

Environmentally Guided Optimization of Nano-Flux Activated Tungsten Inert Gas Welding: A Hybrid Experimental and Machine Learning Framework

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Abstract

Sustainable manufacturing increasingly requires a comprehensive understanding of the environmental consequences associated with process-level decisions in advanced welding technologies. In nano-flux activated tungsten inert gas (A-TIG) welding, variations in process parameters can simultaneously influence weld characteristics, electricity consumption, processing time, and auxiliary material use, highlighting the need to consider technical and environmental performance together. This study develops an integrated experimental–computational framework combining design of experiments (DoE), life cycle assessment (LCA), sensitivity analysis, response surface methodology (RSM), and machine learning (ML) to evaluate and optimize nano-flux A-TIG welding of AISI 316L stainless steel. A total of 37 welding experiments were conducted using central composite and Box–Behnken designs by varying welding current, travel speed, and $\text{SiO}_2/\text{TiO}_2$ nano-flux composition. Cradle-to-gate environmental impacts were quantified in SimaPro using the EPD 2018 method and the Ecoinvent 3 database. Latin hypercube sampling (LHS) was employed to expand the parameter space and support global sensitivity analysis and surrogate-model development. The results showed that welding current was the dominant contributor to most environmental impact categories, whereas increasing travel speed generally reduced environmental impacts through lower electricity consumption and shorter welding time. Nano-flux composition exhibited weaker but nonlinear effects, particularly on photochemical ozone creation potential. RSM-based optimization identified 75% SiO_2 , 115 A, and 110 mm min^{-1} as the preferred operating condition, providing a balance between weld geometry and environmental performance. The developed ML surrogate models achieved high predictive accuracy, with R^2 values exceeding 0.90 for most impact categories, enabling rapid sustainability-oriented evaluation of process conditions without repeated LCA simulations.

1. Introduction

Activated tungsten inert gas (A-TIG) welding is an assisted variant of the conventional tungsten inert gas process in which a thin layer of activating flux is applied to the workpiece surface prior to welding [1, 2]. Such nano-scale flux layers have also been explored in other manufacturing and surface-engineering processes [3]. In A-TIG welding, the activating flux enhances weld penetration through arc constriction, reversal of Marangoni-driven fluid flow, and other reported mechanisms affecting heat transfer and molten pool dynamics, thereby enabling significantly deeper penetration compared with conventional TIG welding [4, 5]. For stainless steels and other difficult-to-weld alloys, these advantages make A-TIG attractive for improving productivity, limiting distortion, and reducing joint preparation requirements [6–8].

Recent research has increasingly focused on nano-sized activating fluxes, particularly TiO_2 - and SiO_2 -based formulations, because of their strong surface activity and their influence on bead shape, penetration, and microstructure [9, 10]. Previous studies on nano-flux A-TIG welding have primarily focused on weld geometry and mechanical performance, while Machine Learning (ML), Design of Experiments (DoE), and Response Surface Methodology (RSM) have been widely applied for welding optimization [11–14]. In parallel, Data-driven surrogate modeling has emerged as a computationally efficient approach for accelerating repetitive Life Cycle Assessment (LCA) calculations [15]. However, the environmental implications of process parameter variation in nano-flux A-TIG welding, particularly through integrated LCA–ML frameworks, remain largely unexplored.

This gap is important because the environmental burden of welding is strongly affected by process settings such as current, travel speed, shielding gas consumption, electricity demand, and auxiliary material use [16, 17]. LCA provides a systematic way to quantify these burdens, but single-point LCA comparisons are not sufficient to describe how impacts change across a process window [18, 19]. In addition, repeated LCA calculations can be expensive when many parameter combinations must be evaluated. For this reason, sensitivity analysis and surrogate modeling can be valuable complements to LCA, allowing broader exploration of the design space and faster prediction of environmental performance [20].

Accordingly, this study develops an integrated DoE–LCA–sensitivity–RSM–ML framework for nano-flux A-TIG welding of AISI 316L stainless steel. Experimental data from central composite design (CCD) and Box–Behnken design (BBD) were used to build parameterized life cycle inventories and evaluate weld geometry. Latin Hypercube Sampling (LHS) expanded the parameter space for sensitivity analysis and surrogate model training. The resulting trends guided RSM optimization toward conditions that reduce impact while maintaining acceptable weld geometry.

2. Experimental Methods

2.1. Experimental design and welding data

Bead-on-plate Activated tungsten inert gas (A-TIG) welds were produced on AISI 316L stainless steel to investigate the effects of welding current, travel speed, and activating flux composition on weld geometry and environmental performance. The welding experiments were conducted using a non-consumable tungsten electrode and 99% argon shielding gas. No filler metal was used, and each weld was produced over a 100 mm length. The activating flux consisted of nano-sized SiO₂ and TiO₂ powders with particle sizes of 20–30 nm dispersed in methanol to form a homogeneous paste. The mixture was stirred at 600 rpm for 20 min at 20°C and applied uniformly over a 10 × 100 mm area on the steel surface. The weld region was bounded using adhesive tape, and the flux layer thickness was controlled using a 0.2 mm gauge to improve repeatability. Welding was performed using a Gaam Electric PSQ250 AC/DC power source equipped with a single-axis motion system for travel speed control (Fig. 1). The experimental factors and their ranges are listed in Table 1. Welding current and travel speed were treated as continuous variables, while flux composition was defined by the SiO₂/TiO₂ fraction. The experimental campaign was designed using a combination of CCD and BBD. For each experimental run, weld bead width (WBW) and depth of penetration (DOP) were measured from polished cross-sections. These responses were selected to characterize weld geometry, since greater penetration and smaller bead width are generally desirable for improved joint efficiency and reduced heat-affected zone overlap in multi-pass welding [21, 22].

Table 1
Process parameters and their ranges used in the A-TIG welding experiments

Parameter	Value / Range	Unit	Type
Welding current	80 – 160	A	Variable
Travel speed	80 – 120	mm.min ⁻¹	Variable
SiO ₂ /TiO ₂ fraction	0 – 100	%	Variable
Shielding gas	Argon	–	Constant
Gas flow rate	10	L.min ⁻¹	Constant
Arc length	3	mm	Constant
Electrode diameter	2.4	mm	Constant
Torch angle	90	°	Constant
Weld length	100	mm	Constant

2.2. Life Cycle Assessment

Life Cycle Assessment (LCA) is an internationally standardized methodology for evaluating the potential environmental impacts associated with a product, process, or service throughout its life cycle. It provides a systematic framework for defining the assessment objective, compiling life cycle inventory data, evaluating environmental impacts, and interpreting the results. LCA has been increasingly applied to manufacturing and welding processes to assess their environmental

performance and identify important process-level contributors. In the present study, the LCA framework was implemented in accordance with the principles established in ISO 14040 [23], while the methodological requirements and guidelines specified in ISO 14044 were followed throughout the assessment [24]. The overall LCA framework adopted in the present study is illustrated in Fig. 2.

The first phase of the assessment involves defining the goal and scope of the study, including the objective, intended application, system boundary, and Functional Unit (FU), which serves as the reference basis for all environmental calculations. Careful definition of these elements is particularly important when applying LCA to emerging or process-specific technologies, for which system boundaries and inventory assumptions can substantially affect the assessment results [25]. Depending on the purpose of the assessment, different system boundaries may be adopted, including cradle-to-gate and cradle-to-grave approaches. In the present study, a cradle-to-gate system boundary was selected to evaluate the environmental performance of the Activated tungsten inert gas (A-TIG) welding process. Accordingly, the assessment included the upstream production of the AISI 316L stainless-steel plate, ER316L filler wire, activating flux, shielding gas, electricity generation, and the foreground A-TIG welding process, while the use phase, recycling, and end-of-life treatment were excluded. The FU was defined as the production of a continuous 100 mm bead-on-plate A-TIG weld on AISI 316L stainless steel using a 100 × 50 × 5 mm substrate.

The second phase, Life Cycle Inventory (LCI), involves the systematic compilation and quantification of all relevant input and output flows associated with the product system. Previous life cycle assessments of manufacturing processes have demonstrated the importance of accounting for material consumption, energy requirements, and associated process flows when quantifying environmental burdens [26]. Comparative assessments of industrial processes have likewise shown that process energy demand and resource consumption can strongly influence the resulting environmental profile [27]. In the present study, the foreground inventory was established using experimentally measured process data, including the consumption of electrical energy, AISI 316L base metal, ER316L filler wire, activating flux, methanol solvent, and argon shielding gas during the A-TIG welding process. Electrical energy consumption was quantified using experimentally measured arc voltage together with an engineering model for total machine input power calibrated against rated inverter performance. The electrical energy consumption per weld was calculated according to Eq. (1) where P_{in} is the total input power (W) and where t_{weld} is the welding time (min), calculated as 100 divided by the travel speed.

$$E_{total} = \frac{P_{in} \cdot t_{weld}}{60,000}$$

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For shielding gas, a constant argon flow rate of 10 L.min⁻¹ was used. The mass of argon consumed per weld was determined from the welding time, volumetric gas flow rate, and argon density according to Eq. (2):

$$m_{Ar} = Q \cdot t_{weld} \cdot \rho_{Ar}$$

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where m_{Ar} is the mass of argon consumed per weld, Q_{Ar} is the volumetric gas flow rate, t_{weld} is the welding time, and ρ_{Ar} is the density of argon. As an illustrative case, a representative welding condition of 120 A, 100 mm min⁻¹, and 50% SiO₂ resulted in an electrical energy consumption of approximately 0.042 kWh per weld. The activating flux was prepared by mixing SiO₂ and TiO₂ nanopowders with methanol as a solvent. The flux composition varied from 0 to 100% SiO₂, with powder masses and methanol volumes linearly interpolated between five discrete mixture ratios. A methanol density of 0.791 g.mL⁻¹ was used to determine its mass contribution. Flux preparation was performed using a magnetic stirrer, with its electricity consumption measured as 0.001 kWh per weld. All welding runs were conducted on AISI 316L substrates using a constant base-metal mass of 0.196 kg per 100 mm bead length. TiO₂ and SiO₂ nanoparticles were modeled as foreground materials within the LCA. The material-specific assumptions for nanoparticle production were developed from

published studies addressing the synthesis of silica and titanium dioxide nanoparticles. For SiO_2 , reported synthesis routes and material characteristics were considered when defining the representative production pathway [28], while recent studies have provided additional information on alternative preparation routes for TiO_2 nanoparticles [29]. A recent synthesis study of SiO_2 nanoparticles obtained from natural sand was also considered in defining the representative silica production route adopted in the present inventory [30]. Because the experimental work was conducted in Iran, the electricity supply conditions were explicitly considered in the LCA model, particularly because the national electricity generation profile can influence the environmental burdens associated with electricity-intensive processes [31]. In the absence of industrial-scale inventory data for nanoparticle production under Iranian conditions, laboratory-scale production pathways reported in the literature were adapted to represent the synthesis of the nanoparticles used in the present study. For TiO_2 nanoparticles, published life cycle impact assessments covering physical, chemical, and biological synthesis routes were used to inform the environmental inventory assumptions [32]. Additional life cycle assessment studies of nanoparticle production were considered to account for the influence of synthesis conditions and process configuration on the associated environmental burdens [33]. For silica-based materials, recent comparative life cycle assessment of synthesis at different production scales was used to support the inventory assumptions adopted for the SiO_2 component [34]. Background processes were linked to the Ecoinvent 3 database, while regional relevance was incorporated through the selected electricity supply conditions and the foreground process assumptions.

The third phase, Life Cycle Impact Assessment (LCIA), converts the quantified inventory results into potential environmental impacts through characterization models. In the present study, LCIA was performed using the EPD 2018 method in SimaPro 9.1 with the Ecoinvent 3 cut-off database. The midpoint impact categories evaluated were acidification, eutrophication, global warming potential (GWP), photochemical oxidant creation potential (POCP), abiotic depletion of elements (ADE), abiotic depletion of fossil fuels (ADF), water scarcity, and ozone depletion potential (ODP).

2.3. LHS-Based Sensitivity and Surrogate Modeling

Latin hypercube sampling (LHS) is a space-filling sampling technique that enables efficient exploration of a multidimensional input space by distributing sample points across the defined ranges of the input variables [35]. To extend the discrete experimental design to a continuous parameter space, LHS was used to generate 200 parameter combinations within the ranges of welding current, travel speed, and $\text{SiO}_2/\text{TiO}_2$ flux composition. The sampled space covered welding currents from 80 to 160 A, travel speeds from 80 to 120 $\text{mm}\cdot\text{min}^{-1}$, and flux compositions from 0 to 100%. The application of LHS for efficient exploration of welding-process parameter spaces has recently been demonstrated in both wire arc additive manufacturing and laser welding studies [36, 37]. The generated LHS points were then evaluated using the parameterized LCA model to obtain the corresponding environmental impact indicators, thereby generating an expanded synthetic dataset covering the process design space. To represent flux composition as a continuous variable, powder masses and methanol volumes were linearly interpolated between the experimentally defined formulations containing 0, 25, 50, 75, and 100% SiO_2 . These discrete formulations were retained as the experimental reference points for subsequent validation. The resulting LHS–LCA dataset was subsequently used for sensitivity analysis and machine-learning surrogate modeling. Sensitivity assessment combined distribution analysis, Spearman rank correlation, and multiple linear regression with interaction terms to identify the dominant environmental drivers and the direction of their effects across the investigated design space. The use of space-filling sampling followed by sensitivity analysis has also been reported in recent welding-process studies to quantify the influence of process variables and their interaction effects [38].

The LHS-based sensitivity assessment indicated that welding current had a dominant positive influence on most environmental impact indicators, whereas increasing travel speed generally reduced the predicted impacts. These findings were incorporated into the RSM-based optimization framework by introducing preferential weighting toward lower current and higher travel speed while retaining weld quality as the primary optimization objective. In this manner, environmental considerations were incorporated into the optimization process without replacing the primary geometric response

functions, namely depth of penetration (DOP) and weld bead width (WBW). This approach allowed the optimization framework to account for the environmental implications of process conditions while maintaining weld geometry as the principal performance criterion.

To enable rapid prediction of environmental impacts throughout the investigated parameter space, machine-learning regression models were developed using the LHS–LCA dataset. The input variables were welding current, travel speed, and flux composition ($\text{SiO}_2/\text{TiO}_2$ fraction), while the outputs were the midpoint environmental impact indicators obtained from the LCA model. Six regression algorithms were evaluated, including Polynomial Regression, Random Forest (RF), Gaussian Process Regression (GPR), Support Vector Regression (SVR), Extreme Gradient Boosting (XGBoost), and Artificial Neural Networks (ANN). These models were selected to represent a range of learning approaches with different levels of complexity, flexibility, and interpretability.

The LHS dataset was divided into training (80%) and testing (20%) subsets using a fixed random seed. Prior to model development, the dataset was screened using Z-score analysis and isolation-based outlier detection, and no significant anomalous observations were identified. Model performance was evaluated on the held-out test set using R^2 , RMSE, and MAE, while 5-fold cross-validation was applied to the training subset to assess model robustness. The 37 experimental observations obtained from the CCD and BBD designs were not used for model training and were reserved for external validation of the ML surrogate models. The trained models were subsequently used to predict environmental impacts at selected process conditions and to support the integrated process-optimization framework.

Validation was conducted at two levels. First, the predictive adequacy of the RSM models was assessed using the available experimental results within the investigated process window, while any independent confirmation experiments, where applicable, were used to verify the optimized weld geometry. Second, the selected ML surrogate models were externally validated by comparing their predicted environmental impacts with the corresponding SimaPro-calculated impacts for the experimental conditions excluded from the LHS training dataset. This two-level assessment provided separate verification of the weld-geometry prediction and environmental-impact prediction components of the proposed framework, thereby evaluating the practical applicability of the integrated approach for sustainable Activated tungsten inert gas (A-TIG) welding process optimization.

3. Results and discussion

3.1. Life-Cycle Environmental Performance of the Experimental A-TIG Welding Runs

The cradle-to-gate environmental impacts of the 37 experimental activated tungsten inert gas (A-TIG) bead-on-plate welds produced according to the CCD and BBD designs were quantified using the EPD 2018 method. As shown in Table 2 and Fig. 3(a), the impact values varied across the investigated process window for all midpoint categories, indicating that the process parameters measurably influenced the environmental profile of the welds. The extent of this variation differed substantially among the evaluated categories. POCP exhibited the largest relative variation, whereas ADE and water scarcity changed over comparatively narrower ranges. This difference can be attributed to the varying contributions of process-dependent foreground flows and upstream background processes [39]. In particular, ADE and water scarcity are largely influenced by upstream electricity and steel production datasets, which reduce their sensitivity to changes in local welding parameters. In A-TIG welding, arc power is approximately proportional to the product of welding current and arc voltage. However, arc voltage may also be affected by flux-induced arc constriction, meaning that changes in current do not necessarily produce a strictly proportional change in electrical energy demand. Accordingly, the nonlinear variation observed in GWP reflects the combined effects of current, arc voltage, and welding time associated with the applied travel speed within the investigated process window.

Table 2
Summary of Midpoint Environmental Impacts for the 37 Experimental A-TIG Welding Runs

Impact category	Min	Max	Mean
Acidification (kg SO ₂ eq)	0.02052	0.02300	0.021910
Eutrophication (kg PO ₄ ³⁻ eq)	0.01329	0.01414	0.013776
Global warming (kg CO ₂ eq)	4.911	5.525	5.264
Photochemical O ₃ (kg NMVOC)	0.02847	0.07704	0.06249
Abiotic depletion, elements (kg Sb eq)	4.851×10 ⁻⁵	4.997×10 ⁻⁵	4.933×10 ⁻⁵
Abiotic depletion, fossil fuels (MJ)	48.45	60.75	56.05
Water scarcity (m ³ eq)	2.072	2.311	2.158
Ozone depletion (kg CFC-11 eq)	2.916×10 ⁻⁷	4.010×10 ⁻⁷	3.587×10 ⁻⁷

Figure 3(b) shows a clear increase in GWP with increasing welding current, although the scatter at comparable current levels indicates that current alone does not account for the observed variation, with travel speed and flux composition also contributing to the overall environmental response. The increase in GWP at higher current levels is primarily associated with greater electrical energy demand resulting from increased arc power and the corresponding energy consumption per unit welding length. Where applicable, inverter losses included in the inventory further contribute to the total electricity demand. The resulting increase in electricity consumption is reflected in higher values of electricity-related impact categories, including GWP, acidification, eutrophication, ADF, and ODP [40–42]. Under the electricity mix considered in this study, these changes translate into higher environmental burdens. In contrast, POCP is strongly influenced by the inventory contributions associated with flux preparation, including methanol consumption [43]. Its non-monotonic variation with the SiO₂/TiO₂ ratio indicates that the environmental contribution of flux preparation does not change monotonically across the investigated composition range. This behavior highlights the sensitivity of POCP to the composition-dependent life-cycle inventory of the flux and distinguishes it from categories that are more strongly governed by electricity and material production. Water scarcity exhibits comparatively limited variation because it is predominantly influenced by upstream electricity generation and material production processes rather than by changes in the welding operation itself. Overall, these results demonstrate that the evaluated midpoint categories differ substantially in their sensitivity to process-level changes, which should be considered when interpreting the environmental performance of A-TIG welding under different process conditions [44].

3.2. Sensitivity analysis

The 200 LHS points provided a space-filling representation of the three-dimensional parameter space defined by welding current, travel speed, and SiO₂/TiO₂ fraction. Figure 4(a) shows that the sampling points were distributed throughout the investigated design space without pronounced clustering or apparent regions of poor coverage [45]. The expanded LHS dataset reproduced the main trends observed in the experimental runs, with POCP exhibiting the largest relative variability among the evaluated impact categories.

As illustrated in Fig. 4(b), the Spearman correlation heatmap shows that welding current is positively associated with several impact categories, particularly ADE ($\rho = 0.75$), GWP ($\rho = 0.39$), and acidification ($\rho = 0.38$). In contrast, travel speed exhibits consistently negative associations, with the strongest correlations observed for water scarcity ($\rho = -0.81$), eutrophication ($\rho = -0.54$), and acidification ($\rho = -0.49$). These trends are consistent with the reduction in welding duration and, consequently, in electricity and shielding-gas consumption at higher travel speeds. The SiO₂/TiO₂ fraction shows comparatively weak monotonic associations with the evaluated impact categories ($|\rho| < 0.28$), indicating that its effect is

less directly reflected by monotonic changes in the environmental indicators and may instead depend on nonlinear relationships within the inventory model.

To account for potential interaction effects, multiple linear regression models incorporating two-way interaction terms were fitted separately for each environmental indicator. The resulting standardized regression coefficients (β), presented in Fig. 4(c), indicate that welding current contributes substantially to the variation of most impact categories, whereas travel speed is generally associated with lower impact values. The interaction terms further indicate that the effect of travel speed may depend on the applied welding current. In comparison, the contribution of the $\text{SiO}_2/\text{TiO}_2$ fraction is generally smaller, with its environmental influence showing a more complex, non-monotonic behavior.

3.3. Surrogate regression modeling

Regression-based surrogate models were developed to approximate the environmental response surface generated from the LHS-expanded LCA dataset. Several models with different levels of flexibility and interpretability, including Polynomial Regression, RF, GPR, SVR, XGBoost, and ANN, were evaluated using the training subset and validated on independent test data. The resulting models showed high predictive accuracy across the investigated impact categories. ANN provided the best overall performance for most indicators, whereas RF, Polynomial Regression, and SVR performed better for POCP, ADE, and water scarcity, respectively. As summarized in Table 3, test-set R^2 values exceeded 0.97 for all categories and surpassed 0.99 for several indicators, indicating that the surrogate models accurately reproduced the LCA response trends within the investigated process window. The selected surrogate models were subsequently validated against the independent 37-run experimental dataset comprising the CCD and BBD designs. As shown in Fig. 5, the surrogate predictions exhibit a strong agreement with the corresponding impact values calculated using SimaPro, with external R^2 values exceeding 0.90 for six midpoint categories and reaching 0.995 for POCP. The comparatively lower R^2 values obtained for ADE and water scarcity may be partly attributed to the narrow ranges of their impact values, which can limit the ability of R^2 to reflect predictive performance when the variability in the response is relatively small.

Table 3
Best-performing ML model for each environmental impact category

Impact	Best model	Test R^2	CV R^2	Hyper-parameters
Acidification	ANN	0.9953	0.9821	hidden_layer_sizes= (50,50), activation=relu, max_iter = 1000, random_state = 42
Eutrophication	ANN	0.9923	0.9758	hidden_layer_sizes= (50,50), activation=relu, max_iter = 1000, random_state = 42
GWP	ANN	0.9958	0.9832	hidden_layer_sizes= (50,50), activation=relu, max_iter = 1000, random_state = 42
POCP	RF	0.9976	0.9960	n_estimators = 200, random_state = 42
ADE	Polynomial	0.9938	0.9821	degree = 2, include_bias=False
ADF	ANN	0.9941	0.9866	hidden_layer_sizes= (50,50), activation=relu, max_iter = 1000, random_state = 42
Water scarcity	SVR	0.9783	0.9693	kernel = rbf, C = 10, gamma='scale'
ODP	ANN	0.9925	0.9879	hidden_layer_sizes= (50,50), activation=relu, max_iter = 1000, random_state = 42

3.4. Environmentally informed optimization and validation

The LHS-based sensitivity analysis indicated that lower welding current and higher travel speed were generally associated with lower environmental impacts and therefore provided the basis for the subsequent RSM optimization. From a manufacturing perspective, these conditions correspond to lower heat input per unit weld length and shorter welding times, thereby reducing electricity demand and shielding-gas consumption per unit length. The RSM models developed from the BBD and CCD designs were first compared in terms of their predictive and statistical performance, as summarized in Table 4. The CCD-based models exhibited better predictive capability than the corresponding BBD models for both depth of penetration (DOP) and weld bead width (WBW) and were therefore selected for the optimization stage. ANOVA further confirmed the statistical adequacy of the selected models, with non-significant lack-of-fit tests.

For DOP, the SiO₂/TiO₂ fraction did not exhibit a statistically significant effect, suggesting that flux composition can be adjusted within the investigated range with limited influence on penetration. The desirability-based optimization identified 75% SiO₂, a welding current of 115 A, and a travel speed of 110 mm min⁻¹ as the optimal compromise among the considered responses. This parameter combination represents a balance between achieving the required weld penetration and limiting process-related energy consumption. In addition, the SiO₂-rich flux composition can reduce the upstream environmental burden associated with TiO₂ nanoparticle production [32, 34].

Table 4
Comparison of the RSM models from the BBD and CCD designs

Response	Design	Model type	R ²	Adj R ²	Pred R ²	Adeq Precision
DOP	BBD	Linear	0.8810	0.8535	0.8104	18.5
DOP	CCD	Linear	0.9524	0.9435	0.9316	37.4
WBW	BBD	Quadratic	0.9765	0.9464	0.8179	20.4
WBW	CCD	2FI	0.9607	0.9425	0.8706	32.1

The optimized conditions were subsequently verified experimentally using three independent validation conditions, with each condition evaluated from three replicate measurements. As presented in Table 5, the experimental results showed good agreement with the corresponding RSM predictions, with prediction errors for DOP and WBW remaining around 5% or lower across the three validation conditions. These results confirm the predictive adequacy of the selected RSM models within the investigated process window. The surrogate regression models also showed good agreement with the SimaPro-calculated environmental impacts for the validation conditions, with most relative errors remaining below 4%. The largest deviation, 11.9%, was observed for POCP, which may be associated with the nonlinear dependence of this indicator on flux composition and methanol-related contributions. Figure 6 presents the three experimentally fabricated weld specimens used for experimental validation. The specimens showed consistent bead appearance and similar macroscopic weld geometry across the three validation conditions, providing a visual representation of the experimentally validated welds.

Table 5
Validation of RSM Predictions Using Three Experimental Conditions

Condition	Mixture (SiO ₂ /TiO ₂)	Current (A)	Speed (mm/min)	Predicted DOP (mm)	Measured DOP (mm)	Error (%)	Predicted WBW (mm)	Measured WBW (mm)	Error (%)
1	50	125	110	2.46	2.55	3.53	4.99	5.21	4.22
2	75	115	110	2.26	2.38	5.04	4.55	4.45	2.25
3	30	130	110	2.53	2.51	0.8	5.1	5.22	2.3

The validation results further demonstrated that the selected environmentally favorable conditions were compatible with the target weld geometry, indicating that reductions in energy and material consumption could be achieved without a

substantial loss in the required geometric performance. The consistency of the optimized parameter range, characterized by relatively low current and high travel speed, is also consistent with the trends identified by the sensitivity analysis. From a process perspective, once sufficient flux activation and fusion are achieved, further increases in welding current may increase thermal input without producing a proportional improvement in penetration efficiency [46]. Flux composition played a secondary but environmentally relevant role. Because the $\text{SiO}_2/\text{TiO}_2$ fraction showed no statistically significant effect on penetration, SiO_2 -rich flux compositions can be considered as a means of reducing the upstream environmental burden associated with TiO_2 production while maintaining the targeted weld geometry. Nevertheless, flux composition influenced POCP through changes in methanol-related contributions, highlighting the importance of including auxiliary materials in environmental optimization [47]. Taken together, these findings demonstrate that the proposed framework can provide an efficient means of screening and optimizing A-TIG welding conditions while substantially reducing the need for repeated conventional LCA simulations.

4. Conclusions

This study developed an integrated framework combining life cycle assessment (LCA), Latin hypercube sampling (LHS), response surface methodology (RSM), and machine learning (ML) to evaluate and optimize the environmental performance of nano-flux activated tungsten inert gas (A-TIG) welding of AISI 316L stainless steel. The results demonstrated that welding current was the dominant process variable influencing most of the evaluated environmental impact categories, whereas increasing travel speed generally reduced environmental burdens by decreasing welding duration and associated electricity consumption. In comparison, flux composition exhibited a weaker and more complex influence, with its most pronounced effect observed for photochemical ozone creation potential (POCP), primarily through methanol-related contributions associated with flux preparation.

The sensitivity analysis further confirmed the positive association of welding current with energy-related impact categories and the generally negative association of travel speed with the evaluated environmental indicators. These findings provided the basis for the subsequent RSM optimization, which identified a parameter combination of 75% SiO_2 , 115 A welding current, and 110 mm min^{-1} travel speed as the optimum within the investigated process window. Experimental validation showed that these conditions provided the targeted weld geometry while simultaneously limiting the associated environmental burdens, demonstrating the feasibility of incorporating environmental criteria into A-TIG process optimization without a substantial deterioration in weld performance.

The ML-based surrogate models accurately reproduced the LCA results, with externally validated R^2 values exceeding 0.90 for six of the eight impact categories and reaching 0.995 for POCP. These results demonstrate the potential of surrogate-based modeling to substantially reduce the computational effort associated with repeated LCA evaluations while retaining high predictive accuracy within the investigated parameter space. Overall, the proposed framework provides a systematic approach for integrating environmental assessment with process modeling and optimization in A-TIG welding. Future work should focus on propagating input and model uncertainties, experimentally quantifying process-related emissions, and extending the framework to industrial-scale and multi-pass welding operations.

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Author contributions (CRediT)

Mahdi Mazloom Farsibaf contributed to conceptualization, data curation, formal analysis, investigation, methodology, software, validation, visualization, writing – original draft, and writing. Farhad Rahmati contributed to methodology, formal analysis, investigation, visualization, and writing – review & editing. Farhad Kolahan contributed to project administration, resources, and writing – review & editing. Younes Zarif Javadi Yazdi contributed to investigation and visualization.

Amirreza Banejad contributed to software. Masoud Bavejdan contributed to investigation and data curation. All authors have read and approved the final version of the manuscript and agreed to its submission for publication.

Declarations

Declaration of competing interest

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

Declarations of generative AI and AI-assisted technologies in the writing process

During the preparation of this work, the authors used ChatGPT (OpenAI) in order to improve readability and language. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the published article.

Supplementary information

Not Applicable.

Author Contribution

Mahdi Mazloom Farsibaf contributed to conceptualization, data curation, formal analysis, investigation, methodology, software, validation, visualization, writing – original draft, and writing. Farhad Rahmati contributed to methodology, formal analysis, investigation, visualization, and writing – review & editing. Farhad Kolahan contributed to project administration, resources, and writing – review & editing. Younes Zarif Javadi Yazdi contributed to investigation and visualization. Amirreza Banejad contributed to software. Masoud Bavejdan contributed to investigation and data curation.

Data Availability

All data generated and analyzed in this study, including the experimental, life cycle assessment, and modelling results, are presented in the manuscript.

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Figures

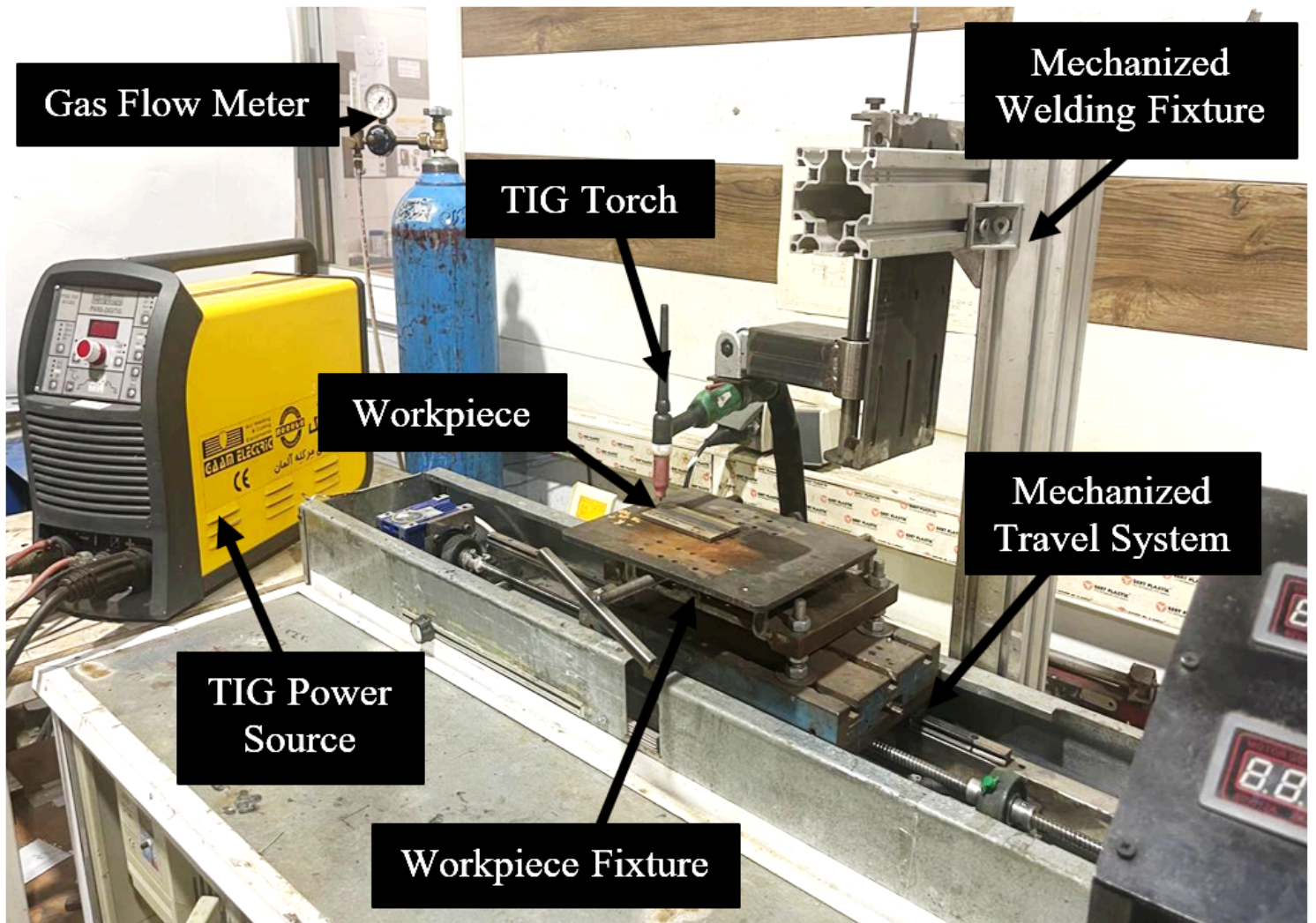


Figure 1

Experimental setup used for Activated tungsten inert gas (A-TIG) welding

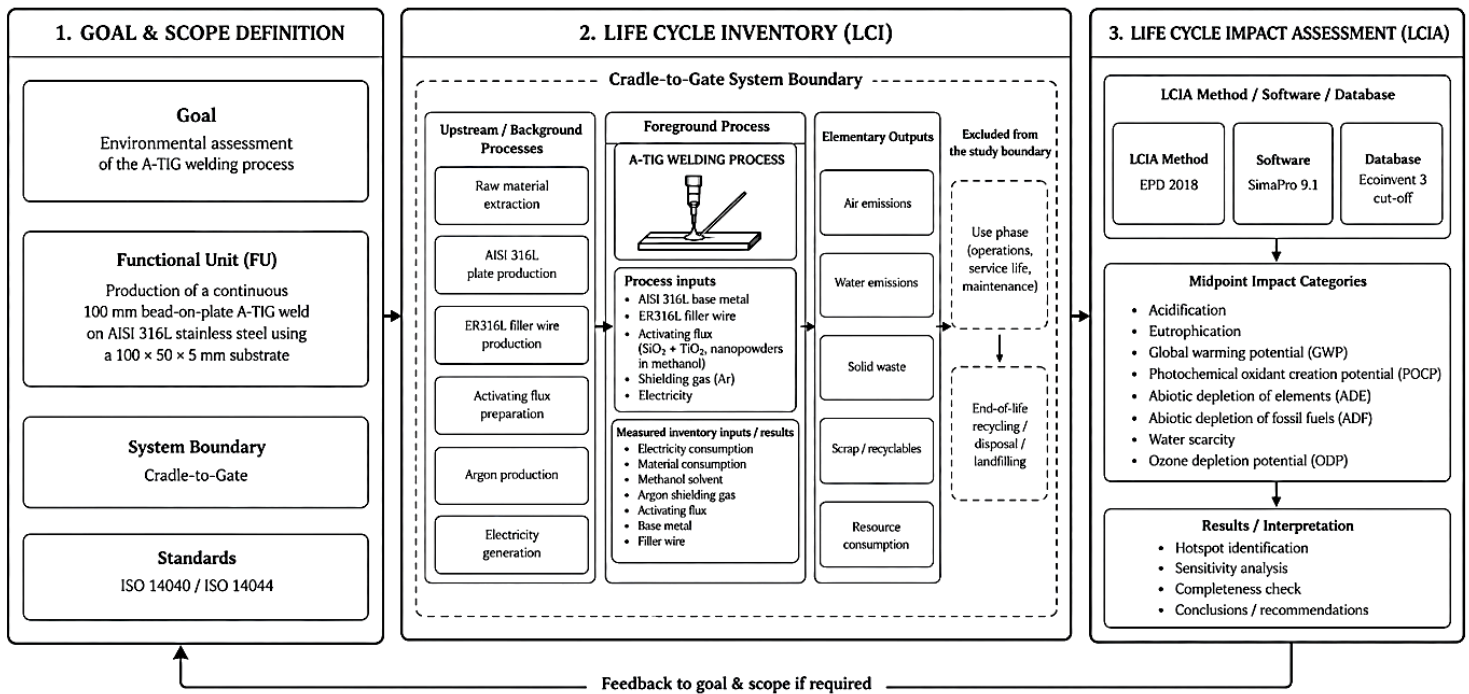


Figure 2

System boundaries and case studies considered for the life cycle assessment (LCA), together with the cross-sectional profiles of A-TIG welds

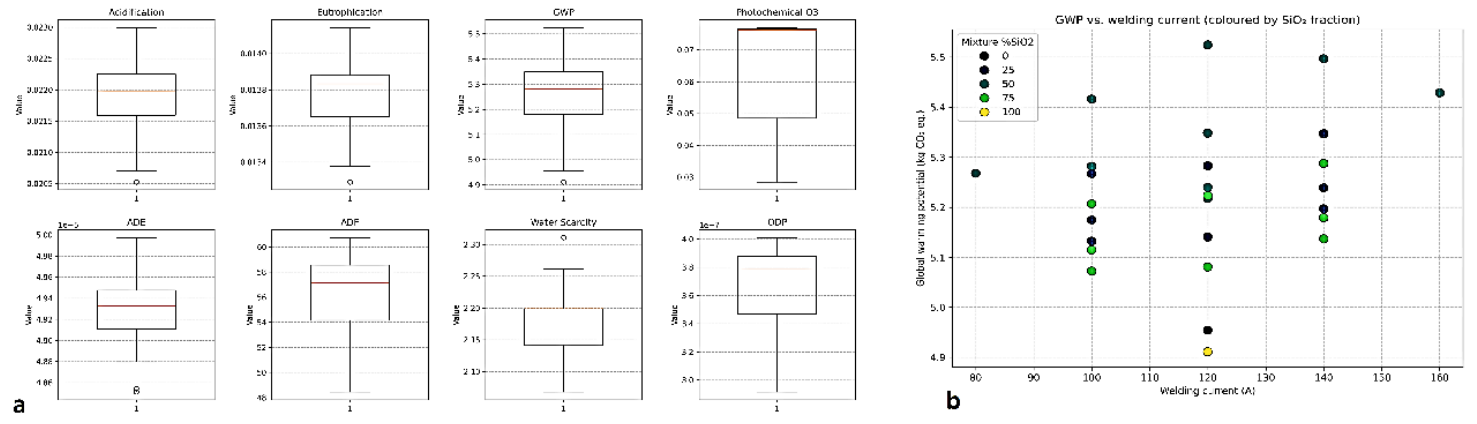


Figure 3

(a) Midpoint environmental impact profiles of the 37 experimental A-TIG welding runs; (b) variation of GWP with welding current at different $\text{SiO}_2/\text{TiO}_2$ fractions.

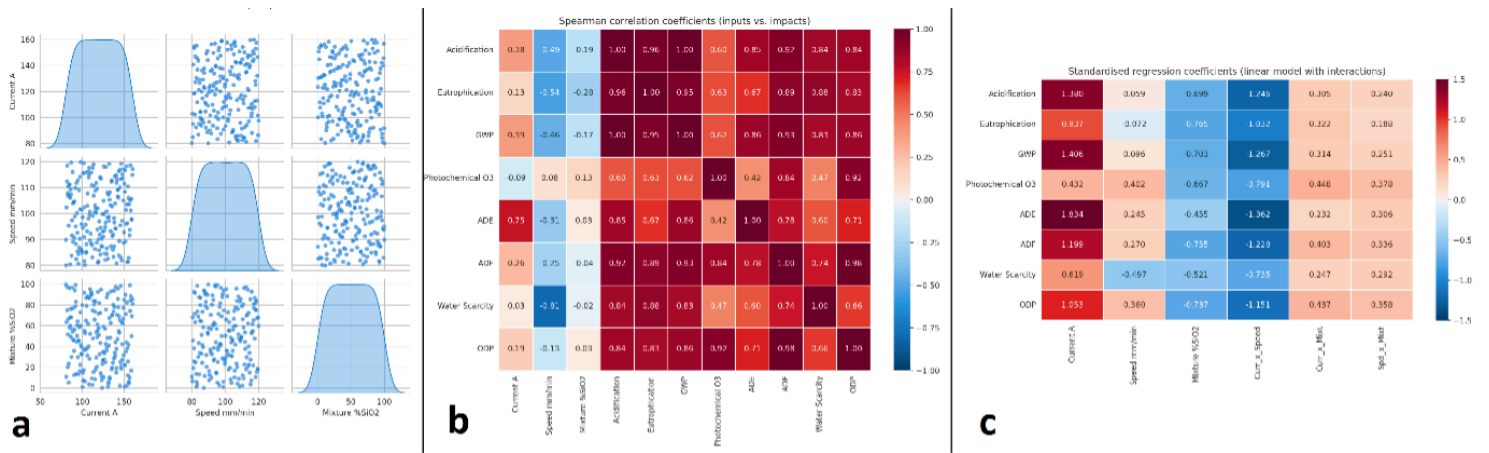


Figure 4

LHS-based sensitivity analysis: (a) design space coverage, (b) Spearman correlation heatmap, (c) standardized regression coefficients

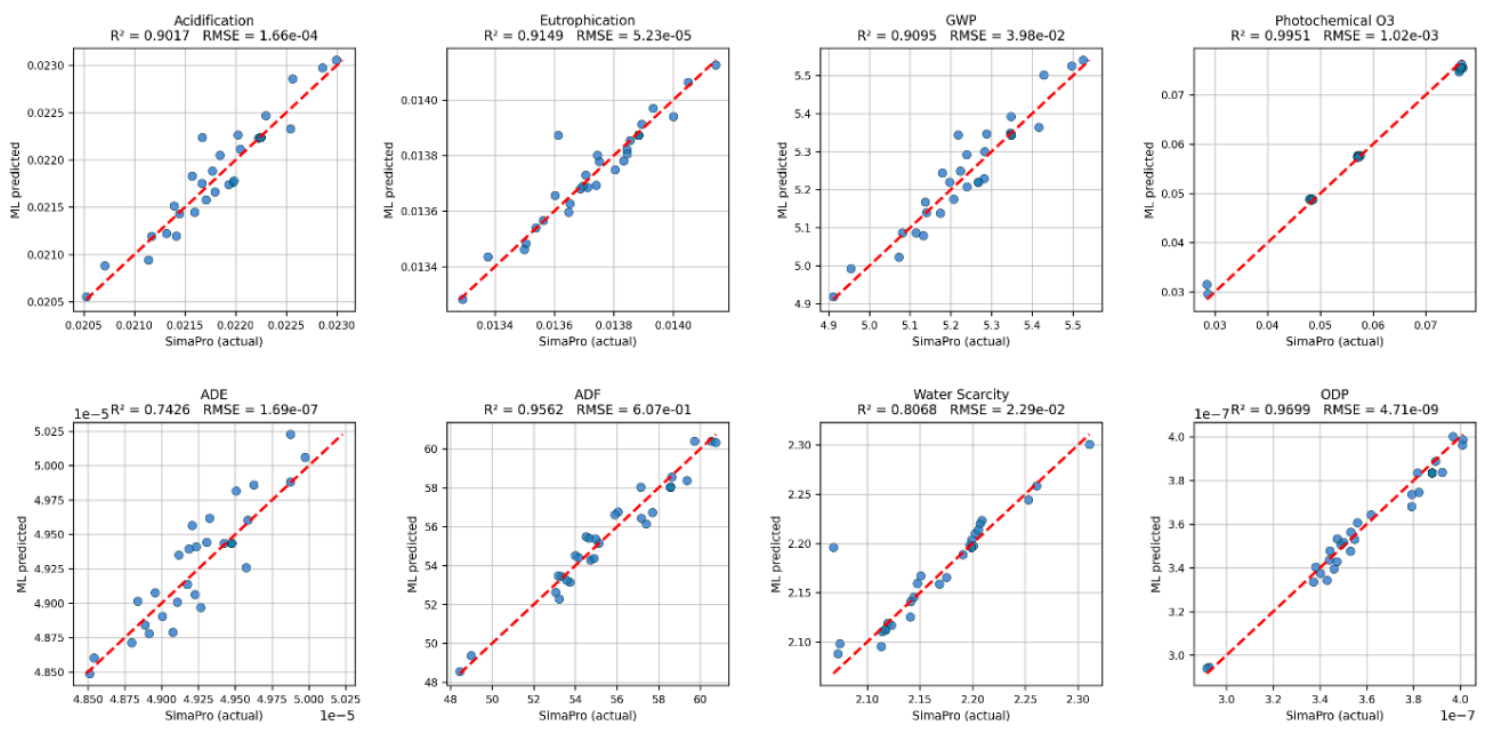


Figure 5

Parity plots comparing surrogate-learning-predicted impacts with SimaPro-calculated values for the EPD 2018 midpoint categories

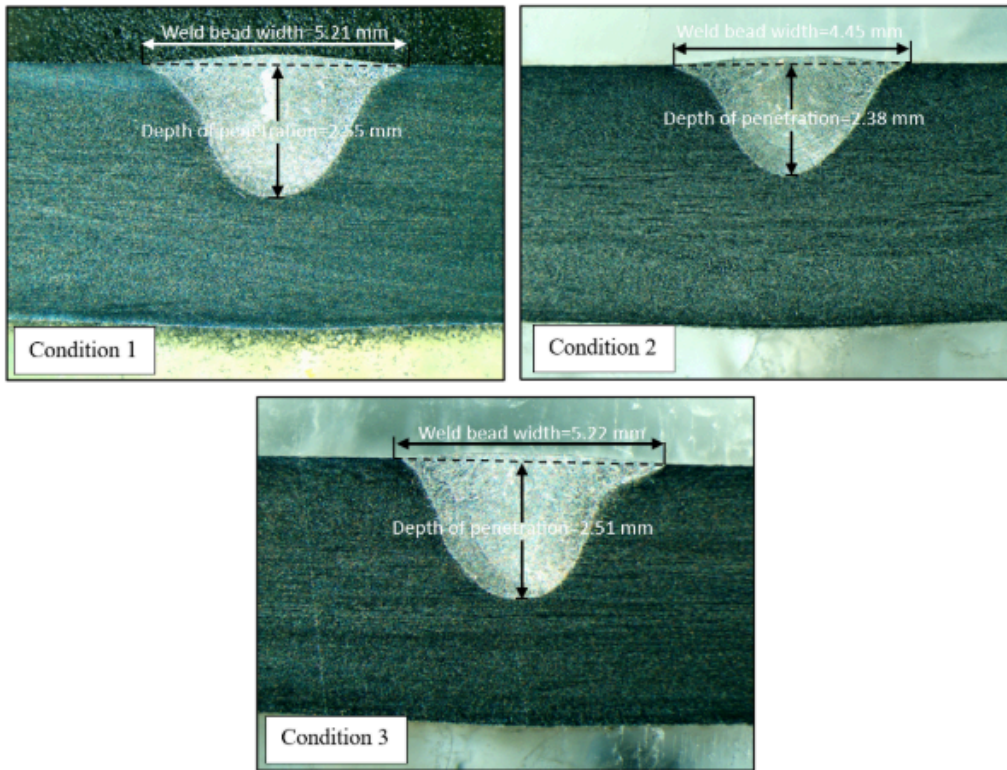


Figure 6

Experimentally fabricated weld specimens corresponding to the three validation conditions.