Simulation of a weld pool interface motion by a variational inequality approach

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Abstract

This work deals with the numerical simulation of the temperature field within the solid part of a metallic piece during a welding process. By using an integral transformation such as the Duvaut’s transform, the direct heat transfer problem is formulated as a parabolic variational inequality in a fixed domain. It consists of determining the temperature distribution in the solid region, coupled with the location and the motion of the weld pool interface and the heat flow crossing it, which is modelled by a Stefan’s condition. The method is applied to numerically solve the solution of a phase change problem formulated in a 2-D cylindrical geometry. The computed temperature field is compared with results given by a standard method.

Keywords: Stefan problem, front of fusion, heat source, Duvaut’s transform, variational inequality, finite element.

1 Introduction

Fusion welding is the most frequently used metal joining method. It is a process by which the edges of two pieces of metal are melted and fused together. This is accomplished by using an intense local energy source. During the heating and cooling cycles while welding, thermal strains occur and generate residual stresses and distortions in the welded structure. One of the major industrial challenges is to predict these mechanical effects. Thus, in order to evaluate these mechanical effects with accuracy, it is necessary to have a thermal model which takes in to account the welding process.
This work focuses on the determination of the temperature field in the work piece without setting in advance the form of heat source which represents the local energy source of the process by solving an inverse thermal conduction problem with a moving boundary. The temperature field during welding can be computed by solving a Stefan problem with convection in the liquid part. Our objective is to find the front position and the convective heat flux on this boundary from solving a pure heat conduction problem only in the solid part and using temperature measurements in the solid part. This approach must allow a simplified but realistic simulation of the temperature field due to the welding process and will finally give reliable model for various operating conditions and process including process involving filler metal transfer as Gas Metal Arc Welding.

Two methods are usually used to obtain the temperature field:

1) One is to solve a magnetohydrodynamic problem coupling the physics of the energy source, its interaction with the welding pool, the energy transfer in the welding pool and its diffusion in the solid ([1]-[2]). Process hypothesis can be done to avoid the coupling with the energy source physic leading to parameters estimations associated with the resolution of the weld pool simulation. This problem is still very complex and still requires important computation facilities and an exorbitant computing time [3].

2) The other one is to use an equivalent source approach [4]. Under this assumption, we use a parameterized heat source distribution representing the energy of the process. A non-linear problem of heat conduction is consequently solved. The parameters of this source model are estimated by solving an inverse problem ([5]-[8]). However, this method shows some limits because it is difficult to obtain in a satisfactory way the form of the pool and the temperature field at the points of measurement. From the mathematical side, this approach is not exactly equivalent to the first method.

The inverse Stefan problem has growing in interest recently ([9]-[13]). However, reliable direct measurements of the temperature profile in the weld pool are difficult due to the small fusion zone, the intense arc plasma and the large temperature gradient. Approaches were performed using only information within the solid part ([14]-[15]). From the point of view of the solid, the heat transfer problem would be rigorously identical to a two phase Stefan problem if we know at any given time the position of the solid-liquid interface and the heat flux crossing it.

1.1 Symbols and notation

\( \lambda_s \): thermal conductivity of the Solid  \( \varphi \): heat flux
\( \rho_s \): density of the Solid  \( T_e \): exterior temperature
\( \rho_L \): density of the Liquid  \( T_0 \): initial temperature
\( c \): heat capacity  \( T_f \): melting temperature
\( L \): latent heat of fusion  i,k: index of nodes
\( t \): time  \( \Delta t \): time step
2 Formulation of the direct problem in the solid

2.1 Geometrical description

Let $\Omega_{\text{tot}}$ be an open bounded set on $\mathbb{R}^n$ ($n = 2, 3$ in our applications), with boundary $\partial\Omega$ and $[0, T_{\text{fin}}]$ a finite interval. $\Omega_s(t) \subseteq \Omega_{\text{tot}}$ is the solid region at time $t \in [0, T]$, so the liquid domain is denoted as $(\Omega_{\text{tot}} \setminus \Omega_s(t))$. Let us denote the interface between solid and liquid as $\Gamma(t)$. We define therefore the following partition: $\Omega_{\text{tot}} = \Omega_l(t) \cup \Gamma(t) \cup \Omega_s(t)$. At a point $X = (x, y, z) \in \Gamma(t)$, the unit normal vector on the interface pointing away from the liquid region is denoted as $\vec{n}$. Let us partition $\partial\Omega$ into three parts $\partial\Omega_D$, $\partial\Omega_N$, $\partial\Omega_C$ on which we apply respectively the boundary condition of Dirichlet, Neumann and Cauchy.

2.2 Governing equation

We write the equations governing the heat transfer in the solid. The convective heat flux from the liquid domain is denoted as $\varphi_L$. The temperature in the solid is negative and is the solution of the heat conduction equation. So $\theta$ is the solution of the following problem in which $\Omega_s(t)$ is unknown:

**Problem 1:**

\[
\rho_s c_p \left( \frac{\partial \theta}{\partial t} + \vec{v}_{\text{torche}} \nabla \theta \right) - \nabla \cdot \left( \lambda_s \nabla \theta \right) = 0 \text{ in } \Omega_s(t) \times [0, T_{\text{fin}}] \\
\theta < 0 \text{ in } \Omega_s(t) \times [0, T_{\text{fin}}] \\
\theta = 0 \text{ on } \Gamma(t) \\
\lambda_s \frac{\partial \theta}{\partial n} = \varphi_L \vec{n} - \rho_s L \left( \vec{v} + \vec{v}_{\text{torche}} \right) \vec{n} \text{ on } \Gamma(t) \\
\theta(x, y, z, 0) = \theta_0(x, y, z) \text{ for } t = 0 \\
\theta = \theta_D \text{ on } \partial\Omega_D \times [0, T_{\text{fin}}] \\
\lambda_s \frac{\partial \theta}{\partial n} = \varphi_N \text{ on } \partial\Omega_N \times [0, T_{\text{fin}}] \\
\lambda_s \frac{\partial \theta}{\partial n} + h \theta = h \theta_e = -h \text{ on } \partial\Omega_C \times [0, T_{\text{fin}}]
\]
The equations (3) and (4) characterize the free boundary. The equation (3) defines the temperature and the (4) writes the energy balance on the free boundary. The isothermal condition specified in (3) is the simplest form of the imposed Dirichlet condition. It is justified only if the free boundary is plane and if the thermodynamic balance is realized. However, the melting balance temperature depends on the surface tension curvature of the free boundary. That’s what we call the Gibbs-Thomson effect. Similarly, the balance temperature may depend also on the speed of free boundary, being known as a kinetic condition.

If we admit that the free boundary is at the thermodynamic balance, we could define $\Gamma(t)$ by:

$$\Gamma(t) = \left\{ (x,y,z,t) \in \Omega_{\text{tot}} \times [0,T_{\text{fin}}] \mid \theta(x,y,z,t) = 0 \right\}$$

so that $\theta(x,y,z,t) > 0$ ($< 0$) correspond to the liquid (solid).

In those conditions, we define the normal vector of $\Gamma(t)$ by

$$\vec{n} = \frac{\nabla \theta(x,y,z,t)}{||\nabla \theta(x,y,z,t)||}$$

If the surface is sufficiently regular, we can write:

$$\Gamma(t) = \left\{ (x,y,z,t) \in \Omega_{\text{tot}} \times [0,T_{\text{fin}}] \mid S(x,y,z) - t = 0 \right\}$$

where $S(x,y,z)$ indicate the time for which the point $(x,y,z)$ changes phase. We can therefore write

$$\vec{n} = \frac{\nabla \theta(x,y,z,t)}{||\nabla \theta(x,y,z,t)||} = \frac{\nabla S(x,y,z)}{||\nabla S(x,y,z)||}$$

Let us denote $\varphi_n = \vec{\varphi}_L \cdot \vec{n}$ and $\vec{v}_n = \vec{v} \cdot \vec{n}$.

If we calculate the differential of the equation defining $\Gamma(t)$:

$$S(x,y,z,t) - t = 0 \Rightarrow \nabla S(x,y,z),\vec{v} = 1 \Rightarrow v_n = \vec{v} \cdot \vec{n} = \frac{1}{||\nabla S(x,y,z)||}$$

By using the equations (3) and (4), we can rewrite below the equation (4):

$$\lambda_S \nabla \theta \cdot \nabla S(x,y,z) = \varphi_n ||\nabla S(x,y,z)|| - \rho_S L \left[ v_n + \varphi_{\text{torche}} \nabla S(x,y,z) \right]$$

on $\Gamma(t)$

3 Transformation

The front of fusion divides the total domain into two sub domains, the liquid pool and the solid domain. When this front propagates, these two sub domains are redefined, therefore to solve uniquely the heat transfer problem in the solid part by using for example a finite element method, we have to re-mesh it at each time step. Let us recall that our objective is to work only in the solid domain and
on a fixed mesh. So, to overcome these difficulties, we will introduce an integral transformation (transformation of Duvaut).

\[
\begin{align*}
\{ & u(x, y, z, t) = \int_t^{T_{\text{fin}}} \theta(x, y, z, \tau) d\tau & \text{in } \Omega_S(T_{\text{fin}}) \\
& u(x, y, z, t) = \int_t^{T_{\text{fin}}} \theta(x, y, z, \tau) d\tau & \text{in } \Omega_S(T_{\text{fin}}) \\
& u(x, y, z, t) = 0 & \text{in } \Omega_l(t)
\end{align*}
\]

We impose \( X = (x, y, z) \rightarrow \frac{\partial u(X, t)}{\partial t} = -\theta(X, t) \) in \( \Omega_{\text{tot}} \).

The new variable \( u \) is continuous and its first derivatives are continuous in the whole domain; this is proved in [15]. So a variational formulation of the problem in \( u \) can be introduced.

**DEFINITION 1** We note \( u_d, \phi_N \) and \( u_C \) the Duvaut’s transform of the boundary condition \( \theta_D, \varphi_N \) and \( h\theta_e \).

### 3.1 Formulation of the transformed problem

The following problem in \( u \) is equivalent to the problem defined by equations (1) to (8).

**Problem 2** Find \( u \) such that:

\[
\rho_S c_p \left( \frac{\partial u}{\partial t} + \vec{v}_{\text{torche}} \nabla u \right) - \lambda_S \Delta u = -\left( \phi_n \left\| \nabla S \right\| - \rho L \left( 1 + \vec{v}_{\text{torche}} \nabla S \right) \right)
\]

in \( \Omega_s(t) \setminus \Omega_s(T) \times [0, T_{\text{fin}}] \) \hspace{1cm} (10)

\[
\rho_S c_p \left( \frac{\partial u}{\partial t} + \vec{v}_{\text{torche}} \nabla u \right) - \lambda_S \Delta u = -\rho_S c_p \theta(X, T_{\text{fin}})
\]

in \( \Omega_s(t) \) \hspace{1cm} (11)

\[
u(X, t) = 0 \hspace{1cm} \text{in } \Omega_l(t) \hspace{1cm} (12)
\]

\[
u(X, t) < 0 \hspace{1cm} \text{in } \Omega_s(t) \times [0, T_{\text{fin}}] \hspace{1cm} (13)
\]

\[
u(X, 0) = S(X) \int_0^{T_{\text{fin}}} \theta(X, 0) d\tau \hspace{1cm} \text{in } \Omega_s(0) \setminus \Omega_s(T_{\text{fin}})
\]

\[
u(X, 0) = \int_0^{T_{\text{fin}}} \theta(X, 0) d\tau \hspace{1cm} \text{in } \Omega_s(T_{\text{fin}})
\]

\[
u(X, 0) = 0 \hspace{1cm} \text{in } \Omega_l(0) = \text{initial liquid}
\]
\begin{align*}
\frac{\partial u(X,t)}{\partial n} &= \phi_N \quad \text{on } \partial \Omega_N \quad (16) \\
\frac{\partial u(X,t)}{\partial n} + hu(X,t) &= u_C \quad \text{on } \partial \Omega_C \quad (17)
\end{align*}

In this problem \( \Omega_S(t) \) and therefore \( S(X) \), are unknown.

**Theorem 1**: If \( u \) is defined by Duvaut’s transform (9), with \( \theta \) solution of problem 1, then \( u \) is the solution of problem 2 (Proof [15]).

### 3.2 Inequality formulation in \( u \) in the known domain \( \Omega_{tot} \)

The unknown domain \( \Omega_S(t) \) appears explicitly in the preceding problem (10) – (17). Our objective is to be able to work in a fixed and known domain. We present an inequality system, verified by \( u \) in \( \Omega_{tot} \), equivalent to the problem 2. To simplify the second member of heat equation, we introduce the following definition.

We define a function \( H(X,t) \) such that:

\[ H(X,t) = \begin{cases} 
- \left( \nabla S \cdot \nabla \cdot (1 + \nabla \cdot \nabla S) \right) & \text{in } \Omega_S(t) \setminus \Omega_S \times [0, T_{fin}] \\
- \rho_S c_p \theta(X, T_{fin}) & \text{in } \Omega_S(T_{fin}) \\
> 0 & \text{in } \Omega(t)
\end{cases} \quad (18)
\]

The function \( H(X,t) \) depends on \( \rho_n \) and \( S(X) \), so it is unknown. We introduce a set of equations defined on \( \Omega_{tot} \), equivalent to the problem 2.

**Problem 3** Find \( u \) such that

\[ \rho_S c_p \left( \frac{\partial u}{\partial t} + \nabla \cdot \nabla u \right) - \lambda_S \Delta u - H(X,t) = 0 \quad \text{in } \Omega_{tot} \times [0, T_{fin}] \quad (19) \\
\rho_S c_p \left( \frac{\partial u}{\partial t} + \nabla \cdot \nabla u \right) - \lambda_S \Delta u - H(X,t) \leq 0 \quad \text{in } \Omega_{tot} \times [0, T_{fin}] \quad (20) \\
u(X,t) \leq 0 \quad \text{in } \Omega_{tot} \times [0, T_{fin}] \quad (21)
\]

\[ u(X,0) = \int_0^{S(X)} \theta(X,0) d\tau \quad \text{in } \Omega_S(0) \setminus \Omega_S(T_{fin}) \quad (22) \]

\[ u(X,0) = \int_0^{T_{fin}} \theta(X,0) d\tau \quad \text{in } \Omega_S(T_{fin}) \quad (23) \]

\]
\[ \lambda \frac{\partial u(X,t)}{\partial n} = \phi_N \quad \text{on } \partial \Omega_N \]  
\[ \lambda \frac{\partial u(X,t)}{\partial n} + h u(X,t) = u_C \quad \text{on } \partial \Omega_C \]  

**Theorem 2:** the equation system (10) – (17) is equivalent to the *problem 3* defined on \( \Omega_{\text{tot}} \) (Proof [15])

### 4 Variational inequality formulation

\( u \) and the first partial derivatives of \( u \) are continuous in \( \Omega_{\text{tot}} \), so a variational formulation of *problem 3* can be done.

**DEFINITION 2:** Let us define a bilinear application \( a(,) \) on a Hilbert’s space \( V \) and a linear application \( b() \) on \( V \) by:

\[
\lambda \nabla \cdot \nabla \int_{\Omega_{\text{tot}}} \lambda
\\nabla u \cdot \nabla v \, dX
\]

\[
\int_{\partial \Omega_N} \phi_N v d\Gamma + \int_{\partial \Omega_C} \frac{\partial u}{\partial n} v d\Gamma + \int_{\Omega_{\text{tot}}} H v dX
\]

(26)

By using Riesz’s theorem [20] the variational problem is defined as follows:

**Problem 4** (Variational inequality) Find \( u \) such that

\[
\int_0^{T_{\text{fin}}} \left( \rho_S c_p \left( \frac{\partial u}{\partial t} + \nabla_{\text{torche}} \nabla u \right), v - u \right) dt + \int_0^{T_{\text{fin}}} a(u,v-u) dt \geq \int_0^{T_{\text{fin}}} b(v-u) dt \quad \forall v
\]

(27)

**Theorem 3:** If \( u \) is the solution of the problem 3, then \( u \) is the solution of the variational *problem 4* (Proof [15]). The unicity of this problem is presented in [15] and proved in [16], [18] and [19].

### 4.1 Numerical resolution of the variational inequality

To solve the variational problem (27), we discretise the inequality by a finite element method. Numerical computational has been performed by cast3M (http://www-cast3m.cea.fr). The finite - element formulation is given below:

For \( t \in [0, T_{\text{fin}}] \), let us denote as \( \underline{U}(t), \underline{V}(t), \frac{\partial \underline{U}}{\partial t}(t), \frac{\partial \underline{V}}{\partial t}(t) \) and \( H \) the

\( \mathbb{R}^{n_{bn}} \) vector defined by:

\[
\frac{\partial \underline{U}}{\partial t} = \left[ \frac{\partial u_1}{\partial t}(t), \frac{\partial u_2}{\partial t}(t), \ldots, \frac{\partial u_{n_{bn}}}{\partial t}(t) \right]^T
\]

\[
\underline{U} = [u_1(t), u_2(t), \ldots, u_{n_{bn}}(t)]^T, \quad \underline{V}U = \left[ \frac{\partial u_1}{\partial X}(t), \frac{\partial u_2}{\partial X}(t), \ldots, \frac{\partial u_{n_{bn}}}{\partial X}(t) \right]^T
\]
Problem 5 : (Approximated system, Inequality system in $\mathbb{R}^{nbm}$) For a given $U_0 \in \mathbb{R}^{nbm}$, find $U_{i+1} \in K^i_R$ for $i = 0, \ldots, nT-1$ such that for each $V_{i+1} \in K^i_R$

$\left( \left( \frac{MT}{\Delta t} + kK^T \right) U_{i+1} + MT \nabla U_{i+1} - V_{i+1} \right)_{R^{obs}} \geq \left( \frac{MT}{\Delta t} U_i + MT H_{i} - U_{i+1} \right)_{R^{obs}} \tag{28}$

So, we solve the direct problem, i.e. "to find $u$ knowing $H$", by finding a solution of the approximated problem (28).

5 Application to a two-dimensional axisymmetric case

In the standard method (with Lagrange multiplier) we involve the heat transfer problem with a gaussian heat flux as presented in Figure 1.

The results obtained by solving the transformed problem with variational inequality are compared with the standard method (Figure 2).

$\theta = \frac{T - T_j}{T_j - T_c}$, $T_j = 1450^\circ C, T_0 = T_e = 20^\circ C, h = 20$ so the problem in $\theta$ is formulated

$\rho_S c_p \frac{\partial \theta}{\partial t} - \nabla \cdot (\lambda_S \nabla \theta) = 0$ in $\Omega_S(t) \times [0, 200]$ 

$\theta < 0$ in $\Omega_S(t) \times [0, 200]$ , $\theta(x, y, z, 0) = -1$

$\theta = 0$ on $\Gamma(t), \lambda_{S} \frac{\partial \theta}{\partial n} = \phi_0 \tilde{n} - \rho_S L \tilde{v} \tilde{n}$ on $\Gamma(t)$;

$\theta = 0$ on $\partial \Omega_{D} \times [0, 200]$, $\lambda_{S} \frac{\partial \theta}{\partial n} = \phi_0 \partial \Omega_{N} \times [0, 200]$, $\lambda_{S} \frac{\partial \theta}{\partial n} + h \theta = -20$ on $\partial \Omega_{C} \times [0, 200]$

Duvaut's transform:

$u(x, y, z, t) = \int_{t}^{S(x, y, z)} \theta(x, y, z, \tau) d \tau$ in $\Omega_S(t) \setminus \Omega_S(200)$

$u(x, y, z, t) = \int_{t}^{200} \theta(x, y, z, \tau) d \tau$ in $\Omega_S(200)$

$u(x, y, z, t) = 0$ in $\Omega_1(t)$

Formulation of transformed problem

$\left[ \rho_S c_p \frac{\partial u}{\partial t} - \lambda_S \Delta u - H(X, t) \right] u = 0$ in $\Omega_{tot} \times [0, 200]$

$\rho_S c_p \frac{\partial u}{\partial t} - \lambda_S \Delta u - H(X, t) \leq 0$ in $\Omega_{tot} \times [0, 200]$
\[ H(X,t) = \begin{cases} 
- \left( \varphi_n \| \nabla S \| - \rho_L L \right) & \text{in } \Omega_S(t) \setminus \Omega_S \times [0, 200] \\
- \rho_S c_p \theta(X, 200) & \text{in } \Omega_S(200) \\
> 0 & \text{in } \Omega_S(t) 
\end{cases} \]

Gaussian Heat Flux \( h = 20 \)

**Figure 1:** Two-dimensional model.

\[ u(X, t) \leq 0 \text{ in } \Omega_{tot} \times [0, 200] \]
\[ u(X, t) = 0 \text{ on } \partial \Omega_D, \]
\[ \lambda \frac{\partial u(X, t)}{\partial n} = \phi_N \text{ (on } \partial \Omega_N ) = \begin{cases} 0 & r = 0, 0 < z < b \\
f(r) & 0 < r < c, z = 0 \\
0 & r = a, 0 < z < b \end{cases} \]
\[ \lambda \frac{\partial u(X, t)}{\partial n} + 20u(X, t) = 20(t - 200) \text{ on } \partial \Omega_C, \]
\[ u(X, 0) = -S(X) \text{ in } \Omega_S(0) \setminus \Omega_S(200), u(X, 0) = -200 \text{ in } \Omega_S(200) \]

**Figure 2:** Comparison of variational inequality (cross) and the solution of standard method (black line) at \( t = 10s, 150s, 200s. \)
6 Conclusions

A direct heat transfer model is developed to the determination of weld pool interface location and the convective heat flux crossing it without setting in advance the form of heat source. By using Duvaut’s transform the direct heat transfer problem is formulated as a parabolic variational inequality in a fixed domain. The numerical solution of the variational inequality problem is equivalent to that obtained by a standard method. Now this method can be applied to solve the inverse heat transfer problem which aims to reconstruct the motion of the free boundary.

References


