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MODELING THE EFFECT OF SURFACE ACTIVE ELEMENTS ON WELD POOL FLUID FLOW, HEAT TRANSFER AND GEOMETRY

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ABSTRACT

The influence of sulfur on the heat flow and fluid flow and the transient development of the weld pool was quantitatively evaluated for two heats of Type 304 stainless steel containing 90 and 240 ppm sulfur, respectively. A transient heat transfer model was utilized to simulate the heat flow and fluid flow in the weld pool during stationary laser and gas tungsten arc (GTA) spot welds. A recently developed surface tension model was utilized to calculate the temperature coefficient of surface tension ($\frac{d\gamma}{dT}$) as a function of temperature and sulfur content. This allows a realistic evaluation of the effect of surface-active elements on the fluid flow and weld geometry. The computed results indicate that during stationary welding, the weld pool surface temperatures are fairly high. As a consequence, the temperature coefficient of surface tension becomes negative and a radially outward or a bifurcated flow of weld metal occurs even when the weld pool contains a significant amount of sulfur. The predictions of the model were verified by comparing the calculated and experimentally observed fusion zone geometry. The results indicate very good agreement between the predicted and experimentally observed fusion zone geometry, for both laser and gas tungsten arc (GTA) spot welds, due partly to the accurate treatment of surface tension gradient driven flows.

THE DEVELOPMENT of the weld pool size and shape is influenced by the simultaneous occurrence of several important physical processes. These include the amount of heat transferred from the heat source to the workpiece, the fluid flow in the weld pool, and the accompanying convective heat transfer. Recent studies[1-11] have demonstrated that, in most cases, the fluid flow and the heat transfer in the weld pool is controlled by the spatial variation of surface tension (surface tension gradient) that exists on the weld pool surface. The surface tension gradient arises from the spatial variation in surface temperature and the temperature dependence of surface tension. The spatial variation of surface tension causes the molten metal to be drawn along the surface from the region of lower surface tension to that of higher surface tension and this may result in very large surface flows. For pure metals and alloys the temperature coefficient of surface tension ($\frac{d\gamma}{dT}$) is negative. Thus, the surface tension is highest near the solid-liquid interface (lower temperature), causing the flow to be outward and away from the center of the pool. However, surface-active elements such as sulfur or oxygen can produce a positive $\frac{d\gamma}{dT}$ resulting in a higher surface tension at the center of the pool causing an inward flow. The effect of surface-active elements has been investigated in detail by Heiple et al.[1,12-15] Their results indicate that surface-active elements significantly alter the surface tension of the weld metal thereby altering the flow field in the weld pool. Of particular significance is the reversal of flow which can occur in the presence of relatively small amounts of surface-active elements, causing a deep penetration. Sundell et al.[9] have experimentally investigated the effect of sulfur, silicon, cerium, oxygen and nitrogen on GTA weld penetration. Their results indicate that these elements can directly or indirectly influence the weld pool shape and size.

Several investigations of the effect of surface-active elements on weld penetration have been carried out for GTA welding of steels. While the effect has been identified, the extent and the nature of the influence of surface- active elements on weld pool fluid flow and depth of penetration remain to be clarified. A quantitative understanding of the effect of surface-active elements on weld pool fluid flow and fusion zone shape can be achieved by mathematical modeling. Prior modeling efforts[3-11] aimed at understanding surface tension gradient driven flow in the presence of surface- active elements considered a specified constant positive $\frac{d\gamma}{dT}$ which cannot be justified based on the physical phenomena governing the process. Therefore, in the present analysis a more realistic procedure that considers the temperature coefficient of surface tension as a function of the surface temperature and the amount of surface- active element in the melt was utilized.

Experimental surface tension data are seldom available for any material throughout the temperature range of interest. Sundell et al.[9] have obtained surface tension data for different heats of stainless steels with various levels of surface-active elements. It must be noted,

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however, that their results extend only over a limited temperature range from approximately 1800 to 2200K. Since it is difficult to experimentally obtain surface tension data at all temperatures and compositions of interest, in the calculations presented here a recently developed formalism[16] to calculate $\frac{d\gamma}{dT}$ as a function of temperature and the amount of surface-active elements in the base metal was used. This paper presents the result of an experimental and theoretical investigation aimed at understanding the effect of surface-active elements on the evolution of weld pool shape and size during GTA and laser welding conditions. The computational model was used to simulate the fluid flow, temperature distributions and the weld pool shape and size, and the results were correlated with the experimental observations.

MATHEMATICAL MODELING

Figure 1 is a schematic drawing of the weld pool showing the region of interest. The energy exchange between the heat source and the metal surface produces a molten pool that grows due to conduction and convection. For laser welding, the development of the weld pool is governed by buoyancy and surface tension forces. In addition, during GTA welding, the electromagnetic force produced can significantly influence the development of the weld pool. A computational model[17] using a finite difference analysis (FDA) was appropriately modified to investigate transient, two dimensional heat flow and fluid flow problems associated with laser and GTA welding processes. The mathematical formulation can consider, depending on the process, buoyancy, electromagnetic, and surface tension driving forces in the solution of the overall heat transfer conditions associated with welding. The theoretical analysis in this study considers the effect of surface-active elements on the weld pool fluid flow by calculating $\frac{d\gamma}{dT}$ as a function of temperature and activity (wt% of surface-active element). This approach differs significantly from previous modeling efforts which have considered $\frac{d\gamma}{dT}$ as a specified constant that was assumed to be independent of the temperature. The temperature dependent surface tension force is calculated for the two heats of Type 304 SS based on the sulfur content in the base metal according to the model noted in the previous section. The details of the mathematical model are presented elsewhere[18] and will not be reproduced here. The data used for the computational study are presented in Table 1.

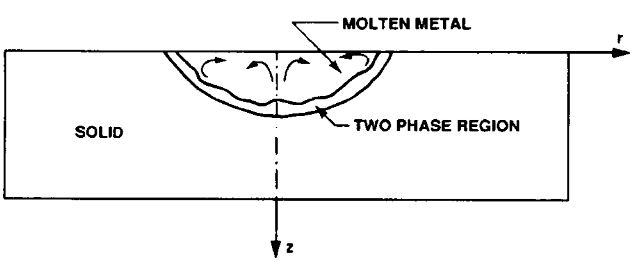

Fig. 1. Schematic drawing of the weld pool showing the region of interest.

Table 1. Data Used For Calculations

Laser power	500 watts
Laser beam radius	0.17 mm
Absorptivity	15%
GTA welding current	150 A
GTA welding voltage	14 V
Arc efficiency	80%
Arc radius	3 mm
Effective viscosity of molten metal	0.5 g/cm s
Effective thermal conductivity of molten metal	0.37 cal/cm-s-K

EXPERIMENTAL PROCEDURE

The materials used in this study consist of two heats of Type 304 stainless steel and their compositions are given in Table 2. Stationary welds were made on 30 × 30 × 6 mm samples at the center of the specimen using conventional GTA and laser welding processes. The welding parameters used in this investigation are given in Table 3. Details of the experimental set-up and the welding equipment used are presented elsewhere[19] and will not be reproduced here.

Table 2. Alloy Composition (Wt %)

Element	Heat **A**	Heat **B**
Cr	18.27	18.28
Ni	8.73	9.46
Mn	1.71	1.88
C	0.025	0.031
Si	0.35	0.50
P	0.026	0.022
S	0.009	0.024
Mo	0.27	0.31
V	0.10	0.08
Nb	0.01	0.01
Ti	<0.01	<0.01
Co	0.14	0.15
Cu	0.19	0.15

The fusion zone size, shape and structure were examined by light microscopy. Particular care was taken to ensure that the samples were sectioned along the center of the weld. The specimens were prepared using standard procedures and then etched using HNO_3 and H_2O.

RESULTS AND DISCUSSION

TEMPERATURE DEPENDENCE OF SURFACE TENSION - The temperature coefficient of surface tension was calculated as a function of temperature and activity for the entire temperature range of interest. The calculated $\frac{d\gamma}{dT}$ for the two heats of Type 304 SS (90 and 240 ppm sulfur) as a function of temper-

Table 3. Welding Parameters

GTA Process	
Current	150 A
Voltage	14 V
Weld duration	5 s
Shielding gas	20 cfh argon
Laser Beam Process	
Power	500 watts
Weld duration	5 s
Shielding gas	20 cfh argon

ature is given in Fig. 2. For the heat containing 90 ppm of sulfur, $\frac{d\gamma}{dT}$ is positive until about 2200K. For a sulfur content of 240 ppm $\frac{d\gamma}{dT}$ is positive until approximately 2450K (see Fig. 2). As the melt surface temperature increases beyond these temperatures, $\frac{d\gamma}{dT}$ becomes negative. For a tool steel containing 100 ppm sulfur, Heiple et al.[1] have indicated that this critical temperature is 2300K as determined by Gogiberidze et al.[20] Thus, the data is in general agreement with our calculations. Our results are also consistent with the experimental measurements of surface tension for stainless steel by Sundell et al.[9] Their results show that heats containing surface-active elements initially exhibit a positive $\frac{d\gamma}{dT}$. As the temperature of the melt increases beyond a critical temperature, $\frac{d\gamma}{dT}$ becomes negative, and increasing the sulfur content changes the temperature dependence of the surface tension gradient.

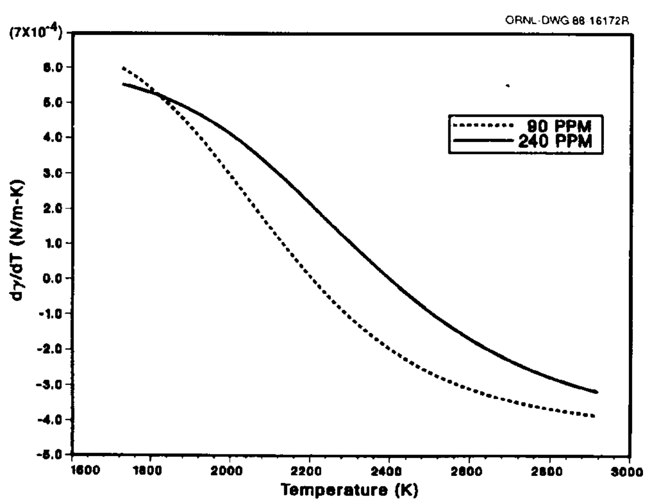

Fig. 2. Calculated temperature coefficient of surface tension ($\frac{d\gamma}{dT}$) as a function of temperature and sulfur content.

The change in $\frac{d\gamma}{dT}$ from a positive value at low temperature to a negative value at high temperature has serious consequences on the weld pool fluid flow and heat transfer, and the ultimate development of the weld. Directly below the welding heat source, a hot zone exists where the temperature experienced by the molten weld metal is likely to be above the critical temperature such that a negative $\frac{d\gamma}{dT}$ prevails in this region. This would result in two surface tension gradients to exist on the weld pool surface: a positive surface tension gradient at the periphery of the weld pool and a negative surface tension gradient at the center of the weld pool. Depending on the relative magnitude of the two driving forces that the weld may encounter, either a radially outward flow or a radially inward flow, or even a combination of both resulting in complex bifurcated flow, may develop.

GTA WELDS - The flow and temperature fields during GTA welding were simulated for both heats (90 ppm and 240 ppm sulfur) of Type 304 SS. First, the results for the heat containing 90 ppm sulfur are presented. Figure 3 is a composite transverse section showing the calculated temperature and flow fields and the experimentally observed weld pool geometry for a stationary GTA weld after 5 s. The major vortex near the weld pool surface is dominated by the surface tension gradient effect causing a radially outward flow. Away from the weld pool surface, near the centerline of the weld pool, the flow field is controlled by the electromagnetic force. The maximum radial surface velocities are of the order of 0.12 m/s. The calculated velocities appear to agree qualitatively with earlier theoretical investigations for a wide variety of materials in which surface velocities ranging from 0.05 m/s (ref. 21) to 1 m/s were reported.[8,10,11,17] All these studies assumed a constant $\frac{d\gamma}{dT}$ ranging from -0.01×10^{-3} N/m·K to -0.35×10^{-3} N/m·K. The higher velocities of 1 m/s were obtained for a $\frac{d\gamma}{dT}$ of -0.35×10^{-3} N/m·K.[8,10,11]

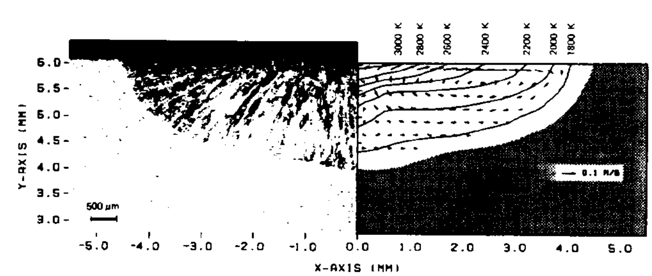

Fig. 3. Composite section showing the calculated temperature and flow fields and the experimentally observed weld pool geometry for a stationary GTA weld after 5 s (heat A containing 90 ppm sulfur).

The simulated results clearly show the influence of convection on the temperature distribution in the weld pool. Even though there exist opposing surface tension gradient effects on the weld pool surface, the negative $\frac{d\gamma}{dT}$ that is present over much of the weld pool surface, associated with the higher temperatures, prevails and controls the surface flows. The calculated flow field is radially outward, transporting heat from the center to the periphery. In the interior of the weld pool, the effect of the surface flows on the total flow behavior diminishes. This is particularly evident at the center of the pool where the inward flow due to the electromagnetic force transports relatively hot liquid from the surface to the interior, shifting the isotherms downwards and increasing the depth of the weld pool in this region.

The results of the previous experimental investigations studying the effect of sulfur on the weld pool fluid flow suggest that the amount of sulfur has to exceed a critical level before observing flow reversal.[1,15] Heiple et al.[1] have reported that the addition of 50 ppm of sulfur increased the depth/width ratio of a GTA weld in 21-6-9 stainless steel by over 80%, suggesting that an inward flow of the liquid melt in the weld pool occurred. Since the alloy used in the present investigation has 90 ppm sulfur, it is surprising that the calculated results indicate an outward flow instead of a radially inward flow as suggested by the earlier investigations. This discrepancy is likely to be due to the fact that the previous experimental results were obtained for linear (moving arc) welds. The GTA welding parameters in these studies were: a welding current of 150 A and a travel speed of 2.12 mm/s (5 ipm).[1] For the same welding current (150 A), the surface temperatures in the weld pool would be significantly lower for a moving arc weld due to lower heat input. For example, Sundell et al.[9] have reported peak temperatures of $\approx$ 2100K for linear welds on stainless steels. Under such conditions, the flow field would be radially inward since $\frac{d\gamma}{dT}$ would be positive everywhere on the melt surface (see Fig. 2). On the other hand, for stationary welds the calculated results from this study show that much of the weld pool surface is above 2200K and therefore a negative $\frac{d\gamma}{dT}$, which causes a radially outward flow, is present.

In the interior of the weld pool, the electromagnetic force prevails, resulting in a small flow in the radially inward direction and causing increased local penetration near the root of the weld. The inflection in the fusion zone interface is due to this flow reversal. The calculated velocities in the interior of the weld are at least an order of magnitude less than the surface velocities. For the conditions investigated, the overall effect of the electromagnetic force on the weld pool development is relatively weak compared to the effect of the surface tension gradient. This is to be expected since the welding current used in this investigation is relatively low. Heiple et al.[13-15] have shown that for low welding currents (<150 A) the surface tension gradient at the weld pool surface is the dominant force driving fluid flow in the weld pool.

In order to quantitatively evaluate the effect of the higher sulfur content on the weld penetration and geometry, the flow and temperature field after 5 s were modeled for a sulfur content of 240 ppm. The $\frac{d\gamma}{dT}$ was evaluated for the higher sulfur content as a function of temperature (see Fig. 2). Figure 4 shows the composite transverse section of the weld showing the calculated and experimental results after 5 s of welding. The positive $\frac{d\gamma}{dT}$ at the periphery significantly influences the local flow field. As a result, the radially inward flow near the solid-liquid interface increases with time. The predicted flow field has a strong effect on the development of the weld pool as can be seen from Fig. 4. The radially outward loop near the centerline transports heat radially outward from the center of the pool. However, in this case, the relatively hot liquid metal is met by a radially inward flow that transports heat from the sides to the interior. The ensuing convective heat transfer produces an almost cylindrical weld puddle with increased depth of penetration primarily at the periphery instead of at the center of the weld pool. The calculated weld pool shape is in excellent agreement with the actual shape, as shown in Fig. 4. The calculated temperature fields show the significant influence the modified flow (due to the higher sulfur content) has on the temperature distribution in the weld pool. The resulting temperature field is considerably different and has a profound influence on the bead shape.

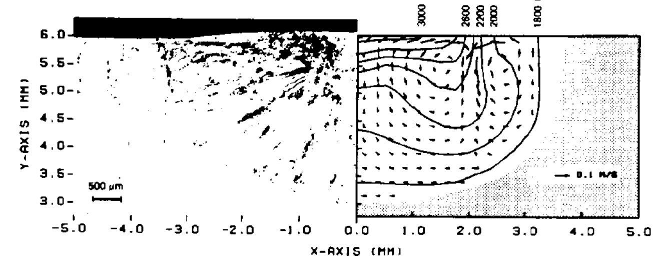

Fig. 4. Composite section showing the calculated temperature and flow fields and the experimentally observed weld pool geometry for a stationary GTA weld after 5 s (heat B containing 240 ppm sulfur).

The results presented in this section clearly show the influence of a surface- active element such as sulfur on the flow and temperature fields during stationary welding, and the resulting effect on the weld pool shape and size. There is overwhelming experimental evidence that small variations in sulfur can cause significantly different penetration behavior. The present investigation confirms that sulfur can cause variations in the bead geometry by altering the surface tension gradient and thereby altering the fluid flow and convective heat transfer in the weld pool. However, the effect of sulfur on the flow reversal and the bead geometry is not as pronounced in this study as that reported by the earlier investigations.[1,12-15] This weaker influence of sulfur on the bead geometry is attributed to the higher surface temperatures observed during stationary welding compared to linear welding. To illustrate this effect, the flow field and the temperature field during linear GTA welding were calculated in a two-dimensional plane along the welding direction, for the heat containing 240 ppm sulfur. The welding parameters used were: welding current of 150 A, arc voltage of 14 V, and a welding speed of 2.5 mm/s. The results of the calculation are presented in Fig. 5. Figure 5a shows a radially inward flow in the weld pool, as suggested by previous experimental investigations, resulting in increased depth of penetration. Figure 5b shows the calculated temperature distribution in the weld pool. The calculated peak temperature at the surface is on the order of 2500K, considerably below the peak temperatures of more than 3000K found for the stationary welds. The result is that a positive $\frac{d\gamma}{dT}$ exists over most of the weld pool surface. This explains the calculated inward flow in the case of linear GTA welding.

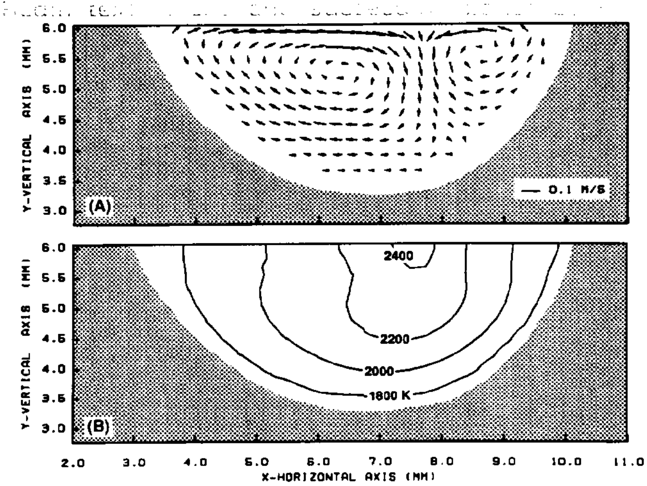

Fig. 5. Calculated heat flow and fluid flow during linear GTA welding of Type 304 SS containing 240 ppm sulfur (150 A, 14 V, 2.5 mm/s). A - Flow field; B - Temperature field.

The results presented show that while sulfur in the base metal can alter the flow field and thereby influence the weld penetration, the extent of this effect is a strong function of the temperature field in the weld pool. The results also show that the temperature dependence of $\frac{d\gamma}{dT}$ must also be taken into account. To illustrate the importance of considering $\frac{d\gamma}{dT}$ as a function of temperature and sulfur content, the fluid flow and the consequent weld pool shape and size were calculated assuming a constant positive $\frac{d\gamma}{dT}$ of 0.15×10^{-3} N/m·K. The computed flow field and temperature field for GTA welding after 2 s are presented in Fig. 6. The results show an inward flow pattern causing a very large depth of penetration, considerably more than the actual experimentally observed depth.

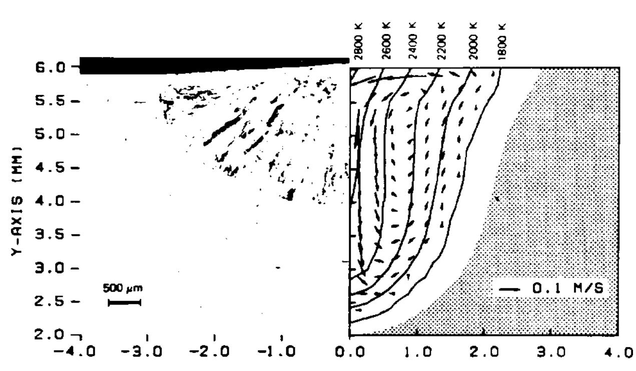

Fig. 6. Comparison of the calculated (for a constant $\frac{d\gamma}{dT}$ of 0.15×10^{-3} N/m-K) and experimentally observed GTA weld fusion zone after 2 s (heat B containing 240 ppm sulfur).

LASER WELDS - The flow and temperature fields during laser beam welding were simulated for the heat containing 90 ppm sulfur. Figure 7 is a composite transverse section of the weld pool showing the calculated flow and temperature fields and the experimentally obtained pool geometry after 2 s. The results show a single coherent vortex during laser beam welding. As discussed earlier, during laser beam welding the driving forces for convection in the weld pool are surface tension and buoyancy. Due to the high surface temperature, $\frac{d\gamma}{dT}$ is largely negative causing a radially outward flow at the weld pool surface. This flow is augmented by the buoyancy driven flows in the interior of the pool. In the absence of any significant opposing forces, the resulting fluid flow pattern consists of a single coherent loop. The maximum radial velocity at the weld pool surface is of the order of 0.7 m/s. The higher velocity is to be expected as the temperature gradient on the weld pool surface is significantly higher than during conventional GTA welding. The radially outward flow produces a relatively shallow weld pool (depth/width ratio of 0.28) by transferring the heat from the center to the periphery. The calculated temperature distribution is similar to that obtained for GTA welding.

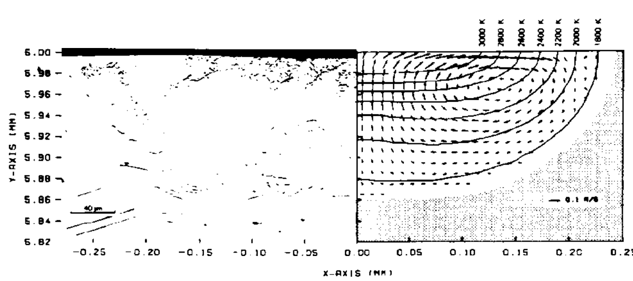

Fig. 7. Composite section showing the calculated temperature and flow fields and the experimentally observed weld pool geometry for a stationary laser beam weld after 2 s (heat B containing 90 ppm sulfur).

The predicted and experimental results obtained after 5 s of laser beam welding are very similar to that obtained after 2 s and therefore not presented here. During laser welding, the use of a laser beam focussed on a very small area results in higher power density, causing a rapid increase in the local temperature of the material. At the same time, the energy supplied to the weld is relatively low, producing a small weld in comparison to the overall size of the specimen. Therefore, a 'quasi-steady' state is achieved very quickly as the energy supplied to the weld is rapidly conducted away by the base metal.

The calculated results showed very little difference in the overall shape or size of the pool for the heat containing 240 ppm sulfur compared to the heat containing 90 ppm sulfur. This is to be expected as the surface temperature as well as the surface temperature gradient are considerably higher during welding using a high energy laser beam. Consequently, a very large hot zone exists on the weld pool surface where the temperature is well above the critical temperature such that a negative $\frac{d\gamma}{dT}$ prevails over much of the weld pool surface. Therefore, minor variations in surface-active elements (within the allowable limits) are not expected to produce any major variations in the penetration depth.

SUMMARY AND CONCLUSIONS

1. The effect of sulfur on the weld pool fluid flow and heat transfer was computationally modeled by considering $\frac{d\gamma}{dT}$ as a function of temperature and sulfur content. This allowed for the realistic simulation of the effect of surface-active elements on the fluid flow and the weld geometry.
2. The calculations of $\frac{d\gamma}{dT}$ indicate that for certain alloys, $\frac{d\gamma}{dT}$ can change from a positive value at relatively low temperature to a negative value at high temperature resulting in complex flow and temperature fields. The results confirm the significant influence of weld pool fluid flow and convective heat transfer on the development of the weld pool.
3. For the welding conditions investigated, surface tension gradient was the predominant driving force for fluid flow in the weld pool.
4. Surface-active elements such as sulfur increased the depth of penetration by modifying the surface tension gradient driven flow. However, the observed increase in penetration was considerably less than the values reported by earlier investigations. This is likely to be due to the fact that previous investigations were done for linear welds where the surface temperatures are considerably lower than those obtained for stationary welds. This was further confirmed by the results obtained for laser welding. The higher surface temperatures during the high energy density process caused a negative $\frac{d\gamma}{dT}$ to exist over much of the weld pool surface resulting in relatively low weld penetration.
5. The predictions of the model were verified by direct correlations with the experimental observations. The excellent agreement with experiment is attributed to the more realistic treatment of the surface tension gradient driven flows that occur during welding.

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