk fluid motion: molten metal is directed downward from the arc center, flows along the solid–liquid boundary toward the rear, and finally recirculates toward the pool front. At 200 ppm (Fig. 9A), thermal energy remains confined near

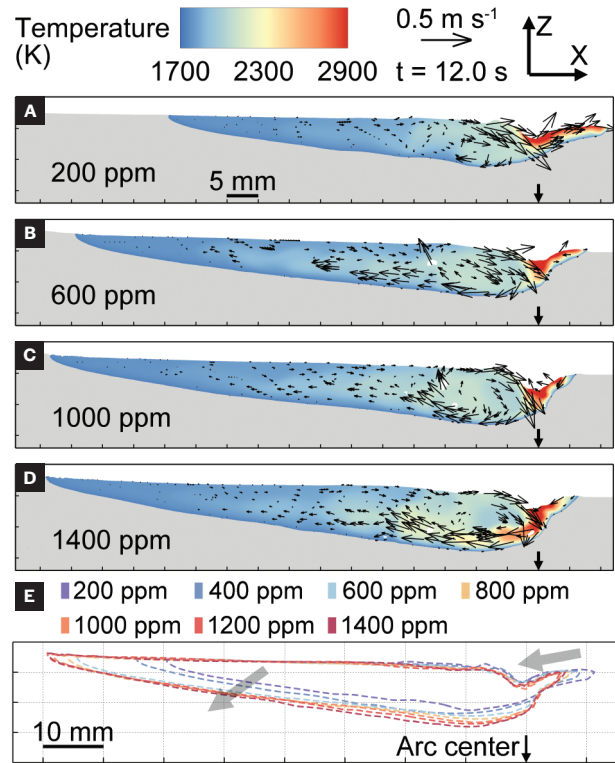


Fig. 9 — Comparison of temperature distribution and flow field on the symmetry plane of the molten pools using the O Transport Model with varying oxygen contents at $t = 12.0 \text{ s}$: A — Case 1 (200 ppm); B — Case 3 (600 ppm); C — Case 5 (1000 ppm); D — Case 7 (1400 ppm). E — comparison of internal fusion boundary profiles for all simulated cases (Cases 1–7). Note: Intermediate cases are omitted for brevity.

the free surface with a shallow vortex core. With increasing oxygen (Figs. 9B–D), however, high-temperature isotherms penetrate progressively deeper. Concurrently, the vortex core shifts downward and rearward, expanding the circulation loop until it reaches the pool bottom at 1400 ppm. This internal flow evolution aligns with the geometric profiles in Fig. 9E as higher oxygen levels increase penetration depth and tail length while narrowing the pool front.

Figure 10 presents the quantitative evolution of molten pool dimensions with increasing oxygen content. A clear monotonic trend is evident: higher oxygen levels result in narrower widths and deeper penetration. Specifically, as shown in Fig. 10A, the molten pool width decreases significantly from the baseline. The most pronounced reductions occur in the lower-to-medium oxygen ranges, notably with a decrease of approximately 1.5 mm observed between 200–400 ppm, followed by a further reduction of 2.2 mm between 600–800 ppm. Beyond 800 ppm, the rate of narrowing diminishes. In contrast, the molten pool depth (Fig. 10B) exhibits a relatively steady, near-linear increase across the entire examined range (200–1400 ppm), reaching a maximum at the highest oxygen level.

Discussion

Role Of Coupled Oxygen Transport and Region-Specific Tension

The simulation results in Fig. 4 primarily confirm the successful implementation of the O Transport Model in resolving oxygen distribution within the molten pool. Unlike the uniform assumption, the computed oxygen field exhibits a distinct topology characterized by localized enrichment near the arc center. Experimental measurements support this spatial pattern. Specifically, measurements in the arc extinction zone revealed an oxygen concentration of 788 ppm, consistent with the local enrichment trend driven by the central oxygen input mechanism. Furthermore, the arc ignition zone showed slightly elevated oxygen levels (654 ppm) compared to the steady-state baseline. This minor increase corresponds to the initial welding stage, where limited base-metal melting results in reduced dilution, leading to a localized rise in oxygen concentration.

Crucially, this non-uniform oxygen distribution physically underpins the superior accuracy of the O Transport Model, which reduces geometric error from 13% to < 0.5% (Fig. 7). The Constant-Oxygen Model fails to match this precision because its uniform assumption neglects the localized γ_{g-l} and γ_{s-l} gradients essential for SAW pool dynamics (Fig. 5B1). In contrast, as shown in Fig. 5B2, the O Transport Model establishes a sharp tension gradient at the boundary between the central γ_{g-l} zone and the peripheral γ_{s-l} zone. This gradient functions as an additional acceleration zone, which synergizes with the electromagnetic constriction force to impart significantly higher momentum to the rear-to-front flow (Fig. 6B). Driven by this immense inertia, the high-velocity fluid does not simply converge and turn downward at the arc center; instead, it redirects laterally, transforming longitudinal converging momentum into robust outward spreading. This intensified convection facilitates heat transfer to the periphery, thereby widening the weld bead while limiting excessive downward penetration. Lacking this supplementary Marangoni acceleration, the Constant-Oxygen Model remains dominated by centripetal constriction, yielding the narrower, converging flow pattern seen in Fig. 6A.

Mechanisms Governing Surface Flow Transitions

Phase II employed the O Transport Model for a parametric study (Cases 1–7; 200–1400 ppm) to investigate oxygen-induced pool dynamics. The observed flow transitions are governed by the hydrodynamic collaboration between γ_{g-l} and γ_{s-l} (Figs. 8 and 9). Specifically, the γ_{s-l} region functions as a static low-tension baseline, imposing a persistent inward pull at the zonal boundary. In contrast, the steep gradients within the γ_{g-l} region render it the dynamic determinant; its gradient direction fundamentally inverts with varying oxygen content, thereby dictating the net flow pattern.

The variation of γ_{g-l} and γ_{s-l} along the molten pool centerline is analyzed in Fig. 11 for all parametric cases. At low oxygen levels (e.g., 200 ppm), Fig. 11 reveals a distinct γ_{g-l}

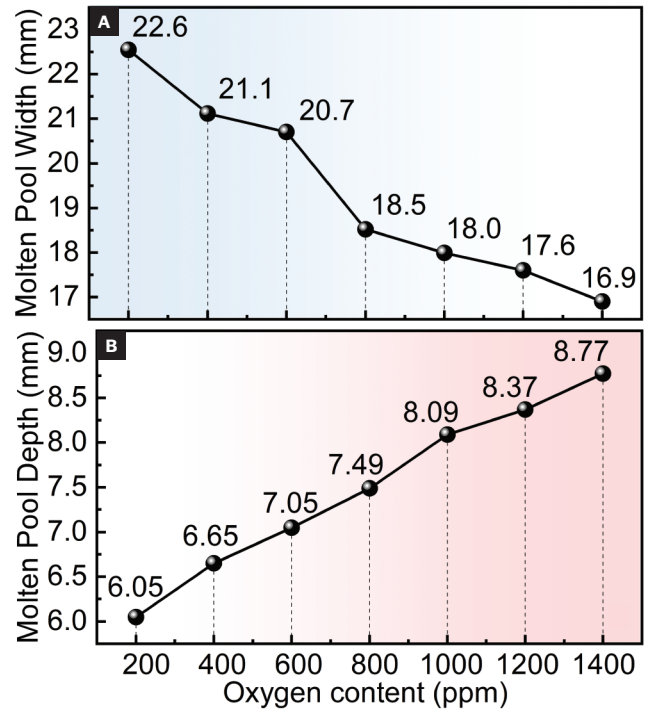


Fig. 10 — Quantitative variation of molten pool dimensions as a function of oxygen content (Cases 1–7) at $t = 12.0$ s: A — Molten pool width; B — molten pool depth.

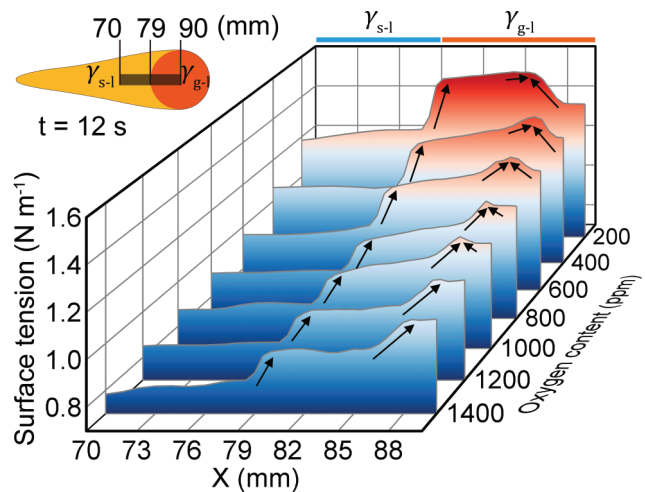


Fig. 11 — Comparison of γ_{g-l} & γ_{s-l} along the centerline from 70 to 90 mm on the upper surface of the molten pools for all parametric cases (Cases 1–7) at $t = 12.0$ s.

valley within the arc cavity. This local minimum generates a positive tension gradient pointing outward from the arc center. This centrifugal force effectively drives the dominant spreading flow observed in Fig. 8A. However, as the oxygen content increases, the central γ_{g-l} valley is progressively flattened. By 1000 ppm, Fig. 11 shows that the profile has inverted into a monotonic gradient decreasing from the center. This inversion implies that the driving force within the central region is now centripetal. Crucially, this force now

aligns synergistically with the inward pull originating from the boundary between the γ_{g-l} and γ_{s-l} zones. Consequently, the centripetal force becomes overwhelmingly dominant, establishing the vigorous centripetal flow pattern seen in high-oxygen cases (Fig. 8D).

Correlation Between Internal Hydrodynamics and Weld Profiles

The morphological evolution quantified in Fig. 10 provides direct physical evidence of the Marangoni-driven thermal transport. Under low-oxygen conditions, the dominant outward spreading flow confines high-temperature molten metal to the near-surface region. This mechanism promotes lateral thermal erosion of the base metal sidewalls, physically explaining the maximized weld width (22.6 mm at 200 ppm) despite the limited penetration. Conversely, under high-oxygen conditions, the intensified centripetal flow converges at the pool center and plunges downward, forming a deep, penetrative vortex (Fig. 9). This downward convection functions as a ‘thermal drill,’ efficiently transporting enthalpy to the pool bottom. This hydrodynamic mechanism elucidates the monotonic increase in penetration depth and the simultaneous sharp reduction in width observed in the 200–1400 ppm range, as the suppression of outward spreading effectively cuts off the lateral heat flux.

Conclusions

This study develops a comprehensive numerical framework for SAW by coupling a multi-pathway oxygen-transport model with region-specific surface-tension calculations. The key conclusions are summarized as follows:

- γ_{s-l} and γ_{g-l} assume distinct hydrodynamic roles arising from their specific distribution characteristics. The region governed by γ_{s-l} exhibits negligible internal gradients due to quasi-uniform temperature and oxygen fields, yet imposes a stable inward baseline force via the sharp tension step relative to the higher γ_{g-l} zone. Conversely, the central γ_{g-l} region is dominated by steep gradients driven by significant temperature and oxygen variations.
- Increasing oxygen content induces a fundamental reversal in the surface flow pattern by inverting the central γ_{g-l} gradient. Low oxygen levels generate a centrifugal γ_{g-l} gradient that drives outward spreading, whereas high oxygen levels invert this into a centripetal γ_{g-l} gradient, establishing a dominant inward centripetal flow.
- This flow governs the molten pool dimensions. Outward spreading promotes lateral thermal convection, maximizing width. Conversely, the high-oxygen centripetal flow creates a “thermal drill” effect that drives a monotonic increase in penetration depth while simultaneously constricting width by redirecting lateral heat.
- By integrating coupled oxygen transport and region-specific surface tensions, the proposed framework offers an enhanced physical description of the SAW process. Comparison with experimental data demonstrates that this approach successfully reproduces the weld-bead geometry, reducing the discrepancy in weld width from 13.2% to less than 0.5%.

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tion accounts for thermal buoyancy. The slag layer is treated as a continuous fluid phase; melting/solidification of the slag is neglected due to limitations of the Finite Volume Method. The governing equations for continuity, momentum (Navier-Stokes), energy, and VOF phase fraction are:

$$\nabla \cdot \mathbf{v} = 0 \quad (\text{A1})$$

$$\rho \left[\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right] = -\nabla p + \mu \nabla^2 \mathbf{v} + \mathbf{S}_f - \mu \tau \mathbf{v} \quad (\text{A2})$$

$$\rho \left[\frac{\partial h}{\partial t} + (\mathbf{v} \cdot \nabla) h \right] = \nabla \cdot (\kappa \nabla T) + S_h \quad (\text{A3})$$

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{v} \phi) = 0 \quad (\text{A4})$$

Enthalpy h and liquid fraction f_L are defined as:

$$h = \int_{T_0}^T C_p dT + f_L \Delta L_m \quad (\text{A5})$$

$$f_L = \begin{cases} 0 & (T \leq T_s) \\ \frac{T - T_s}{T_L - T_s} & (T_s < T \leq T_L) \\ 1 & (T > T_L) \end{cases} \quad (\text{A6})$$

Welding Model

The total thermal efficiency η comprises contributions from the arc η_a , droplets η_d , and slag η_s (Refs. 55, 56). In this study, η was determined to be 0.82. Specifically, this value was selected from the reasonable range reported in the literature (Ref. 2) and determined via a posteriori fine-tuning to match the experimental cross-sectional area of the weld bead.

$$Q = \eta UI = \eta_a UI + \eta_d UI + \eta_s UI \quad (\text{A7})$$

$$\eta = \eta_a + \eta_d + \eta_s \quad (\text{A8})$$

η_d is derived from the wire feed rate, and η_s from the experimental slag consumption rate:

$$\eta_s = \frac{\dot{m}_f C_{pf} (T_{m,flux} - T_0)}{UI} \quad (\text{A9})$$

$$\eta_d = \frac{\dot{m}_d \left(\int_{T_0}^{T_d} C_p dT + \Delta L_m \right)}{UI} \quad (\text{A10})$$

Appendix A: Governing Equations and Physical Models

Governing Equations and Assumptions

The molten pool dynamics are modeled under the assumptions of an incompressible, laminar, Newtonian fluid within a fixed Cartesian coordinate system. Specifically, the laminar assumption prevents the artificial damping of surface tension gradients caused by the amplification of VOF spurious currents in standard turbulence models. Symmetry allows for a half-domain simulation. The Boussinesq approxima-

The arc heat input follows a Gaussian distribution:

$$q_a(x, y, K_a) = K_a \frac{\eta_a UI}{2\pi\sigma_a^2} \exp\left(-\frac{(x - v_w t)^2 + y^2}{2\sigma_a^2}\right) \quad (A11)$$

$$K_a = \frac{\eta_a UI}{\iint_{\Omega} \frac{\eta_a UI}{2\pi\sigma_a^2} \exp\left(-\frac{(x - v_w t)^2 + y^2}{2\sigma_a^2}\right) dS} \quad (A12)$$

The Gaussian distribution parameter σ_a was set to 0.002 m based on a posteriori calibration against experimental weld cross-sections. The initial range for σ_a was selected with reference to (Ref. 57). Although directly measuring σ_a in SAW remains a significant challenge; it was kept constant across all simulations to ensure consistent heat input and enable meaningful comparison between different oxygen levels.

Slag heat input follows a ring-shaped distribution (Refs. 55, 56) defined within the radius $\sqrt{(6\sigma_a^2)} \leq \sqrt{(x - v_w t)^2 + y^2} \leq L_w$ then:

$$q_s(K_s) = K_s \frac{\eta_s UI}{\pi(L_w^2 - 6\sigma_a^2)} \quad (A13)$$

$$K_s = \frac{\eta_s UI}{\iint_{\Omega} \frac{\eta_s UI}{\pi(L_w^2 - 6\sigma_a^2)} dS} \quad (A14)$$

The arc pressure adopts the same Gaussian distribution as the arc heat model:

$$p_a(x, y, K_p) = K_p \frac{\mu_m I^2}{8\pi^2\sigma_a^2} \exp\left(-\frac{(x - v_w t)^2 + y^2}{2\sigma_a^2}\right) \quad (A15)$$

$$K_p = \frac{\mu_m I^2}{4\pi \iint_{\Omega} \frac{\mu_m I^2}{8\pi^2\sigma_a^2} \exp\left(-\frac{(x - v_w t)^2 + y^2}{2\sigma_a^2}\right) dS} \quad (A16)$$

In the VOF method, the interface is treated as a finite-thickness transitional region rather than an idealized zero-thickness surface. All surface forces are converted to volumetric sources via the Continuum Surface Force model.

The electromagnetic force is specifically represented by components in the XYZ axis direction:

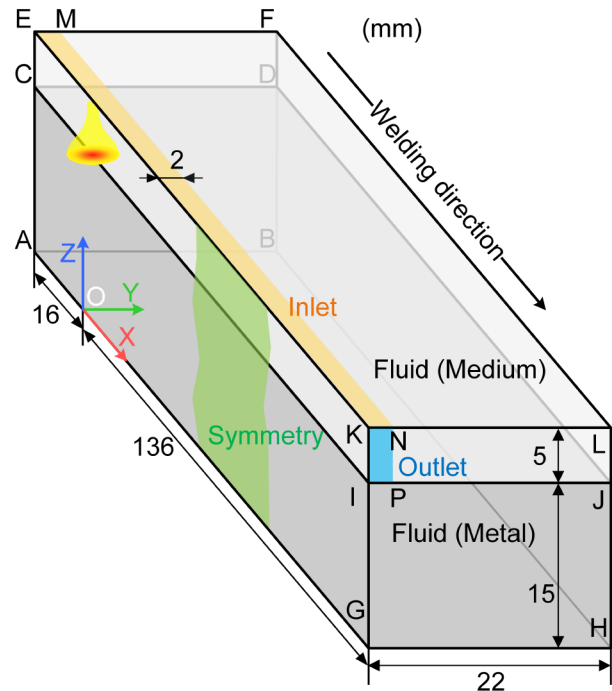


Fig. A1 – Schematic diagram of the computational domain for SAW.

Table A1 – Boundary Conditions External to the Computational Domain

	Momentum	Energy
Pressure Outlet (IKNP)	Atmosphere Pressure	$T = 300 \text{ K}$
Symmetry (AEKG)	$V_y = 0, \partial V_x / \partial y = 0, \partial V_z / \partial y = 0$	$\partial T / \partial \mathbf{n} = 0$
Metal Side Surface (ACDB, BDJH, GIJH, and ABHG)	$\mathbf{v} = 0$	$k \partial T / \partial \mathbf{n} = k(T_{n+1} - T_n) / \Delta y$ (Ref. 58)
Medium Side Surface (CEFD, DFLJ, PNLJ, and MFLN)	$\mathbf{v} = 0$	$k \partial T / \partial \mathbf{n} = h_c(T - T_o)$

$$r = \sqrt{(x - v_w t)^2 + y^2} \quad (A17)$$

$$J_z = \frac{I}{2\pi} \int_0^\infty \lambda J_0(\lambda r) \exp\left(-\frac{\lambda^2 \sigma_a^2}{2}\right) \frac{\sinh(\lambda z)}{\sinh(\lambda \Omega(x, y))} d\lambda \quad (A18)$$

$$J_r = \frac{I}{2\pi} \int_0^\infty \lambda J_1(\lambda r) \exp\left(-\frac{\lambda^2 \sigma_a^2}{2}\right) \frac{\cosh(\lambda z)}{\sinh(\lambda \Omega(x, y))} d\lambda \quad (A19)$$

$$B_\theta = \frac{\mu_m I}{2\pi} \int_0^\infty J_1(\lambda r) \exp\left(-\frac{\lambda^2 \sigma_a^2}{2}\right) \frac{\sinh(\lambda z)}{\sinh(\lambda \Omega(x, y))} d\lambda \quad (A20)$$

$$F_{Ex} = -J_z \times B_\theta \frac{x - v_w t}{r} \quad (A21)$$

$$F_{Ey} = -J_z \times B_\theta \frac{y}{r} \quad (A22)$$

$$F_{Ez} = -J_r \times B_\theta \quad (A23)$$

In the vertical direction, gravity and thermal buoyancy are also taken into consideration:

$$F_b + F_g = \rho g \beta (T - T_0) - \rho g \quad (A24)$$

The above volumetric forces are incorporated as source terms.

Geometric Configuration

The computational domain (152 mm × 22 mm × 20 mm; see Fig. A1) is meshed with 1.045 million hexahedral elements (0.4 mm in size). The domain comprises a metal phase ($Z \in [0, 15]$ mm) and a secondary medium phase ($Z \in [15, 20]$ mm).

Boundary Conditions

Droplet transfer is simulated via a pulsed velocity inlet (EMNK) at constant temperature (3000 K). Additionally, the oxygen content of the droplet, denoted as α_{o_d} , represents the oxygen contribution along path I.

$$\phi(v_{inlet}, f_{droplet}, t) = \begin{cases} 1 & v_{inlet} t - \frac{v_{inlet} \text{floor}(f_{droplet} t)}{f_{droplet}} \leq \frac{4}{3} r_{inlet} \\ 0 & v_{inlet} t - \frac{v_{inlet} \text{floor}(f_{droplet} t)}{f_{droplet}} > \frac{4}{3} r_{inlet} \end{cases} \quad (A25)$$

$$\phi_{IJKL} = \begin{cases} \phi(v_{inlet}, f_{droplet}, t) & (x - v_w t)^2 + y^2 \leq r_{inlet}^2 \\ 0 & (x - v_w t)^2 + y^2 > r_{inlet}^2 \end{cases} \quad (A26)$$

$$f_{droplet} = \frac{\dot{m}_d}{\pi r_{inlet}^2 \alpha \rho} \quad (A27)$$

Other boundary conditions are listed in Table A1.

Appendix B: Nomenclature

Table B1 — Nomenclature and Constants Used in the Simulation Model

Symbol	Nomenclature
A	Temperature coefficient of surface tension for pure metal ($\text{N m}^{-1} \text{K}^{-1}$)
a_o, a_s	Concentration of active elements O, S (mass-%)
B_θ	Magnetic field angular component (T)
C_p	Specific heat ($\text{J kg}^{-1} \text{K}^{-1}$)

Table B1 -continued

Symbol	Nomenclature
F_b	Buoyancy (N m^{-3})
F_g	Gravity (N m^{-3})
F_{Ex}, F_{Ey}, F_{Ez}	EMF component in x, y, z direction (N m^{-3})
f_{droplet}	Droplet transfer frequency
f_L	Liquid fraction
g	Gravitational acceleration (m s^{-2})
ΔH^0	Standard heat of adsorption (J mol^{-1})
h	Enthalpy (J kg^{-1})
h_c	Convective heat transfer coefficient ($\text{J m}^{-2} \text{s}^{-1} \text{K}^{-1}$)
I	Arc current (A)
J_0, J_1	Zero and one order Bessel function
J_r, J_z	Current density radial and vertical component (A m^{-2})
K_a, K_s, K_p, K_o	Global control parameter
κ	Thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$)
k_o, k_s	Rate constant related to entropy of segregation
L_w	Slag shell half width (m)
ΔL_m	Melting latent heat (J kg^{-1})
$\dot{m}_p, \dot{m}_d$	Flux and wire consumption rate of flux (kg s^{-1})
$\dot{m}_o$	Oxygen increment per unit time (kg s^{-1})
$\mathbf{n}$	Normal of free surface (m)
N_p, N_j	Mole fractions of components
p_a	Arc pressure (N m^{-2})
Q	Total effective thermal power (W)
q_a, q_s	Arc and slag heat flux (W m^{-2})
q_o	oxygen mass flux ($\text{kg m}^{-2} \text{s}^{-1}$)
R	Gas constant ($\text{J mol}^{-1} \text{K}^{-1}$)
r_{inlet}	Radius of the molten droplet (m)

Table B1 -continued

$\mathbf{S}_f$	Momentum source term (N m^{-3})
S_h	Energy source term (W m^{-3})
S_0	Scalar source term ($\text{kg s}^{-1} \text{m}^{-3}$)
T	Temperature (K)
T_0	Ambient temperature (K)
T_L, T_S	Liquidus and solidus temperature (K)
T_d	Droplet temperature (K)
$T_{m, \text{flux}}$	Slag temperature (K)
t	Time (s)
U	Arc voltage (V)
$\mathbf{v}$	Velocity vector (m s^{-1})
v_{inlet}	Velocity of the droplet (m s^{-1})
v_w	Welding speed (m s^{-1})
Γ_{s1}, Γ_{s2}	Surface excess at saturation (mol m^{-2})
α	Height of the droplet cylinder in the velocity inlet (m)
β	Expansion coefficient (K^{-1})
γ_{g-l}	Gas/liquid metal surface tension (N m^{-1})
γ_{s-l}	Slag/liquid metal surface tension (N m^{-1})
γ_{g-s}	Gas/slag surface tension (N m^{-1})
γ^0	Surface tension of pure metal at the melting point (N m^{-1})
η	Total thermal efficiency
η_a, η_s, η_d	Arc, slag, and droplet thermal efficiency
μ	Viscosity ($\text{kg m}^{-1} \text{s}^{-1}$)
μ_m	Permeability (H m^{-1})
ζ_i	Surface tension coefficient for the pure oxide
ζ_{ij}	binary interaction parameter between components
ζ_{s-l}	Surface tension coefficient
ρ	Density (kg m^{-3})

Table B1 -continued

Symbol	Nomenclature
σ_a	Gaussian distribution parameter (m)
τ	Momentum decay coefficient (m^{-2})
ϕ	Phase fraction
$\psi_{W,BM}, \psi_{W,d}$	Area of base metal and molten droplets comprising the weld bead (m^2)
Ω	free surface function

Appendix C: Parameters

Table C1 – Constant Physical Parameters of the Base Metal

Properties	Value
Density (kg m^{-3})	7270
Liquidus Temperature (K)	1787
Solidus Temperature (K)	1738
Latent Heat of Fusion (J kg^{-1})	2.72×10^5
Expansion Coefficient (K^{-1})	1.2×10^{-5}
Magnetic Permeability (H m^{-1})	1.26×10^{-6}

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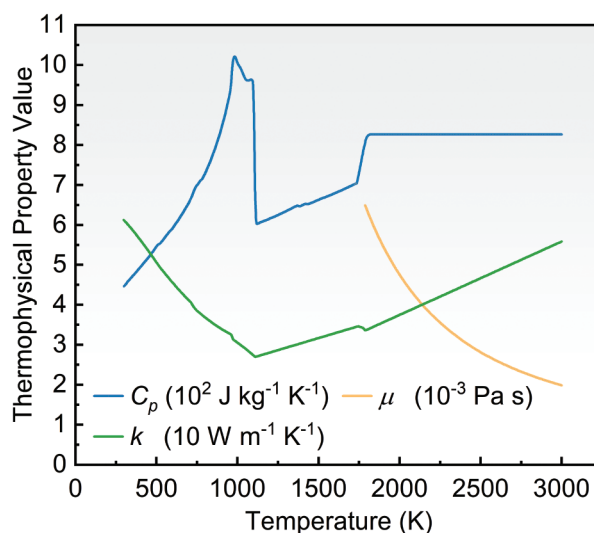


Fig. C1 – Temperature-dependent thermophysical properties.