MACROSCOPIC MODELING OF MARANGONI FLOW AND SOLUTE REDISTRIBUTION DURING LASER WELDING OF STEEL

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Abstract

Fluid flow driven by thermocapillarity (Marangoni) and / or thermo-solutal effects during laser welding results in a concentration inhomogeneity in the resolidified weld pool. To predict the resulting distribution of alloy elements in a multicomponent steel subjected to laser welding, calculations are presented, taking into account solute, heat, mass and momentum conservation in two dimensions. The simulation is based on the volume-averaged two-phase model of alloy solidification presented by J. Ni, and C. Beckermann [1]. It describes mushy zone flow by considering an anisotropic permeability of the dendritic region. At the free surface, Marangoni or surface tension driven flow is described by a corresponding boundary condition. To evaluate the influence that different temperature dependencies of the surface tension gradient $\partial\gamma/\partial T$ exert on the weld pool, comparative calculations of the distribution of temperature, velocity, fraction of solid and alloy concentration are performed as a function of time.

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Introduction

To achieve good results in the simulation of solidification it is necessary to consider both macroscopic and microscopic processes. On the one hand macroscopic temperature and flow fields are highly influenced by microscopic solidification and segregation effects. On the other hand the local solute redistribution is a result of the development in time of these temperature and flow fields.

In addition to thermo-solutal convection effects caused by density gradients inside the melt there is a class of surface tension driven effects, called Marangoni convection. These convection effects due to surface tension gradients do not play a great role in casting processes because the temperature gradients are comparatively small. The situation during a laser welding process is different. The high power coupled into a small area creates steep temperature gradients. The resulting Marangoni convection can completely overlie thermo-solutal convection. Thus the weld pool and the final solute redistribution are significantly altered.

To predict the resulting distribution of alloy elements in a multicomponent steel subjected to laser welding, calculations are presented, taking into account solute, heat, mass and momentum conservation in two dimensions. Special emphasis is placed on the investigation of the influence of different behavior of Marangoni convection caused by different temperature dependencies of surface tension.

Numerical Procedure

Basic Relations

For this research a two dimensional model of Ni and Beckermann [1] was extended to the simulation of Marangoni convection. It is based on an implicit FDM-solver using the SIMPLER algorithm proposed by Patankar [2]. The microscopic conservation equations are integrated over a representative 'averaging volume' to yield a set of macroscopic equations. Three microsegregation models, the lever-rule, the Scheil-model and a 'backdiffusion-model' can be chosen. The latter takes into account the typical solidification specifications of steel. The reduced permeability of the mushy zone was taken into account introducing an anisotropic permeability tensor that uses the angle of dendrite growth given by the local temperature gradient. During the derivation of the macroscopic conservation equations the following simplifications were made: stationary solid phase, Boussinesq approximation in the description of thermo-solutal convection, thermodynamic equilibrium and full mixture inside the averaging volume, and no diffusive cross effects between the alloy elements. A summary of the method can be found in Schneider and Beckermann [3]

Marangoni Convection

Marangoni convection is driven by local variations of the surface tension γ. Surface tension gradients result in flows towards regions with higher values of γ. Viscosity couples the surface velocity into the fluid and may cause convection rolls. Two kinds of effects can be observed: *thermal* and *solutal Marangoni convection*. The governing equation describing both effects is:

$$\tau_{st} = \mu\left(\frac{\partial u}{\partial y}\right) = \left(\frac{\partial \gamma}{\partial T}\right)\left(\frac{\partial T}{\partial x}\right) + \sum_i \left(\frac{\partial \gamma}{\partial a_i}\right)\left(\frac{\partial a_i}{\partial x}\right) \quad (1)$$

where τ_{st} is the shear stress caused by the surface tension gradients, and which has to be balanced by inertia forces of the fluid, μ is the viscosity, u is the velocity component parallel to the surface, x and y are the coordinates parallel and perpendicular to the surface, T is the local temperature, and a_i is the thermodynamic activity of alloy element i. The velocity gradient $\partial u / \partial z$ applied to the flow field as a Cauchy boundary condition on the liquid/gas boundary of the surface.

The surface tension gradients $\partial\gamma/\partial T$ and $\partial\gamma/\partial a_i$ are found to depend strongly on the local temperature and activity respectively. A semi-empirical equation set up by P. Sahoo *et al.* [4] for binary metal-solute systems gives the following expression for the temperature and activity dependence of surface tension:

$$\gamma(T, a_s) = \gamma_m^0 - A(T - T_m) - RT\Gamma_s \ln\left(1 + k_1 a_s e^{-(\Delta H^0 / RT)}\right) \qquad (2)$$

In equation (2) γ_m^0 is the surface tension of the pure metal at the melting point, A represents $-\partial\gamma/\partial T$ for the pure metal, T_m is the melting point of the pure metal, Γ_s is the surface excess of the solute species at saturation, a_s is the activity of the species (in wt %), ΔH^0 is the standard heat of adsorption and k_1 is a constant which is related to the entropy of segregation.

Even if we are not considering a binary alloy, the equation can be taken as a first approach to a good qualitative description of Marangoni convection. As generally the solutal Marangoni convection is considered to be much smaller than thermal convection, in this work the solutal effect has been disregarded. Nevertheless $\partial\gamma/\partial T$ depends on the local activity a_s. Differentiation of Eq. (2) with respect to T yields:

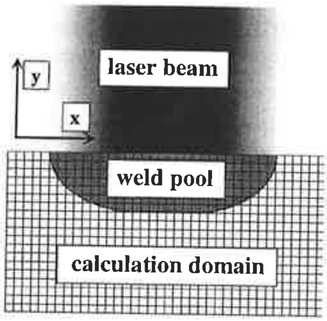
$$\frac{\partial\gamma}{\partial T} = -A - R\Gamma_s \ln\left(1 + K_{seg}\, a_s\right) - \frac{K_{seg}\, a_s}{1 + K_{seg}\, a_s} \frac{\Gamma_s \Delta H^0}{T} \quad \text{where} \quad K_{seg} = k_1 e^{-(\Delta H^0 / RT)} \qquad (3)$$

In our calculations the activity a_s was taken to be equal to the local concentration of the highly surface active component sulfur, initially set at 0.014 wt%. Table I shows the constant values used for the calculations, presented by P. Sahoo *et al.* [4] for a binary Fe-S system and by R.T.C. Choo *et al.* [4] for the industrial steel AISI 304. They only differ in the value for ΔH^0, the standard heat of adsorption, that Sahoo found to be the critical parameter of $\partial\gamma/\partial T$. Since the equidistant grid is not able to resolve the steep velocity gradient in the extremly thin surface layer, Eq. (3) was scaled by a relaxation factor to model the velocity decrease inside the surface element.

Apart from using this equation some preliminary calculations were made to investigate the possible different behavior of surface tension. Positive and negative temperature dependencies were tried and the results compared to those of calculations without Marangoni convection.

Setup for the Calculations

The setup used for the calculations, Fig. 1, was a spot welding process of an infinite 2D-plate with a thickness of 6 mm. A 12 × 6 mm section of this plate (fixed grid of 80 × 40 square volume cells), consisting of the industrial multi-component steel GS60 (Table II), was simulated. It was melted by a stationary laser beam with vertical incidence. The initial temperature of the calculation domain was set at 300 K. The boundary conditions at the top and bottom surface were air convection and radiation. On the top surface the laser energy was brought in as a stationary heat flux. The gauss-shaped laser beam with a diameter (intensity decay to $1/e$ of maximum value) of 4.6 mm was to provide a maximum heat flux of 10^8 W/m^2. The laser beam was to be switched off after three seconds and the calculation continued until complete resolidification of the weld pool. Since vaporization at the surface was not modelled, the surface temperature was explicitly limited to 2500 K. This causes the steepest temperature



$A = 4.3 \times 10^{-4}$ N/(m·K)
$R = 8314.3$ J/(mol·K)
$\Gamma_s = 1.3 \times 10^{-8}$ mol/m^2
$k_l = 3.18 \times 10^{-3}$
$\Delta H^0 = -1.88\times10^8$ J/mol (AISI 304)
$= -1.66\times10^8$ J/mol (Fe-S)

Table I - Constant values used in Eq. (3), determined by P. Sahoo *et al.* [4] for an Fe-S system and R.T.C. Choo *et al.* [5] for AISI 304.

Figure 1 – Principal setup for the calculations showing the 12×6 mm steel block with the incident gauss-shaped laser beam.

Alloy element	C	Mn	Si	S	P	Ni	Cr	Cu	Mo
wt %	0.420	0.800	0.600	0.014	0.015	0.100	0.100	0.100	0.020

Table II: Composition of the industrial multi-component steel GS60.

gradients and the strongest Marangoni effects to occur at the borders of the weld pool. To simulate infinite dimension at the lateral boundaries, the temperature gradients were continued, multiplied by a relaxation factor 0.8.

Results and Discussion

Different Shapes of the Weld Pool

A series of three calculations were made to investigate the influence of different temperature dependencies of surface tension onto the flow field and the shape of the weld pool. The surface tension gradient $\partial\gamma/\partial T$ was to take the constant values:

- -10^{-5} Marangoni convection towards lower temperatures;
- 0 no Marangoni convection at all;
- 10^{-5} Marangoni convection towards higher temperatures.

The results show that Marangoni convection can dominate thermo-solutal convection and that it can change the shape of the weld pool significantly by changes in the heat transport behavior (Fig.2). For the negative gradient, Fig. 2a), Marangoni convection amplifies the thermal convection rolls. Hot melt is quickly driven off the center and the weld pool becomes larger. For the positive gradient, Fig. 2c), Marangoni convection compensates and inverts the thermal convection rolls. Hot melt is driven towards the bottom of the weld pool and its depth increases. The calculated pool shapes correspond to the results presented by K.A. Pericleous and C. Bailey [6] and Y.P. Lei *et al.* [7]

Due to the comparable handling of all alloy elements (all partitioning coefficients $\kappa_i < 1$; values following Böhmer *et al.* [8]; assumption of infinitely fast solute diffusion in the solid on a microscopic scale, i.e. a lever-rule type model), the concentration deviations are qualitatively the same for all components. In general the segregations differ only quantitatively. As a representative example Fig. 2 shows the macro segregation of carbon (right).

The calculation without Marangoni convection, Fig. 2b), shows an enrichment of up to 60 % of the initial concentration near the surface in the middle of the weld pool. This is due to the fact

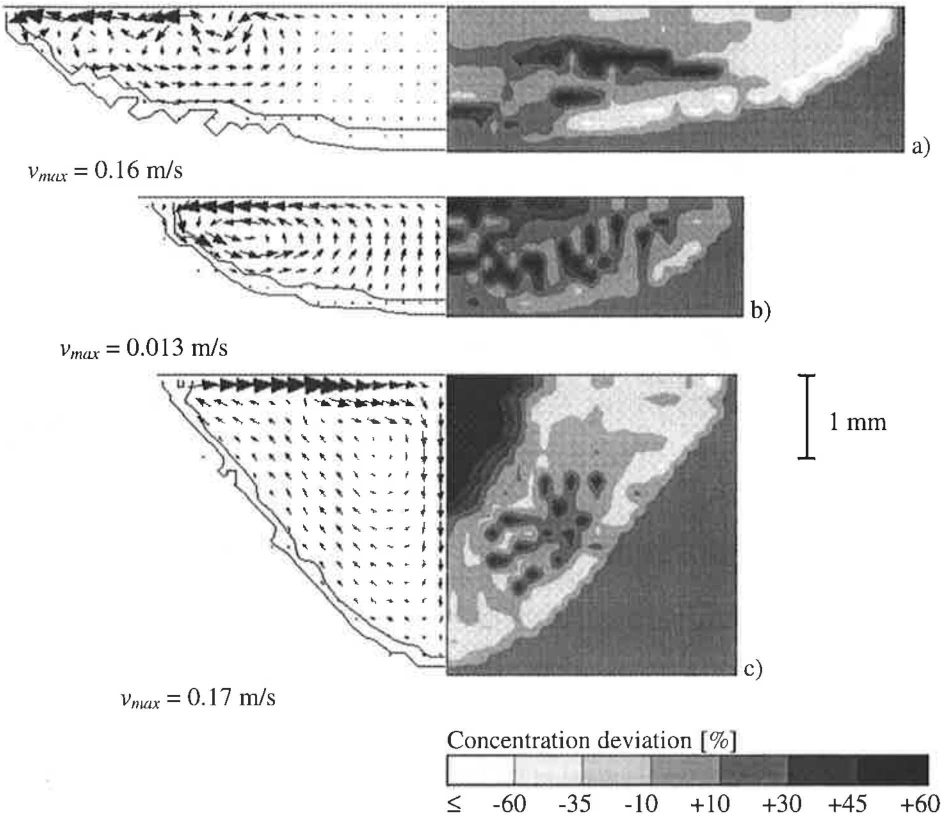


Figure 2 - Influence of different temperature dependencies of the surface tension. $\partial\gamma/\partial T$ = *const* taking the values a) -10^{-5}, b) 0, c) 10^{-5}. Shape of the weld pool and fully developed flow field after 3 s (left; notice the different maximal velocities); the border lines show the mushy zone with fraction solid between 0.3 and 0.98; concentration deviation from the initial carbon concentration after total resolidification (right).

that the melt solidifying last is enriched the most. For $\partial\gamma/\partial T < 0$, Fig. 2a), the high velocities result in a good mixture of the weld pool. The enriched melt is transported towards the outer parts of the pool and mixed well by the strong convection rolls. For $\partial\gamma/\partial T > 0$, Fig. 2c), the flow is directed towards the center. The enriched melt is not spread out all over the pool, but concentrated near the center. The dark spots in Fig. 2b) and 2c) cannot easily be interpreted. parts of it are enclosed by completely solidified regions. The dark spots are the areas that During the rapid solidification of these parts of the pool the mushy zone becomes instable and solidify last. We have so far not discovered whether these segregations are due to a physical effect or if they are numerical artefacts. Possibly they could be compared to the single spots appearing during the calculations of segregation channels presented by M.C. Schneider and C. Beckermann [9]. Due to the steep temperature gradients in the weld pool the mushy zone is quite narrow and the spots could result from an effect that is not completely developed.

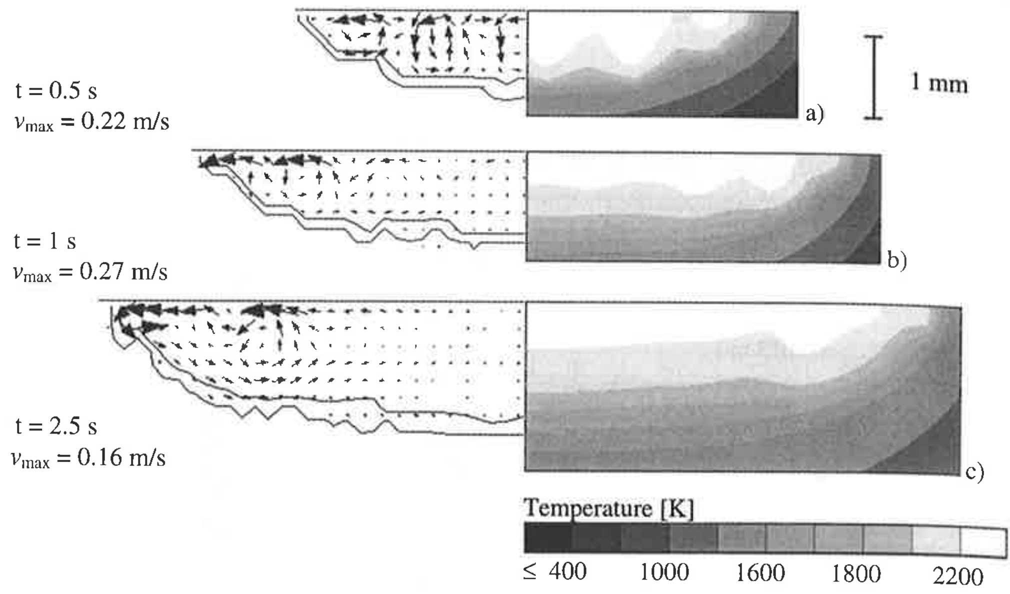


Figure 3 - Development of small Marangoni driven convection rolls in the flat weld pool. Shape of the weld pool and flow field (left); the border lines show the mushy zone with fraction solid between 0.3 and 0.98; temperature distribution in the pool (right) after 0.5 s, 1 s and 2.5 s.

<u>Small Convection Rolls in the Flat Weld Pool</u>

A detailed view of the development of the flow field for $\partial\gamma/\partial T < 0$ shows an interesting effect. At the beginning of the melting process the melt pool is still flat. The high temperature gradients at the surface cause a fast Marangoni flow in the surface layer. This material transport is compensated by a back flow at the bottom of the pool. Induced by instabilities the friction between the surface flow and the bottom flow causes the formation of small convection rolls, Fig. 3a). The traces of the vertical melt transport can be found in the structure of the corresponding temperature profile. As the melting process advances and the maximum temperature shifts towards the margins of the pool, the convection rolls shift in the same direction, too, Fig. 3b). After 2.5 s, when the weld pool has grown deeper, the small cells have been dissolved to produce a single, larger, slower roll, Fig. 3c). Apart from this a small cell remains at the place where the Marangoni convection hits the border of the pool.

<u>Application of an Analytical Expression for $\partial\gamma/\partial T$</u>

To test the influence of a more realistic approach to describe $\partial\gamma/\partial T$, calculations were made using Eq.. (3) with the parameter values taken from P. Sahoo *et al.* [4] and R.T.C. Choo *et al.* [5] (Table I), taking into account the influences of temperature and the concentration of the highly surface active component sulfur on the behavior of the surface tension. The results for the calculation using the constant values of AISI 304 are shown in Fig. 4. The flow field, Fig. 4a), shows a point on the surface where the Marangoni induced velocities change the direction. This occurs at a temperature of about 2300 K, Fig. 4b). At this temperature $\partial\gamma/\partial T$ changes the sign. The two opposite surface flows result in a downward flow of hot melt. As

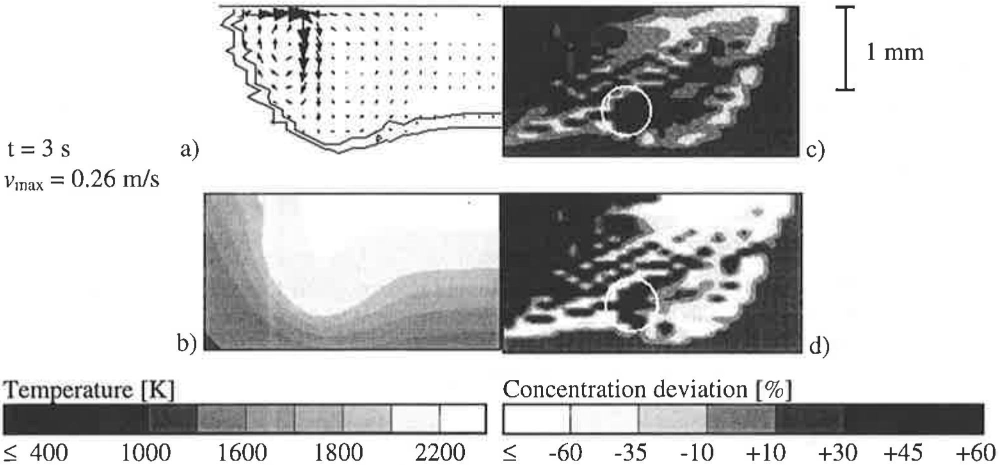


Figure 4 - Calculation using the temperature and concentration dependence of $\partial\gamma/\partial T$ proposed by P. Sahoo *et al.* [4] and the constant values for AISI 304 (Table I). a) Shape of the weld pool and fully developed flow field; the border lines show the mushy zone with fraction solid between 0.3 and 0.98; b) Temperature distribution at the end of the welding period (3 s); c), d) Concentration deviation of the initial carbon and sulfur concentrations. The white circles show a segregation area probably caused by a downflow of enriched melt.

already seen in Fig. 2c), this leads to an increase in depth of the weld pool at this point, Fig. 4a).

The segregation of carbon, Fig. 4c), and sulfur, Fig. 4d), at the end of resolidification shows a high enrichment in the middle of the weld pool, where the material finally solidifies. A small segregation near the bottom of the pool (white circles) may result from the transport of enriched melt by the Marangoni induced downflow. As already mentioned the concentration distributions of carbon and sulfur qualitatively do not vary much, but obviously the effect is stronger for sulfur.

Comparative calculations varying the critical parameter ΔH^0 showed a strong dependence of the weld pool shape on that value. Increasing ΔH^0 lowers the temperature T_{cM} where Marangoni convection changes its direction. For $\Delta H^0 = -1.88\times10^8$ J/mol (AISI 304) T_{cM} becomes 2287 K, for $\Delta H^0 = -1.66\times10^8$ J/ mol (Fe-S) 2020 K. This means that for the Fe-S system the point of the downward flow is shifted to the extreme edge of the weld pool and the pool shape becomes similar to that resulting from $\partial\gamma/\partial T < 0$ (Fig. 2a)).

Conclusions

The behavior of $\partial\gamma/\partial T$ has a big influence on the shape of the weld pool, the development of the flow field and, hence, on the resulting distribution of the alloy elements. The Marangoni convection mainly determines the characteristics of heat and mass transport. The changes in heat transport result in variations of depth, width and shape of the weld pool. The changes in mass transport alter the final distribution of the alloy elements. The quality of the prediction of pool shape and segregations depends strongly on the quality of the thermodynamic data used in the equation for $\partial\gamma/\partial T$.

The possibility of predicting segregation effects opens the way to a better investigation of solutal Marangoni convection. The interaction between Marangoni induced flow and flow determined segregation can be analyzed.

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