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POWERS IN METHYLENE BLUE TESTING SINCE 1974

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COMPUTATIONAL WELD ANALYSIS FOR LONG WELDS

by

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A thesis submitted to
the Faculty of Graduate Studies and Research
in partial fulfillment of
the requirements for the degree of

Doctor of Philosophy

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COMPUTATIONAL WELD ANALYSIS FOR LONG WELDS

Abstract

Due to the limited capacity of computers, we are not yet able to run analyses for large welds or multi-pass welds. However, one can decompose the analysis for large welds into three stages, i.e., starting transient, ending transient and a long period of a quasi-steady state in between. This thesis aims at computing physical changes in large welds, especially during the quasi-steady state period.

In the first part of the thesis, a detailed analysis of temperatures, microstructures and thermal stresses has been performed based on the assumption of steady state. For thermal analyses, a finite element method using a transformed Eulerian formulation is described. The method incorporates the addition of filler metal in a natural manner. Strategies have been developed to analyze the evolution of microstructures in the steady state thermal field. History dependent parameters are integrated along streamlines. A data structure to assist in creating those streamlines and setting starting conditions for each streamline is developed. The method also applies to the temperature field at a specific step in the Lagrangian formulation. Thus, it can reveal values of past thermal analyses. In thermal stress analysis, a formulation has been developed with features from both the Lagrangian formulation and the Eulerian formulation. The same data structure has been used. The mesh sits on an Eulerian frame but deforms as if in the Lagrangian frame. Therefore, it is suitable for steady state problems with free boundaries. A significant gain in computing speed and/or spatial resolution over transient analyses has been achieved.

In the second part, a new model for decoupling the transient heat equation from the weld pool fluid mechanics is presented. In the weld pool, the temperature field is prescribed. Experimental data were used to test the methodology. The compound weld pool shape produces a heat-affected zone (HAZ) containing a "bay" region. The computed thermal cycle in the "bay" region is shown to be consistent with experimental measurements.

Finally, to facilitate thermal analysis of welded pipe joints, thermal shell and shell-brick transition finite elements are developed. Some techniques have been applied such as automatic shell creating and weld path locating. Results are presented for a test problem.

献给亲爱的父母和尊敬的老师

DEDICATED TO MY PARENTS AND TEACHERS

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Nomenclature

Bold Face Characters

α (Chapter 2)

α (Chapter 4)

$\hat{\alpha}$

c_p

k

E

ν

h

D

Q

q_n

σ

σ'

$\delta\sigma$

${}^i\sigma^n$

${}^i\bar{\sigma}$

${}^i\sigma_y$

${}^i\bar{\epsilon}^p$

e

δe

u

δu

f

t

Vectors and Matrices

Reciprocal of diffusivity

Average coefficient of thermal expansion

Weight in α -method

Volumetric specific heat

Thermal conductivity

Young's modulus

Poisson's ratio

Surface convective coefficient

Modified material property tensor

Distributed heat source

Scalar external flux

Stress tensor

Trial stress

Stress correction

Stress tensor at n -th iteration in i -configuration

Effective stress in i -configuration

Instantaneous yield stress

Effective plastic strain in i -configuration

Strain tensor

Strain correction

Displacement vector

Displacement correction

Body force vector

Time

t_0	Initial time
Δt	Time increment
$\mathbf{F}$	Deformation gradient tensor
$\mathbf{J}$	Jacobian matrix
$\mathbf{H}$	Transformation matrix
$\mathbf{K}$	Effective stiffness Matrix
$\mathbf{N}$	Matrix of basis function
W	Test function
T	Temperature function
$T_{,x}$	First order derivative of temperature in x direction
$T_{,xx}$	Second order derivative of temperature in x direction
T_t	Time derivative of temperature
T_0 (Chapter 5)	Temperature at the origin of a source, the peak temperature
T_m	Melting point temperature
T_0	Ambient temperature
$\dot{T}$	Material derivative of temperature
φ	Transformed function from T function
Ω	Observed domain
Γ	Boundary of the domain
Γ_i	Part of the boundary
$\mathbf{n}$	Outward normal vector
n_i	Component of $\mathbf{n}$
v	Weld speed
$r, s, t; \xi, \eta, \zeta$	Local curvilinear coordinates
$\mathbf{x}$	Vector pointing to point P in reference configuration
$\mathbf{x}$	Vector pointing to point P in i-deformed configuration
x^l, y^l, z^l	Local Cartesian coordinates
x, y, z_0	Origin of the local Cartesian coordinate system

x, y, z	Cartesian coordinates
ξ, y, z	Cartesian coordinates with origin at center of heat source
Δx	Space increment
$a_1, b_1, c_1, a_2, b_2, c_2$	The sizes of heat source ³ , ellipsoids
$\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3$	Base vectors of the laminar coordinate system
$\mathbf{r} ; \xi$	Base vectors of local curvilinear coordinate system

Chapter 1 Introduction

1.0 Characteristics of Welding Processes

In the 8th edition of the Welding Handbook, the American Welding Society (AWS) Committee on Definitions and Symbols defines a weld as follows: [1]

Weld. A localized coalescence of metals or nonmetals produced either by heating the materials to the welding temperature, with or without the application of pressure, or by the application of pressure alone, with or without the use of filler metal.

The key words in this definition have remained unchanged for a long time [2]. In other words, the characteristics of welds have not changed although the technology of welds has notably developed. Welds are characterized by their localized coalescence. A weldment is locally heated in most welding processes, therefore, the temperature distribution in the weldment is not uniform, and structural and metallurgical changes take place as welding progresses along a joint. Typically, the weld metal and the heat-affected zone (HAZ) next to the weld are at temperatures substantially above that of the unaffected base metal. As the welding electrode moves away, the weld pool solidifies and the HAZ cools down and shrinks. Microstructures in the HAZ vary according to the cooling rate. Residual stresses arise due to this uneven heating and cooling cycle.

1.1 Computational Weld Mechanics

Failures in welded structures are frequently associated with the welds. Weld processes used to be designed by rules of thumb and trial and error tests. Although there are many approved welding procedures available today for reference, engineers still lack confidence on the design procedure of a typical joint because of the unknown quality after welding. Expensive tests often have to be repeated several times before weld processes can be approved for critical structures, such as nuclear reactors, bridges and oil pipelines. Not only are the tests expensive, but they are also unreliable, because it is difficult to test the structures under real service conditions. Many failures happen after a long time in service. In addition, measurements at a few scattered sampling points can hardly give a complete picture of the full physical states, e. g., microstructures and residual stresses.

Computational Weld Mechanics (CWM) has struggled hard in the past decade to simulate or predict on computers the physical phenomena in welds. By doing so, scientists are hoping to use science to replace individual experiences and expensive tests in design. This thesis will not give a general review of the development of CWM, since reviews have been published in references [3, 4, 5]. Recent contributions of the team led by Professor Goldak of Carleton University are fully described in references [6, 7, 8]. With the rapid decline of computer prices and the development of CWM itself, people can now see the dawn of a full scale welding simulation on computers --- welding with data rather than with power and metals.

Current active topics in CWM include the simulation of heat and fluid flow in the weld pool and the prediction of heat transfer, microstructures and residual stresses in the HAZ. Since the simulation of heat and fluid flow in the weld pool is very complicated, it remains at a less mature stage. While the need to predict temperatures, microstructures and residual stresses in welds is more pressing, coupling the heat and fluid flows in the weld pool to the prediction of temperatures in the HAZ has not been realized yet. Ignoring the real weld pool, a popular and effective method treats the heat input from arc as a distributed heat source.

Coupling the heat transfer in the HAZ to the analysis of microstructures and residual stresses has progressed rapidly. However, the changes in microstructures and stresses have not yet been coupled back to the temperature field in large scale analysis because of the computational cost. Improving the efficiency with acceptable accuracy is still a heavy task, even with coupling in one direction. It is impossible to list all papers on this topic here. Good references from some recent conference proceedings are [9,10,11].

The current ability of CWM is restricted by computer capacity. Only single pass welds have been analyzed in depth. The full scale computations of temperatures, microstructures and residual stresses are rarely performed and are limited to short welds, approximately 5 cm long, at medium resolution or medium length welds, less than 1 m long, at coarse resolution. Boundary conditions are usually applied improperly because only a very small part of the geometry is used. Coupling temperatures, microstructures and stress analyses is often clumsy.

While long welds on large structures are more important in the welding world, the computational capability favors small welds. Furthermore, many large welds can not be

replaced by other manufacturing processes, e.g., the welds on pipelines or pressure vessels. It is these welds that need more attention to their quality, and to their safety.

This thesis aims at improving the efficiency and accuracy in modeling large welds. In the first part of the thesis, detailed analyses of temperatures, microstructures and stresses are performed under the steady-state assumption, which is true for long welds except at the starting and ending stages. In the second part, two techniques are developed to improve the accuracy and efficiency in either transient or steady-state analysis. A heat source model is implemented to model complex heat source shapes in large and deep welds. Thermal shell, as well as thermal shell-brick transition elements, are implemented to reduce unnecessary degrees-of-freedom.

1.2 Steady State

What is a steady state? A steady state is a physical field that does not change with time in some reference frame, i.e., the time derivatives are zero. In manufacturing processes, there exists a class of problems that have steady states more or less under a localized load. A few examples of such processes are sheet rolling, extrusion, wire drawing, continuous casting and long welds. Except at the start and the end of a pass, the processes approach the steady state of their physical fields for some specific frames. The fields can be scalar, vector or tensor.

A steady-state temperature field implies that, to the domain of the field, the incoming heat and the outgoing heat are constant and match each other. Here, the match of the constant incoming and the constant outgoing is not only meant in a weak or average sense but also pointwise. The boundary conditions of a problem must be constant and satisfied with respect to time.

Let us observe two adjacent elements in an infinite domain. First, suppose there is no mass moving between the elements. The amount of diffusion between these two elements is proportional to the difference of their temperatures. If the first element is a heat source and at a constant temperature, then heat will keep moving into the second element as long as the second remains at a lower temperature. The steady state is reached when they have the same temperature, or when the heat from the first element to the second equals the outgoing heat from the second either to the rest elements of the domain or to the outside through the free surfaces. At the beginning, the temperature in the second element may rise quickly because the incoming heat is large. This in turn, increases the outgoing heat.

When the second element reaches steady state its outgoing flux equals its incoming flux. At that moment, the temperature distribution is constant in the second element, as well as in the whole domain. The problem becomes a static boundary problem. In order to distinguish this state from the one we discuss below, we label this state a first type steady state governed only by heat conduction.

If two elements lie in a stream tube, the constant movement of mass inside the tube accelerates heat transfer. If the upstream end is a constant-temperature heat source, the steady state is reached when the outgoing heat through the wall of the tube and the downstream end equals the input heat at the heat source. The mass movement may help little to create the steady state in the whole domain. But locally, when mass moves at a high speed and the variation of the heat lost from the wall can be ignored, the difference between two elements will soon become small and stable.

Now, if two adjacent elements are in two adjacent stream tubes, no mass can transfer between the two elements. When the first is the heat source, heat diffuses to the second element according to their difference in temperatures. If mass flows at a constant speed in the second element, the incoming material of the second element will be heated by the heat source. In this instance, the outgoing heat from the second element will include the convective term. The faster the mass moves and the higher the temperature in the element is, the larger the lost heat is due to convection. Therefore, the second element can reach a steady state at a temperature when the outgoing heat due to diffusion is stable or can be ignored. This steady state is a localized one, since diffusion is still dominant in some other elements, e.g., the element downstream of the heat source. We note this type of steady state as the second type in the sake of convenience. Most welds usually reach this type steady state instead of the first type.

Experiment shows that in welding [12], the temperature distribution around the heat source soon becomes steady, if the weldment is long enough compared to the extent of heat. This is evidently an evolutionary procedure. It is important here to note two conditions. First, the weldment must be long enough or infinite. Welding on a short piece will stop before the steady state is reached. Second, the observed domain must be tied to the electrodes of welds, i.e., it is an Eulerian space. The steady-state field forms first in a volume around the heat source. Initially, the temperature distribution around the heat source becomes steady in a very small volume not long after a weld starts. As the weld continues, the volume containing the steady-state temperature field grows constantly until it

covers the full domain. When it covers the full domain, the temperature in the volume won't change when the weld continues. At this stage, all heat input from the heat source equals the heat lost from the free surfaces of the volume due to radiation and convection. The temperature stays at room temperature in the down stream metal after this full size volume. This full size steady state is the first type described in previous paragraph. In an infinite domain, it can be reached even if the welding electrode is stationary.

In most welding practices, however, a steady state can not fully develop before the weld stops, because the natural convection and radiation are usually low on free surfaces. Most welds have true steady-state temperature fields only around the heat source. They are premature or not a fully developed steady state. The size of a premature steady-state temperature field grows constantly because heat diffuses at some boundaries. People often refer to this premature steady state as the **quasi-steady state**. It has the characteristics of the second type steady state. Cutting a piece from the quasi-steady state temperature field, we can find that the heat balance inside the piece is mainly due to the convection of mass. In this thesis, the quasi-steady state and the fully developed steady state are not identified separately, because we are interested only in a finite observed space, which is assumed to contain a fully developed steady state. The world outside this observed space is not of interest.

Although the steady state does exist in a finite volume around the heat source, it is difficult to analyze it mathematically. The steady-state problem is simply a boundary-value problem. The distribution of a physical quantity, or field, is fully determined by the distribution of the quantity, or its derivatives, at the boundary of the analyzed domain. Since the boundary enclosing the steady state field evolves in welding, we can not know the distribution of temperature or flux at the boundary until it reaches the fully developed steady state. Since most welds we are modeling are quasi-steady state, the downstream flux at the boundary is unknown. Suppose that we know the correct shape of the heat source, i.e., the boundary condition for the incoming heat is known and fixed, and we may, then, have only two choices to decide the boundary conditions for the out going heat. Yet both approximate a quasi-steady state.

(1). In analytical solutions, people often assume that the length of weldments is infinity and welds go from negative infinity to positive infinity, or *vice versa*. Under this assumption, used by Rosenthal [13], either that temperature equals ambient values or the flux equals zero can be chosen for the boundary condition. This is true for a fully

developed steady state and for the steady state close to the weld pool in a quasi-steady state. However, it is difficult to implement in the finite domain which we usually use in the FEM.

(2). In numerical modeling, a finite domain is often used. The boundary condition is assumed to satisfy the outgoing heat dominated by mass convection. Since there is always some unknown diffusion flux at the down-stream boundary, the boundary condition is satisfied only in a weak sense. Since the diffusion takes only a small percentage of the outgoing heat, it can be argued that the error introduced at the down-stream boundary will not seriously distort the whole temperature field.

There are some restrictions of a steady state formulation on a weld. The weld speed must be constant. The power input from the weld electrode to base metal must be constant. The weld has to be on prismatic structures with the weld path parallel to the prismatic axis. When the weld is on a circumference of a large diameter pipe, it can be treated as an analog of a prismatic structure. Although steady-state formulations have these shortcomings, they do have advantages for long welds.

Although a step-by-step transient solution is simple, its capability has been actually restricted by computer capacity. The cost is high. When most metal experiences a steady-state thermal cycle in a long weld, analyzing what happens in the steady state is apparently very important. Compared to one step in a steady-state formulation, a transient solution needs about a hundred time steps to approach the steady-state field around the heat source. A steady state formulation would significantly reduce the computational cost.

Unless we change meshes at every time step, as proposed by McDill, *et al.* [14], or permit accuracy and resolution to vary along the weld, a very fine mesh along the weld path is needed to accommodate rapidly varying temperature gradients around the heat source. Before the heat source arrives and after the heat source has left, temperature gradients tend to be shallow. Often, a large number of degrees of freedom are only an extra burden to the step-by-step transient analysis. With steady-state formulations, meshes can be optimized to correctly predict temperature fields. Resolution can be at least 10 times higher with the same number of degrees of freedom.

A problem can arise when the mesh is not fine enough to describe the heat source in a step-by-step transient solution. Looking at Figure 1.1, the highest temperature oscillates along the weld path. The data in this figure are computed with a transient analysis on a

mesh of a half meter length, with low resolution along most of the weld path. There is a fine mesh area at the middle of the weld path, on which the heat source performs better and a higher maximum temperature can be seen. On the coarse mesh, the heat source can not perform properly, resulting in lower peak temperature. Because of the discretization in the time dimension, even though the mesh is fine along all weld path, what we analyze is a sequence of arc spot welds rather than a continuous arc weld. Spots are scattered according to the time steps used. The steady-state formulation assumes material flowing through mesh continuously. The same peak temperature will be experienced by all material points along a flow line.

Figure 1.1 Maximum temperature versus time in a coarse mesh. The heat source jumps due to the time step. Finely meshed area in the middle raises the temperature.

When filler metal is added to the weld pool, mass can not be conserved in a Lagrangian formulation without a mesh change after the weld pool. When essential boundary conditions are applied, ignoring the filler metal in the thermal analysis may cause the heat input from arc to be underestimated. The added filler metal is at a high temperature, playing an important part in delivering heat from the arc. Changing the mesh

at each time step would cost extra computing time and add complexity to programming. The steady state formulation allows filler metal to be added naturally. The mesh simply describes the weld pool and adds filler metal from the arc. There are no new elements to create. Thus it supports welds with filler metal in a natural and elegant manner.

1.3 Outline of the Thesis

In chapter 2, 3 and 4, detailed analyses for a steady state weld are described. Pictures of temperatures, microstructures and stresses in the steady state are shown. The analyses are based on an Eulerian frame through which material moves at a constant weld speed. However, the steady-state formulations presented in these chapters are not necessarily the Eulerian formulation as described in literature. But, they are formulations that need only one step to analyze. Bergheau *et al* did a three-dimensional simulation of a laser surface treatment on a moving frame with steady state [15]. However, few details about their formulations and results were given.

Chapter 2 calculates temperatures efficiently in transformed Eulerian formulation. Filler metal addition is described.

Chapter 3 analyzes the evolution of microstructures in a weld under steady state conditions. The history dependent parameters are integrated along flow lines. A data structure to assist in creating flow lines and initializing starting conditions for the flow lines is described. The method is shown to be fast and efficient. The data structure is a general one and plays an important role in Chapter 4 too.

Chapter 4 develops a formulation for strain and stress analysis with features from both Lagrangian and Eulerian formulations. It can analyze a free-boundary problem under the steady state condition. A significant gain in computing speed and spatial resolution over transient analysis has been achieved.

Chapter 5 presents a new model for a complex weld pool. Correctness of heat input, i.e., the incoming heat distribution, is critical for the analysis inside the HAZ. It can be expected that different shapes of the heat source will result in different temperature contours, microstructures, as well as strain and stress distributions in the HAZ. The new model prescribes the temperature field in the weld pool. With these essential boundary conditions the 3-dimensional temperature field is computed outside of the weld pool. The experimental data from Barlow [67] are used to test the methodology.

Chapter 6 develops thermal shell and shell-brick transition finite elements to improve the efficiency and accuracy of thermal analysis. The advantage of using a thermal shell is to reduce by half the degrees of freedom and the bandwidth, so that the cost is reduced by a factor of eight for direct solvers. Even more important, numerical conditioning often requires brick elements to be constrained to length to thickness aspect ratios less than 10:1. The aspect ratio of length to thickness of thermal shells is not constrained. This often allows one four-node quad shell to replace several eight-node brick elements. To reduce the time to prepare input files and reduce the probability of error, the creation of the shell and shell-brick transition elements are done automatically from a mesh consisting of brick elements only. The weld path is specified as a curve in space with start and end points. The effectiveness of the method is demonstrated in a thermal analysis of a pipe tee-joint weld.

Smalltalk, an object-oriented programming tool, has been used in the work of this thesis, which manipulates geometry effectively in creating meshes, weld paths and stream lines. Together with the solver written in C and Fortran it provides a rich environment for modelling welds.

Chapter 2 Steady State Thermal Analysis of Welds with Filler Metal Addition

2.0 Introduction

Rosenthal [13] and Rykalin [16] independently solved the heat equation for moving heat sources in the 1930s. Their solution, which was an Eulerian formulation, was the principal method for computing the steady state temperature fields in welds until the 1980s. In the 1980s, the finite element method (FEM) became popular for computing the transient temperature fields in welds. The transient Lagrangian formulation allowed complex geometry, and non-linear equations. Many successful 3-dimensional transient analyses on welds have been reported that used Lagrangian FEM formulations as summarized in [7]. Approximations to the steady state temperature field were obtained by running a transient analysis until it approached the steady state.

Today there are three major difficulties in computing the temperature field in the heat affected zone of a long weldment. (1) Around the heat source, a fine discretization of space is required to accommodate the sharp gradient properly. In a Lagrangian formulation, this requires a very fine mesh along the weld path unless the mesh can be changed dynamically [17]. As a result, the size of weld is limited by the computer memory and speed, and the resolution achieved is usually lower than desired. (2) A fine time discretization is required to lessen the effect of "spot welding". Since so many time steps are needed to reach the steady state, an analysis of a medium sized weld can require a day or longer on a personal work station, such as an Apollo DN-4000. (3) The addition of filler metal is usually ignored in current Lagrangian FEM formulations because the complexity and cost of changing the geometry or mesh between time steps to accommodate the added filler metal are so critical. Since the filler material will release a large amount of enthalpy behind the weld, it can significantly alter the cooling rate and temperature distribution after the weld pool, especially in the HAZ. The added filler metal is, therefore, important in the subsequent microstructure and thermal stress analyses.

In this chapter, an FEM Eulerian formulation is presented for the steady state temperature field in welds. The differential equation is transformed from the standard

Eulerian formulation to a form that can be solved with a positive-definite symmetric linear equation solver. However, like the Rosenthal solution, it is then limited to constant thermal properties and to nearly prismatic domains with constant cross-section and prismatic axis in the direction of welding. When a solver for asymmetric equations is available, the results from the transformed formula can serve as a good estimate of the nonlinear solution. It can be expected that the nonlinear solver would converge more rapidly if the solution of current formulation is used as the first approximation.

For a steady state solution, no information about the transients on starting and stopping the weld is provided. However, it does allow a much higher spatial resolution in a single computational step than a transient analysis. In addition, adding filler material becomes natural in the analysis.

2.1 Transformed Steady State Eulerian Formulation

In a Lagrangian reference frame, the conservation of energy may be written as

$$\nabla \cdot (k \nabla T) + Q = c_p \dot{T}$$

$$T_{xx} + T_{yy} + T_{zz} + \frac{Q}{k} = \alpha \dot{T} \quad (2.1)$$

where the subscripts represent partial derivatives. The temperature is T ; the thermal conductivity is k ; the volumetric specific heat is c_p ; $\alpha = c_p/k$ is the reciprocal of diffusivity and Q is a distributed heat source.

Suppose that a heat source is moving at a constant speed v in the positive x -direction. We define an Eulerian (moving) frame with origin at the center of the source, and coordinates (ξ, y, z) . The transformation from (x, y, z) to (ξ, y, z) is given by: $\xi = x - vt$, where t is time. Noting that the material time derivative $\dot{T}$ in equation (2.1) becomes

$$\dot{T} = T_t + \frac{\partial \xi}{\partial t} T_\xi = T_t - v T_\xi$$

We obtain the equation of conservation of energy in the Eulerian frame:

$$T_{\xi\xi} + T_{yy} + T_{zz} + \frac{Q}{k} = -\alpha v T_\xi + \alpha T_t \quad (2.2)$$

Here T_t represents the time derivative of temperature at a point fixed with respect to the heat source. In a steady state, this derivative is zero, and so (2.2) becomes:

$$T_{\xi\xi} + T_{yy} + T_{zz} + \frac{Q}{k} = -\alpha v T_{\xi} \quad (2.3)$$

When α and v are constant, equation 2.3 can be made more soluble by the transformation

$$T = T_0 + e^{-\frac{\alpha v \xi}{2}} \varphi(\xi, y, z) \quad (2.4)$$

Substituting this into equation 2.3, we have

$$\begin{aligned} \varphi_{\xi\xi} + \varphi_{yy} + \varphi_{zz} + \frac{e^{-\frac{\alpha v \xi}{2}} Q}{k} &= \frac{(\alpha v)^2}{4} \varphi \\ \nabla^2 \varphi - \frac{(\alpha v)^2}{4} \varphi &= -e^{-\frac{\alpha v \xi}{2}} \frac{Q}{k} = \tilde{Q} \end{aligned} \quad (2.5)$$

Equation 2.5 is symmetric positive definite. After properly transforming the boundary conditions from the T function to the φ function, we can easily solve this equation with the standard Lagrangian FEM code that contains a solver for positive-definite symmetric equations. Equation 2.5 only applies to linear systems (i.e., with α independent of T) because of equation 2.4. In the following examples, the diffusivity is taken as a constant.

2.2 Boundary Conditions

The most convenient domains in which to apply equation 2.5 are prisms with constant cross-sections, as one shown in Figure 2.1. The temperature of the boundary between the weld pool and the solid is prescribed to the solidus temperature. Since an essential boundary condition is used, the heat entering base metal through the interface, Γ_3 , equals the thermal reactions, as in the example of Chapter 5, and the flux due to complex radiation and convection on the surface of the weld pool, need not be taken into account.

From experimental measurements, we know that at a sufficient distance, ξ_n , in front of the weld pool, temperatures remain at ambient temperature; $T = T_0$ when $\xi > \xi_n$ and consequently, $\varphi = 0$ when $\xi > \xi_n$.

Figure 2.1. The Eulerian frame and boundary conditions. Γ_2 is the downstream boundary that is normal to the velocity of the source. On this surface the gradient of the temperature has been prescribed to zero. Γ_3 is the surface of the liquid solid interface of the weld pool. On this surface, which is smooth but with arbitrary orientation and curvature, the temperature has been prescribed. Γ_4 is the surface of the upstream end. The outward normal of the surface is parallel to the velocity of the source. On this surface the ambient temperature of the plate has been prescribed. Γ_1 is the remainder of the boundary surface. The outward normal of the surface is orthogonal to the velocity of the source. On this surface natural convection has been applied.

When the prism boundaries as Γ_1 are not insulated, a boundary flux would have to be applied. For the case of a constant convective coefficient, h , the boundary condition is

$$q_n = -k \nabla T \cdot \mathbf{n}_\Gamma = h(T - T_0) \quad (2.6)$$

where q_n is the scalar external flux and $\mathbf{n}_\Gamma$ is the outward normal vector on the boundary.

We express equation (2.6) in terms of φ , using equation (2.4),

$$k \nabla T \cdot \mathbf{n}_\Gamma = k e^{-\frac{\alpha v \xi}{2}} \left(\nabla \varphi \cdot \mathbf{n}_\Gamma - \frac{\alpha v}{2} \varphi \mathbf{n}_\xi \right) = -h e^{-\frac{\alpha v \xi}{2}} \varphi \quad (2.7)$$

On the side walls of the prism, $\mathbf{n}_r$ is orthogonal to the weld path,

$$\mathbf{n}_r = \begin{bmatrix} 0 \\ n_y \\ n_z \end{bmatrix}$$

Equation 2.7 for the side walls becomes

$$\nabla \varphi \cdot \mathbf{n}_r = -\frac{h}{k} \varphi \quad (2.8)$$

The heat source term has been set to zero. If one wished to include the weld pool, a heat source term exists that could replace the prescribed temperature boundary condition on the solid-liquid interface of the weld pool.

If the domain is long enough or infinite, at the downstream end the temperature will drop to ambient temperature because of the heat dissipation from the surfaces. Either essential or natural boundary conditions can be applied, i.e., $T = T_0$ or $\nabla T \cdot \mathbf{n}_r = 0$ when $\xi \Rightarrow -\infty$. Transforming temperature T to the potential function φ , when $\nabla T \cdot \mathbf{n}_r = 0$ is applied and $\xi \Rightarrow -\infty$,

$$\nabla T \cdot \mathbf{n}_r = e^{-\frac{\alpha \nu \xi}{2}} \left(\nabla \varphi \cdot \mathbf{n}_r - \frac{\alpha \nu}{2} \varphi n_\xi \right) = 0$$

So,

$$\nabla \varphi \cdot \mathbf{n}_r = \frac{\alpha \nu}{2} \varphi n_\xi \quad (2.9)$$

2.3 FEM Formulation

Applying Galerkin's method to equation 2.5, when $\tilde{Q}$ does not exist, gives

$$\int_{\Omega} W \left(\nabla^2 \varphi - \frac{(\alpha \nu)^2}{4} \varphi \right) d\Omega \quad (2.10)$$

for all W in the space of test functions.

For infinite domains the test functions must be specified carefully but for a finite domain the usual Galerkin test functions can be used. Apply Green's identity to equation 2.10,

$$\int_{\Omega} \left[-\nabla W \nabla \varphi - \frac{(\alpha v)^2}{4} W \varphi \right] d\Omega + \int_{\partial\Omega} W (\nabla \varphi \cdot \mathbf{n}_{\Gamma}) d\Gamma = 0 \quad (2.11)$$

Applying the boundary condition in equation 2.8 to the side walls,

$$\int_{\Gamma_1} W (\nabla \varphi \cdot \mathbf{n}_{\Gamma}) d\Gamma = - \int_{\Gamma_1} \frac{h}{k} W \varphi d\Gamma \quad (2.12)$$

If the boundary condition in equation 2.9 is applied on the downstream end,

$$\int_{\Gamma_2} W (\nabla \varphi \cdot \mathbf{n}_{\Gamma}) d\Gamma = \int_{\Gamma_2} \frac{\alpha v}{2} W \varphi n_{\xi} d\Gamma$$

When the end faces are perpendicular to ξ , $n_{\xi} = -1$ at the rear end.

$$\int_{\Gamma_2} W (\nabla \varphi \cdot \mathbf{n}_{\Gamma}) d\Gamma = - \int_{\Gamma_2} \frac{\alpha v}{2} W \varphi d\Gamma \quad (2.13)$$

Putting equations 2.12 and 2.13 into 2.11,

$$\int_{\Omega} \left[-\nabla W \nabla \varphi - \frac{(\alpha v)^2}{4} W \varphi \right] d\Omega - \int_{\Gamma_1} \frac{h}{k} W \varphi d\Gamma - \int_{\Gamma_2} \frac{\alpha v}{2} W \varphi d\Gamma = 0 \quad (2.14)$$

for all test functions W .

2.4 Results

Two test cases, of butt welds, have been analyzed on the same mesh structure, shown in Figure 2.2. The characteristics of this mesh are that the liquid metal in the weld pool is excluded and the weld bead can be seen on the plate after the weld pool to account for the added filler material. The weld pool surface was measured for a weld in which the

Figure 2.2 The FEM mesh is built on an Eulerian frame. The finest mesh is in the front of the weld pool. The element sizes after the weld pool can be changed in analyses, so that more or less material is included.

arc was abruptly stopped and liquid in the weld pool was blown out with an air jet. The empty pool is seen clearly on the mesh in Figure 2.2. The first base metal is aluminum which has a high diffusivity and the second is steel which has a low diffusivity. The surfaces open to the weld pool are prescribed at the melting temperatures of the base metals, which give a boundary condition as discussed in Chapter 5. Both surfaces of the weld joints have been prepared with V grooves. Welds are designed for one pass on each face. The pass on the top surface has been analyzed.

The method can be used immediately to compute the transient temperature on stopping the arc. One need only perform a Lagrangian transient analysis with the steady state temperature distribution as the initial condition.

2.4.1 Test Case 1

The steady state temperature field of an arc weld on an aluminum plate has been computed using the method described. The Eulerian frame is created on a mesh 218 mm long, 165 mm wide, and 19 mm thick. The welding speed was 6 mm per second. The length of the weld pool was 32.5 mm. The center of the pool was 10 mm from the leading edge. The maximum pool width was 15 mm. The deepest point was 10.1 mm. The rough bottom of the empty weld pool suggested that some remainder had been left on the bottom of the weld pool. The real liquid-solid interface, in that case, should be underneath the current bottom. However, the measured weld pool still gives the approximate outline of the real liquid-solid interface. The small difference caused by the rough bottom was ignored in the analysis. The thickness of the frame is the same as the plate in the real weld, but the length and the width follow that of the sample. The length and the width of the real weld are unknown. Nevertheless, the sample piece cut from the welded plate is assumed to be in steady state.

The parameter α was chosen as $\frac{c_p}{k} = 1.76 \times 10^4 \frac{\text{sec.}}{\text{m}^2}$.

Radiation and natural convection are allowed on the top and bottom surfaces, but not on the weld pool, and on the side edges. The front edge has mass flowing in at room temperature. Computational results indicate that the diffusion rate in this case is slower than the weld speed. That is, the temperature drops quickly to room temperature not far ahead of the weld pool. Thus, the assumed boundary condition is satisfied exactly.

The boundary condition at the rear edge could be either essential or natural. For a finite domain, the boundary condition can only be an approximation. It is usually not true that the rear edge is at room temperature, nor is the temperature gradient zero. However, setting the temperature gradient equal zero in the ξ -direction ($T_{\xi} = 0$) is obviously closer to the real solution, since no significant diffusion is assumed at the boundary even though the temperature is high. When $T_{\xi} = 0$ at the rear edge, heat input into the weld pool is balanced with the heat loss through free-surface radiation and convection and hot material flowing out from the rear end. Equation 2.9 is used.

If the downstream length is too short, the temperature gradient on the downstream end may be very different from zero, especially when the end is close to the weld pool. From a short domain, we can not get enough information about the thermal cycle. If the downstream length is too long, the problem can become numerically ill-conditioned (see equation 2.4). A small disturbance of ϕ causes large changes in T when ξ is far from the origin. To choose an appropriate length, the domain length has to be changed dynamically, i.e., it can expand or shrink the rear part. Keeping a fixed, very fine mesh near the weld pool as a kernel, material is then added at the rear end until the temperature field in the kernel is stable. The solution converges from one iteration to the next when temperature difference at any node in the kernel is not greater than some specified tolerance. Numerical experiments have proved that with sufficient material behind the weld pool, convergence is rapid.

Figure 2.3(a) shows the computed isothermal contours. Figure 2.3(b) shows the isothermal contours on the half mesh cut symmetrically along the weld path. The contours show the expected results.

Figure 2.4 compares the FEM 3-D steady state analysis with Rosenthal's 1-dimensional and 2-dimensional analytical model. For steady state in the Eulerian frame, the thermal cycle in the time space is its analog in the geometric space, i.e., the history of a material point is stored in a sorted collection of points along a streamline. The sample points for the FEM analysis were picked parallel to ξ and tangent to the weld pool edge on the top surface. The power inputs used for the analytical models were calculated from the nodal fluxes on the weld pool wall. The one-dimensional model implies the heat input in the whole section normal to the weld path. The two-dimensional model uses the through thickness circle source. The curves indicate that too much heat has entered the material in

Figure 2.3 The isothermal contours in the steady state of an arc weld on aluminum plate, computed by a transformed Eulerian formulation. Because of high diffusivity the density of the mesh around the weld pool could be lower than that for steel. (a) is the whole mesh; (b) is the mesh cut along the weld path.

the one-dimensional or two-dimensional model. However, the influence of the thickness dimension is much less than that of the width.

Figure 2.4 Comparison of thermal cycles in steady state of weld on aluminum. Note the one-dimensional and two-dimensional analytical solutions were calculated by the Rosenthal's model. Since the 1-dimensional model uses a sectional source and the 2-dimensional model uses a circular, through-thickness source, both energy inputs are higher than in reality.

2.4.2 Test Case 2

The second test was performed on a low carbon steel plate, Figure 2.5. The weld speed was 1.5 mm/sec. Estimated unit-length heat input was 1.5 kJ/mm. The diffusivity of steel is smaller than that of aluminum. Thus, for the same welding speed, the Eulerian domain for steel can be smaller than that for aluminum. However, the mesh around the weld pool should be finer in order to describe the sharper gradient. The main purpose of this analysis was to compare the results of a transformed Eulerian formulation with that of a step-by-step Lagrangian formulation and to provide a test case used in the consequent analyses of microstructures and stresses.

To assess the efficiency, an analogous analysis was performed in the Lagrangian formulation, Figure 2.6. Fifty-five time steps were taken to reach a relatively stable

temperature field around the weld pool. The same value of α was used, $\alpha = 10^5 \text{ s/m}^2$. The meshes for both analyses consisted of about 12,000 elements. For constant resolution and accuracy, the elements have to form a dense region along the whole weld path in the Lagrangian frame. Thus, the spatial resolution is obviously higher in the Eulerian frame. Compared with 3 CPU minutes for steady state analysis, 6 hours was used in the 55 steps in the transient analysis. Both analyses were performed on a Sun Sparc II workstation. It is estimated that an analysis using equation 2.3 with Gaussian elimination and an asymmetric solver, for same mesh size, would cost approximately 17 minutes on a Sun Sparc I workstation. Such a formulation with a suitable nonlinear solver, has the advantage that it can be used when α is temperature dependent.

Comparing Figures 2.5 and 2.6, we can find the difference in the contours on the symmetric plane along the weld path. The contours in Figure 2.6 distribute evenly through the thickness after the weld pool. It is apparent that the filler material plays an important part in this difference.

Figure 2.7 compares the thermal history of points on the top surface parallel to the weld path. Because of the differences in the meshes used in the two formulations, the nodal positions are not identical. The millimeters indicate the shortest distance from the weld path. In the Eulerian analysis, the thermal cycle has been extracted from the thermal history of a streamline. The temperature in the Eulerian analysis cools down faster immediately after the peak temperature. Not only is the sample point 0.375 mm farther from the weld pool, it has been also observed that the shapes of ellipsoids used to simulate the weld pool in the Lagrangian frame were different from the measured real weld pool used in the Eulerian frame. Although the maximum length, width and depth are the same for the weld pools in the two reference frames, the measured pool is in fact thinner toward the end of the pool. Therefore, the assumed ellipsoids kept the sample point in higher temperatures when the rear half of the ellipsoids passed the point.

The domain length is quite short in Figure 2.5. It has, however, a high resolution. The temperature is still high (above 500 °C) at the downstream end. In a thermal stress analysis, the residual value at room temperature is quite different from the value present at such a high temperature. There is still a great amount of material shrinkage from 500 °C to room temperature. Furthermore, since the thermal gradients are low below 500 °C, the region cooling from 500 °C to room temperature is much longer than the kernel in Figure 2.5. To provide a suitable temperature field for thermal stress analysis, the observed

Figure 2.5 The isothermal contours in the steady state of an arc weld on low carbon steel, computed by a transformed Eulerian formulation. Because of low diffusivity, the density of the mesh around the weld pool should be higher, especially around the first half of the weld pool. (a) is the whole mesh; (b) is the mesh cut along the weld path.

Figure 2.6 The isothermal contours computed by the Lagrangian formulation. The contours represent the solution in 55 time steps, 67 seconds after striking the weld torch. The velocity and diffusivity used were the same as those used for Figure 2.5. Note that without the addition of filler material the temperature varies less in the thickness direction after the pool passes.

domain has to increase extensively. This will certainly cause some numerical ill-conditioning, as shown in equation 2.4.

Figure 2.7 Comparison of thermal cycles at a point near the weld pool between the Eulerian formulation and the Lagrangian formulation in steady state. The weld is on low carbon steel. The millimeters indicate the distances from the weld pool.

A solution to the problem has been tested using successive steps. First, the whole domain was chopped to several short pieces, then each piece was increased by some length so that the effect of the false boundary condition was reduced in the observation part. Next, the kernel part of Figure 2.5 was taken as the first piece of the divided domain. With excluding the inaccurate downstream part, the kernel part was treated as a heat source for the second piece. By prescribing the upstream section of the second piece with the temperatures field of the first piece, or with the first piece serving as a larger heat source, one can compute the temperature field in the second piece. The calculated temperature field can in turn serve, as the heat source, for the third piece. These steps are repeated until the temperature cools down to the required value. An example of this successive treatment is shown in Figure 2.8, which is prepared for the stress analysis in Chapter 4.

Figure 2.8 A temperature field is prepared for stress analysis. The temperature field was solved in the transformed Eulerian formulation in 3 successive steps. The total length of the mesh is 542.9 mm.

Chapter 3 History & Modelling the Evolution of Microstructures in the Heat-Affected Zone of Steady State Welds

3.0 Introduction

The mechanical properties of metals are sensitive to their microstructure. By intentionally changing the microstructure, people can control the properties to provide the best service. However, not all the changes are beneficial. Many manufacturing processes can produce unfavorable microstructures, which can reduce the reliability and performance of the product. In welding, undesirable microstructures can cause failures and are a serious concern. Whether the microstructural changes bring fortune or catastrophe will depend on people's capability to predict why and how these changes happen. The prediction of the microstructural changes caused by thermo-mechanical processing continues to be an area of great practical benefit.

Although many factors can affect the microstructure of a metal, the thermal cycle is the dominant factor in welding processes. It is the peak temperatures and the heating and cooling rates in the thermal cycle that control the phase changes and microstructures. When the thermal cycle reaches its steady state, the microstructural evolution will, in most cases, also reach a steady state. It was this expectation that motivated this model.

Models that take advantage of the steady state temperature field in long welds are well known. When the temperature field reaches a steady state, each material point along a streamline experiences the same thermal cycle. Could models for the evolution of microstructure be developed to exploit the steady state? Essentially such models reduce the dimensionality from four dimensions (x, y, z, t) to three (x, y, z). The answer shall be in the affirmative. Many simulations done before [18][19] depended actually upon the thermal predictions of Rosenthal's model, which assumed a steady state.

Methods to predict the steady state temperature field around a weld pool were first reported by Rosenthal and Rykalin [13][16]. In Chapter 2, a FEM model of a steady state temperature field around the weld pool was described. Since this is a true three-dimensional model, demonstrated also in Chapter 5, it can investigate different welds in

detail for their unique temperature distributions. Such distributions are sometimes critical to the simulation of microstructures. Compared to a step-by-step Lagrangian formulation for a transient thermal analysis, the cost of computing a steady state temperature field has been reduced from hours or days to minutes. Although the computation of microstructures by following the thermal cycle step-by-step has been reported with a transient thermal analysis in the Lagrangian formulation of FEM, to the author's knowledge, coupling the steady state temperature field with a microstructure prediction has not been published. The difficulty in such a coupling is to extract the thermal cycle from the steady state temperature field.

Since the steady state exists only in welds of simple geometry, e.g., prisms or spiral welds on pipes, the work done here focuses only on welding plates. However, the code developed can be used for prisms with any cross-sectional shape. It can also be used when the plate bends into a circular arc, as in the case of welding large-diameter pipes. The only change necessary is to use a polar coordinate system for the streamlines. Note that the change may not be applicable on thermal analysis in chapter 2.

The microstructure algorithm used here was originally developed by Watt, et al., [20] and Henwood, et al. [21], and enhanced by Khorai [22]. The microstructure algorithm is limited to the heat affected zone (HAZ) in low alloy steels. The major contribution of this thesis to the simulation of microstructures is to create a data structure for the coupling of a steady state thermal field to the formation of microstructures. Some changes have been made in order to satisfy conditions in the weld pool and fusion region.

Streamlines play an important role in this work. In a steady state temperature field described in an Eulerian frame, integration along a streamline gives the thermal history of a material point. In a general FEM mesh with refinement around the weld pool, the creation of streamlines consumes more time than the microstructure calculation itself. Data structures to organize elements, points and streamlines are necessary. The functionality of the data structure is critical to the success of the model.

To catch the thermal cycle in a steady state temperature field, the applied data structure should meet several requirements. The data structure must support efficient ordered traversals of the points on a streamline (starting at the head and proceeding downstream). It must also allow the element that contains the head of a streamline to be found. Lohner used a heap of faces [23], supporting insertion and deletion in $O(\log_2(n))$ operations for n

faces. However, given different sized faces this may require a complete search to find the face containing a point. A data structure has been developed in this thesis to represent properly the streamlines in a steady state field and to meet all the above requirements.

Since the analysis of microstructure has been done by the assumption that it can be separated from the deformation analysis, the streamline created for the fixed points in Eulerian domain, or undeformed geometry, is not a streamline in the deformed configuration. It is in fact a "history line". However, the displacements in the welded structure are not so large that the results of thermal analysis would be expected to alter significantly because of the deformation. Since the algorithm to compute microstructures is applied point-wise, when a full coupling of the thermal analysis with the stress analysis is performed, the microstructures can be easily updated with the new thermal cycle. The "history lines" are still called streamlines in this chapter because the notation is well established in the fluid flow literature.

3.1 Data Structures

3.1.1 Streamlines

The computation of microstructure at a spatial point requires that the thermal history be deduced from a set of elements or nodes in a steady state temperature field. The correct history of a material point at a downstream spatial point can only be revealed by following the streamline from its upstream origin to its downstream destination. For this reason, the streamline collection is organized as described below, and as shown in Figure 3.1.

1. Each streamline has three parts: head, body, and front end condition. The head is the position of the front end where this streamline starts. The body contains a collection of the points on the streamline, ordered from upstream to downstream. Every point X_i with coordinates (x_i, y_i, z_i) in the body stores a pointer to the point, X_{i-1} $(x_{i-1}, y_{i-1}, z_{i-1})$, immediately preceding it. The time increment Δt is easily calculated, since the velocity v is known. In this context, v is the weld speed, the weld path is assumed be along the x axis, and v and x_i are scalars.

$$\Delta t = \frac{\Delta x}{v} = \frac{\Delta x_i - \Delta x_{i-1}}{v}.$$

The front end condition can be either defined from the problem data, if the streamline starts at a free surface of the domain, or interpolated from the computed data within the element in which the streamline starts.

Figure 3.1 The structure of streamlines in a 2-dimensional cross-section of a 3-dimensional FEM Mesh. The direction of flow is from the top to the bottom of the page, corresponding to the x-axis.

2. The streamlines are kept in a global collection, sorted by the x-coordinate of their head positions. The computation loops over the streamlines in the sorted order, proceeding downstream along each streamline. The order guarantees the computing order that is necessary when a given point p represents the start condition of a streamline. When and only when the values of all the points, contained in an upstream element of the point p , have been computed, can a value at p be computed.

To satisfy the requirements in building up the above collection of streamlines, we have created a multi-layered tree structure as described in the section after next section.

3.1.2 The Functionality of the Data Structure

Some functionality will be required in the process to build up the streamlines. Since there are some similarities among all requirements, the functionality asked here will be implemented in the same data structure. The data structure provides the functionality to:

- loop over elements in the order from upstream to downstream.
- find an element containing a given point.
- find all points from a given set lying along a given streamline.

Smalltalk has been used in the implementation of the functionality. With the help of Object Oriented Programming, the data structure has not only been created easily, but been organized nicely also.

3.1.3 Layered Tree Description

The structure chosen can be seen as a 3-layered tree, used to hold either points on a streamline or elements. The layers do not refer to the levels of a regular binary tree. Rather, each layer consists of one or more complete trees, each one hanging off a vertex of a higher level tree. The layers represent the x, y, and z axes respectively, and the ordering within a layer is with respect to the corresponding axis.

A concrete example with 2 layers is shown in Figure 3.2. On the left is the top-level tree, a binary search tree based on x-coordinates. The vertex (3,2,1) lies somewhere in the middle of this tree, with parent (1,2,1) and children (2,2,1) and (4,2,1). However, (3,2,1) is also the root of another tree, which is in the second layer, and whose search ordering is based on y-coordinates. This layer 2 tree contains in addition to the root (3,2,1) the points (3,1,1) and (3,3,1). There may be many such layer 2 trees, each one independent. Furthermore, each vertex of a layer 2 tree may have a subtree in layer 3, whose search order is based on z-coordinates.

The structure may also be viewed as a tree of trees. It has the following useful property when organizing points into streamlines. Every vertex of a tree in layer 2 is the root of a layer 3 tree containing points with identical x and y coordinates sorted in order by z-coordinate. This is precisely the body of a streamline in the z-direction. Similarly, by skipping the first layer, or by changing the layer ordering we can obtain the points on a streamline in the x-direction.

The precise structure of the trees that make up the different layers is not important. While some form of balanced binary search trees would probably provide the best performance, quite good results have been achieved in the current implementation using only sorted lists.

Figure 3.2 An example of the tree structure in 2-d. The vertex $(3,2,1)$ is part of a layer 1 search tree based on x-coordinates, but is also the root of a layer 2 subtree based on y-coordinates.

The same structure can be used for organizing elements in the order that they occur along streamlines. For this purpose we make the simplifying assumption that elements can be replaced for most calculations by their axis-parallel bounding boxes. For many elements in these problems this provides a good approximation of their boundary. For the remainder, it can still reduce the number of elements for which the more expensive calculations are required, and help postpone such calculations as long as possible. This is a common technique in geometric algorithms [24].

The tree ordering in this case is based on the maximum x, y, or z coordinate of the bounding box, depending upon which layer of the tree is being processed. In addition, each vertex of the tree stores the maximum extent (in the appropriate direction) of any of the elements in its subtrees. This allows us to consider only the relevant subtrees in most cases. Note that the streamlines normally flow in the negative x-direction, so the terms “maximum” and “upstream” will usually be synonymous.

Figure 3.3 shows the current implementation of the structure in all 3 levels, with the different layers represented as sorted lists.

Figure 3.3 Tree data structure developed to store elements and to collect points for streamlines. When an element is stored X , Y and Z are the maximum positions of the element's bounding box. For streamlines X , Y and Z are the coordinates of the head.

3.1.4 Locating Elements

The most time-consuming part of the streamline construction is in locating the elements that contain points on the streamline, since there may be several such searches required for each streamline. These searches are required to establish the starting conditions.

At each layer, we isolate the intervals in the direction for that layer that might contain the query point. For example, in the first (x) layer, with the query point $q=(q_x, q_y, q_z)$, with vertices V_i , let $xmin_i$ be the minimum x coordinate of the elements stored in the subtree at V_i and let $xlength_i$ be the largest length in the x direction of elements in the subtree at V_i . Then in searching for the element containing q , we search only those subtrees with $xmin_i \leq q_x$ and $xmin_i + xlength_i \geq q_x$. This process is then repeated for the y and z coordinates in the lower layers of the structure.

Finally, the possible elements containing a point (X_0, Y_0, Z_0) will be reduced to a small number for which precise inclusion tests must be done. This is done by solving the nonlinear equations for r, s, and t.

$$\begin{aligned} g_x &= X_0 - N_i(r, s, t) \quad X_i = 0 \\ g_y &= Y_0 - N_i(r, s, t) \quad Y_i = 0 \\ g_z &= Z_0 - N_i(r, s, t) \quad Z_i = 0 \end{aligned}$$

Using Newton's equation [25]

$$J^k (r^{k+1} - r^k) = -g^k$$

where J is the Jacobian matrix, r is the vector (r, s, t) in curvilinear coordinate system, and g is functions (g_x, g_y, g_z). If write $dr = r^{k+1} - r^k$. $dX = g_x$ and so on for s, t, y and z, the Newton's equation can be written in the form convenient in FEM:

$$\begin{bmatrix} dx \\ dy \\ dz \end{bmatrix} = J^k \begin{bmatrix} dr \\ ds \\ dt \end{bmatrix}$$

To ensure the convergence and improve the solution speed, we project the point first onto the coordinate planes and check whether it is inside the projections of the element bounding box.

3.1.5 Creating Streamlines

Streamlines are defined by a set of points. The points can be element nodes or Gauss quadrature points inside elements. Because the velocity is chosen parallel to the x-axis, the streamlines are always parallel to the x-axis.

The first step in constructing streamlines loops over all points. The tree structure is used to organize the points into streamlines as described above. Having x-layer of the structure tree, the tree structure fills its vertexes with the points according to their y and z coordinates. After all points have been installed, each vertex contains a streamline with one or more points.

Figure 3.4 A collection of streamlines. The heads are arranged such that $X_1 \geq X_2 \geq X_3 \geq \dots \geq X_i \geq \dots \geq X_n$. The number of points in each streamline need not be equal. The arrows indicate the downstream direction.

A controller or tester is set to prevent the streamline passing through an element without including the pointers in the element. This can be the case when all the element edges are not parallel to the coordinate axes. If this happened, the history for the streamline would be not only incomplete but also inconsistent. The distance between a preceding

point and current point is calculated and compared to the length of the element. The distance should not exceed the length.

After streamlines are created, they are collected and sorted according to the position of the head of each streamline, as shown in Figure 3.4. The starting conditions of each streamline can then be found as follows:

Figure 3.5 Numerical representation of all streamlines on a $y = 0$ plane. The lines are the links of points in the x direction. (a) Only the bodies of streamlines are shown. The unstructured mesh with refinement around the weld pool results in short streamlines. There is a controller to prevent a streamline jumping over an element. (b) Those streamlines starting inside an element get their initial data by interpolation from upstream elements which are stored in heads.

By using the technique described above, find an element containing the head of the streamline. Take the maximum x -coordinate of this element plus an increment as a new point, and find a new element containing this new point. The new element is the upstream element of the former one and the new point is the predecessor of the head of the streamline in the direction of flow. In the order in Figure 3.4 all points of the new element would

have been calculated before the new streamline starts. The new element can thus be used as an interpolation basis for the starting condition.

If no such element is found, then the streamline must start in an element on the free surface of the mesh, and a free surface condition can be applied. If the surface is an upstream boundary then cold material with the initial microstructure can be assumed. If the surface is the wall of a weld pool, then a hot material with a pure austenite or delta ferrite structure can be assumed.

Figure 3.5 shows the streamlines on the symmetric plane along a weld path.

3.2 Test Problems and Results

The microstructures were computed first for the temperature field (Figure 3.6) obtained from Chapter 2. The steady state temperature field was computed on a mesh with about 12,000 elements. The welding speed was 1.5 mm per second. Weld pool size and shape were measured from an experimental weld [26]. The maximum length was 35 mm, the maximum width 22 mm, and the maximum depth 11 mm. Estimated from the calculation in the transient analysis in Lagrangian formulation, the gross power input in this weld would be approximately 1.5 KJ/mm. The test plate size was 150 X 40 X 19 mm. The composition was in Table 3.1.

C	Si	Mn	P	S	Al	Nb	N
0.12	0.16	0.91	0.002	0.005	0.04	0.021	0.011

Table 3.1 Chemical composition of the low-alloy steel analyzed.

The second modelling was done on a temperature field (Figure 3.13) taken from the transient thermal analysis in Chapter 5. There was a double weld pool phenomenon in the weld. The speed for this weld was also 1.5 mm per second. Weld pool size and shape are described in Chapter 5. The test plate size was 250 X 160 X 19 mm. The composition was chosen the same as the first test case.

Before welding, the microstructures in the plate for both welds were 20% pearlite and 80% ferrite. The initial grain size of austenite was assumed to be 10 μm .

Figure 3.6 Temperature field in a weld computed by a steady state thermal analysis in Chapter 2. The microstructures in figures 3.7-3.11 were computed for this field.

Figure 3.7 Austenite contours at the ends of streamlines. Since the contour A, which represents 0.0 % austenite, stops before the end, there is no retained austenite in the HAZ.

Figure 3.8 Ferrite contours at the ends of streamlines. After welding, the fraction of ferrite is in the range of 65% to 75%.

Figure 3.9 Pearlite contours at the ends of streamlines. Contour B is typical of the edge of the HAZ.

Figure 3.10 Bainite contours at the ends of streamlines. The amount of bainite in the HAZ within contour C is more than 20%.

3.2.1 Steady State Temperature Field

The figures in this section show the state at the rear end of the mesh or streamlines. In the regular mesh next to the filler material, each element has a depth of 2.375 mm in the y-direction.

Figure 3.7 shows the distribution of austenite. In the upstream area, there is no change from the initial microstructures, since the incoming material has not been affected by the heat input from the weld pool. In the downstream area, all austenite has completely decomposed into its transformation products. This full decomposition indicates that the microstructure of the material flowing out is essentially stable. Although some of these transformation products are metastable any changes which occur only do so very slowly unless there is further heating.

Figures 3.8, 3.9, and 3.10 show the iso-percentage contours of ferrite, pearlite and bainite distributions respectively. In this weld process the cooling rate behind the weld pool is not large enough to form martensite at the downstream end. The final microstructure in the HAZ contains mostly ferrite and a little pearlite. Largely due to the increased austenite grain size, there is about 23 percent bainite adjacent or near the fusion zone. Two to three mm within contour C in Figure 3.10 is predicted a layer with the largest grain size and the most bainite. The cooling rate is almost constant for an isothermal contour as observed in Figure 3.11. The cooling rate defined here is $\Delta T (^{\circ}\text{C}) / \Delta t (\text{sec})$ between two neighboring points along a streamline.

Figure 3.12 shows the estimated austenite grain size in μm . The coarse grained HAZ region is next to the fusion zone. The grains in the HAZ are up to 10 times coarser than the original material. Note that the higher values inside the fusion zone, or weld metal, may not be correct because this microstructure model does not have the ability to predict them. This region is likely weak and brittle since the bainite is formed with large grain size at low cooling rate. If the bainite is formed at higher cooling rates, the region can have an ideal structure, being hard and tough. However, if the cooling rate is high enough to form martensite the region is likely to be very hard and brittle and susceptible to cracking.

Figure 3.11 A bird's-eye view picture of cooling rate contours overlapping the temperature contours (greyed). The range shown is 800 °C to 600 °C. The corresponding range of cooling rate is 20 °C/sec to 8 °C/sec. Note that for an isothermal contour, e.g., 600 °C, the cooling rate at that temperature is very nearly constant.

3.2.2 Clipped Transient Temperature Field

Sometimes an estimate of the steady state microstructures is desired in a temperature field computed by a transient step-by-step analysis. This kind of temperature field is frequently available in published data. To estimate the microstructures is to explore further the values of the old calculations. This test was done on a mesh clipped from the example in Chapter 5.

After about 24 seconds, the weld pool and its surrounding temperature field became stable. The mesh with only the steady-state temperature field was extracted, reducing the mesh size by 2/3.

In a transient study, microstructures are computed after the transient temperature analysis from step to step. After a certain number of time steps the temperature field approaches the steady state in a finite domain. In this domain, however, the computed microstructures may not have necessarily reached a steady state. Before the temperature reaches steady state, the cooling rates are usually higher. The austenite grains tend to grow less. Transformation products that are sensitive to high cooling rates are more likely to form. For these reasons, a Lagrangian formulation will have to run longer to reach the steady state for microstructures than to reach the steady state for the temperature field. Because microstructures are more sensitive to the history, the steady-state microstructure

Figure 3.12 The contours of prior austenite grain sizes are shown. Since the filler material is hot and stays longer at high temperature, above 1104 °C, grains grow very large. Contours A, B, C, and D represent the grain sizes in the HAZ, which are at least 7 times coarser than that in the original base metal.

TEMPERATURE °C

Min. = 20   Max. = 1800

A = 300   B = 500

C = 700   D = 900

E = 1100   F = 1300

G = 1500

Figure 3.13 The temperature field in a weld with a complex weld pool is shown. It has been computed in Chapter 5. The mesh with these steady state contours was cut from a larger mesh in a transient time marching analysis. The microstructures in Figure 3.14 were computed for this temperature field.

Figure 3.14 Microstructures at the end of streamlines. Only the interesting part at the end of the mesh (Figure 3.13) is shown. A "bay" area due to the complex weld pool results in an unusual microstructure. The "bay" area can be clearly seen on (c), (e), and (f), where martensite nucleates, residual austenite remains and the grain size is larger.

forms later than the steady-state temperature field. This delay in the time dimension corresponds to a length in the selected finite domain.

The temperature field adopted is shown in Figure 3.13. An important characteristic of this temperature field is a “bay” area as described in Chapter 5. In the “bay” area, the HAZ stays above the precipitate dissolution temperature, 1044 °C for this material, for a longer period of time and cools later but faster after the weld pool has passed.

Figure 3.14 shows the microstructures at the downstream end, where the material has experienced the entire steady-state thermal cycle. The modelling of steady-state microstructures here predicts that the “bay” is a hard zone with the potential to initiate fractures. In the “bay” area, the austenite grain size is the largest, and so is the percentage of bainite. It is the only place that martensite nucleates under the current weld process conditions.

Chapter 4 FEM Formulation of Steady State Stress Field in Welds

4.0 Introduction

In continuum mechanics, there are two basic descriptions, resulting in two basic formulations, the Lagrangian formulation and the Eulerian formulation. The Eulerian formulation uses spatial coordinates. With the Eulerian formulation material can move in and out of the observed domain, which is fixed in space. The Lagrangian formulation uses material coordinates so that the observed domain deforms and no material moves into or out of the domain. The two formulations are equivalent when the deformation state is independent of time. The Lagrangian formulation is often used as a first choice when the constitutive parameters in the deformation process are history dependent and the deformed geometry is unknown in advance. The Eulerian formulation is preferred when the deformed geometry is known in advance and the process is history independent and at steady state. The arbitrary Eulerian Lagrangian formulation used initially in fluid mechanics [27] [28] and its twin in solid mechanics, the mixed Eulerian Lagrangian formulation of Harber, et al., and Koh, et al., [29][30][31][32], has the capability to solve history independent problems with evolving fields, in which there is often a moving patch with a steady state field. No history dependent variables are involved in Harber's formulation. Ghosh and Kikuchi [33] recently published a paper on the arbitrary Eulerian Lagrangian formulation with the history dependent variables interpolated from a pseudo-material mesh. This results in an added computational cost and a possible loss in accuracy from the interpolation across elements in a C^0 approach. In the Eulerian formulation for stress analysis with history dependence, the history is often embedded in streamlines. The streamlines are formed by the method of characteristics starting from a known boundary. This was done by Dawson [34] for the rolling process, in which the deformed or current boundary locations must be known. The steady state formulation proposed here applies especially to stress analysis with history dependence and with unknown deformed boundary. Its domain has both the characteristics of the Eulerian space and the Lagrangian space. Material moves relative to the Eulerian frame at the welding speed. In the Lagrangian frame, a node in the mesh moves continuously with the deformation.

The Lagrangian formulation or the updated Lagrangian formulation, has dominated computational weld mechanics for more than a decade [35][36][37][38][39][40]. A typical example using the updated Lagrangian formulation [41] has the following computational capabilities. The domain length, the length along weld path, is about half a meter. To reach a relatively stable temperature field, and then a corresponding stress field, 70 to 100 time steps are required. This moves the heat source from one end nearly to the other end. Resolution is usually not satisfied in full scale. To avoid the spot welding effect, as discussed in Chapter 1, **Introduction**, more time steps would be necessary.

The steady state stress field in welding has several distinguishing features. (1) The thermal cycle results in the stress field. Errors in the temperature analysis cause errors in the stress analysis. (2) The mechanical properties of most materials used in welds are temperature and deformation-history dependent. Not only the thermal cycle but also the deformation history has to be considered when the stresses at a material point are computed. However, computations for tracking both the temperature and deformation histories are point-wise. (3) The major part of a thermal cycle in the steady state covers a short distance compared to the length of a long weld path. Therefore, if boundary constraints can be ignored, the analyzed subject is under a steady and localized loading condition, which results in steady-state distortions and residual stresses. (4) The resulting thermal stress is so high that both elastic and plastic deformations must be considered. The problem requires a nonlinear thermo-elasto-plastic solution. (5) The peak temperatures are high enough to cause phase transformations in the material. The expansions and contractions caused by the phase transformation influence the stress state, particularly the final residual stress.

Real welds are often several meters in lengths. On both ends of any weld there will be regions where the stress field is different from that existing over the majority of the weld length. These regions have been called end effects. The differences in the thermal histories between the ends of the weld and the middle of the weld are an important cause of these end transients. Differences in end constraints also contribute in important ways. Under the assumption of the steady state, the starting and ending transient thermal histories will not be considered. Therefore, the end effects are only dependent on the end constraint. For a 1 m butt weld the experimental measurements by Garmon et al. [42] showed about 15 cm on both free ends of a butt weld where longitudinal and transverse stresses were noticeably different. Andersson's [43] 2-D analysis proved this effect. The steady state formulation is expected to be correct on the stable middle part of the weld, if the weld is sufficiently

long. The main inaccuracy caused by the free ends of the Eulerian domain is expected to be near the ends. To analyze a complete weld, a combination of the Lagrangian and Eulerian formulations would be more suitable. Ideally, the starting and stopping transient could be analyzed in steps with a Lagrangian formulation and the middle part of the weld could be analyzed with a steady state formulation.

4.1 Equilibrium Equation

In the welding process, changes in stress caused by deformation are assumed to travel slowly compared to the speed of sound. So, at any instant, an observed group of material particles is approximately in static equilibrium. In either the Lagrangian or the Eulerian reference frame, the partial differential equation of equilibrium is, at any moment,

$$\frac{\partial \sigma_{ji}}{\partial x_j} + f_i = 0 \quad \text{or} \quad \nabla \cdot \boldsymbol{\sigma} + \mathbf{f} = 0 \quad (4.1)$$

where $\mathbf{f}$ is the sum of the body forces.

In the FEM formulation, equation 4.1 can be integrated over the physical domain, or a reference domain with a unique mapping to the physical domain, and written in the matrix form

$$\int_{\Omega} \mathbf{B}^T \boldsymbol{\sigma} \, d\Omega = \mathbf{R} \quad (4.2)$$

$$\mathbf{R} = \int_{\Gamma} \mathbf{N}^T \mathbf{T} \, d\Gamma - \int_{\Omega} \mathbf{N}^T \mathbf{f} \, d\Omega$$

where $\mathbf{N}$ is a matrix of basis functions, $\mathbf{B}$ is a symmetric gradient operator, evaluated in the configuration at current time t , $\mathbf{T}$ is the surface traction exerted on the boundary, Γ , of the domain, and Ω is the domain at the time t . $\boldsymbol{\sigma}$ is the Cauchy stress.

Suppose $\boldsymbol{\sigma}$ consists of two parts, a first guess (trial stress) and a correction, $\boldsymbol{\sigma} = \boldsymbol{\sigma}' + \delta\boldsymbol{\sigma}$, then equation 4.2 can be written as

$$\int_{\Omega} \mathbf{B}^T \delta\boldsymbol{\sigma} \, d\Omega = \mathbf{R} - \int_{\Omega} \mathbf{B}^T \boldsymbol{\sigma}' \, d\Omega \quad (4.3)$$

When $\mathbf{D}$ is a modified material property tensor, including the incremental changes of material properties,

$$\delta\boldsymbol{\sigma} = \mathbf{D}\delta\boldsymbol{\epsilon}$$

$$\delta \epsilon = B \delta u$$

$\delta \sigma$ and $\delta \epsilon$ are corrections to stresses and strains respectively in column forms. δu is the correction to the displacement vector. Put δu into equation 4.3,

$$\int_{\Omega} B^T D B \delta u \, d\Omega = R - \int_{\Omega} B^T \sigma^n \, d\Omega \quad (4.4)$$

δu will approach zero when the configuration approaches the current configuration for equilibrium, or, $\sigma = \sigma'$. A residual load vector persists in equation 4.4 until an exact solution is reached.

$$\int_{\Omega} K \delta u \, d\Omega = \text{residual} \quad (4.5)$$

Non-linear solution methods can be used to solve equation 4.5.

4.2 Initial Condition

Before welding, at time t_0 , the base material is assumed stress or strain free for convenience. If the initial stresses and strains were known, they could be included in the analysis. All displacements at t_0 are set to zero.

4.3 Boundary Condition

With the current computational capacity, it is impossible to analyse a large, welded structure in FEM analysis. Therefore, to analyze large welds, there always is an end effect on a relatively small domain cut from the large weld structure. This is true for both a Lagrangian and an Eulerian formulation. Fortunately, this effect is not so significant in welding process, since the heat source is highly localized and its thermal cycle affects stresses only in a short distance. Experimental and computational results indicate that end effects play a role only for short distances from the end.

4.4 Constitutive Equations

Constitutive equations (stress-strain relations) describe the material response to the strains at the current state. In a numerical approach, it is customary to assume initially that the deformation is elastic. In this thesis, the elasto-plastic constitutive model uses a modified effective-stress-function (ESF) algorithm [47].

The trial stress, ${}^i\sigma'$, at each integration point is assumed to be

$${}^i\sigma^n = \int_0^i D d\epsilon = {}^{i-1}\sigma + \int_{i-1}^i D d\epsilon$$

The superscript i indicates a point on a streamline in space dimension, which is equivalent to t in the time dimension. Similarly, $i - 1$ indicates a point analogous to $(t - \Delta t)$. The incremental trial stress is, therefore,

$$\Delta^i \sigma = \int_{i-1}^i D d\epsilon$$

Including thermal, elastic, plastic, transformation, and creep deformations, the constitutive equations can be written in the form

$${}^iS = \frac{{}^iE}{1 + {}^i\nu} ({}^ie - {}^ie^p - {}^ie^c - {}^ie^{TrP}) \quad (4.6)$$

$${}^i\sigma_m = \frac{{}^iE}{1 - 2{}^i\nu} ({}^ie_m - {}^ie^{th} - {}^ie^{TrV})$$

where at point i ,

$$\begin{aligned} {}^iS &= \text{deviatoric stress tensor} \\ &= {}^i\sigma - {}^i\sigma_m \end{aligned}$$

$$\begin{aligned} {}^ie &= \text{deviatoric strain tensor} \\ &= {}^ie - {}^ie_m \end{aligned}$$

$${}^ie^p = \text{plastic strain tensor}$$

$${}^ie^c = \text{creep strain tensor}$$

$${}^ie^{TrP} = \text{transformation plastic strain tensor}$$

$${}^i\sigma_m = \text{mean stress tensor}$$

$${}^ie_m = \text{mean strain tensor}$$

$${}^ie^{th} = \text{thermal strain tensor}$$

$${}^ie^{TrV} = \text{strain due to volume change in phase transformation}$$

$${}^iE, {}^i\nu = \text{Young's modulus and Poisson's ratio at point } i \text{ corresponding to temperature at point } i$$

Let ${}^{i-1}\mathbf{e}^e$ be the deviatoric elastic strain at point $i-1$, which is the deviatoric elastic strain at point i at $(t - \Delta t)$.

$$\begin{aligned} {}^{i-1}\mathbf{e}^e &= {}^{i-1}\mathbf{e} - {}^{i-1}\mathbf{\epsilon}^p - {}^{i-1}\mathbf{\epsilon}^c - {}^{i-1}\mathbf{\epsilon}^{TrP} \\ &= \frac{1 + {}^{i-1}\nu}{{}^{i-1}E} {}^{i-1}\mathbf{S} \end{aligned} \quad (4.7)$$

We can rewrite equation 4.6 as

$$\mathbf{S} = \frac{{}^iE}{1 + {}^i\nu} ({}^i\mathbf{e}'' - \Delta\mathbf{\epsilon}^p - \Delta\mathbf{\epsilon}^c - \Delta\mathbf{\epsilon}^{TrP}) \quad (4.8)$$

where

$${}^i\mathbf{e}'' = {}^{i-1}\mathbf{e}^e + \Delta\mathbf{e}$$

$\Delta\mathbf{e}$ is the incremental deviatoric strain tensor from $i-1$ to i .

Thermal strain at point i , $\Delta\mathbf{\epsilon}^{th}$, comes from integration of $\dot{\mathbf{\epsilon}}^{th}$ from $i-1$ to i .

$$\Delta\mathbf{\epsilon}^{th} = \int_{i-1}^i \dot{\mathbf{\epsilon}}^{th} dl = \dot{\mathbf{\epsilon}}^{th} \Delta l$$

where

$$\dot{\mathbf{\epsilon}}^{th} = \bar{\alpha} \dot{T} \mathbf{I}$$

$$\dot{T} = \frac{dT}{dl}$$

$\bar{\alpha}$ is related to α by

$$\bar{\alpha} = \alpha + \frac{\partial \alpha}{\partial T} (T - T_{ref})$$

$$\alpha = \gamma \alpha_\gamma + (1 - \gamma) \alpha_\alpha$$

where γ is the percentage of austenite, α_γ is the thermal expansion coefficient in the phase of austenite and α_α is the thermal expansion coefficient in the lower temperature phases. $\bar{\alpha}$ is called the instantaneous coefficient of thermal expansion and α is called the average coefficient of thermal expansion.

When integrating along a streamline from $i-1$ to i , we assume that the temperature along the line changes linearly. We also assume that the material properties are a smooth function of the temperature. So, the mid-point values $^{i-0.5}T$ and $^{i-0.5}\alpha$ can be used as constants to replace T and α in the integration. Thus,

$$\frac{\partial \alpha}{\partial T} \approx \frac{^i\alpha - ^{i-1}\alpha}{^iT - ^{i-1}T}$$

and

$$\int_{i-1}^i T dl = ^iT - ^{i-1}T$$

Therefore,

$$^i\Delta \epsilon^{th} = ^{i-0.5}\alpha(^iT - ^{i-1}T)I + (^i\alpha - ^{i-1}\alpha)(^{i-0.5}T - T_{ref})I$$

The ESF algorithm has been adopted to increase the efficiency of solving for the incremental plastic strain, $\Delta \epsilon^P$, as well as the incremental creep strain, $\Delta \epsilon^C$. A brief description of ESF used in the current case is given in the following. Details of the ESF can be found in Kojic and Bathe [45][46]. Details with combined isotropic-kinematic hardening are given by Oddy [47]. The transformation plasticity formulation is due to Oddy, et al. [48].

A basic equation of thermo-plasticity is, considering isotropic hardening only,

$$\frac{d^i\epsilon^P}{dl} = ^i\Lambda ^iS \quad (4.9)$$

where $\frac{d^i\epsilon^P}{dl}$ are the derivative of the plastic strain at point i with respect to a distance along the streamline, and $^i\Lambda$ is a scalar,

$$^i\Lambda = \frac{3}{2^i\sigma_y} \left[\frac{\partial ^i\bar{\epsilon}^P}{\partial ^i\sigma_y} \frac{\partial ^i\sigma_y}{\partial l} + \frac{\partial ^i\bar{\epsilon}^P}{\partial ^iT} \frac{\partial ^iT}{\partial l} \right]$$

$^i\sigma_y$ is the instantaneous yield stress at point i . $^i\bar{\epsilon}^P$ is the effective plastic strain defined as a function of the effective plastic strain and temperature.

Considering the classical description of creep, the creep strain gradient tensor is given by

$$\frac{d {}^i \bar{\epsilon}^c}{dl} = \frac{3}{2} \frac{\partial {}^i \bar{\epsilon}^c}{\partial l} {}^i S \quad (4.10)$$

where ${}^i \bar{\epsilon}^c$ and ${}^i \bar{\sigma}$ are the effective creep strain and the effective stress, respectively.

For the numerical solution, one can rewrite equation 4.9 and equation 4.10 in the form,

$$\Delta \epsilon^p = \Delta l {}^\tau \Lambda {}^\tau S = \Delta \lambda {}^\tau S \quad (4.11)$$

$$\Delta \lambda = \frac{3}{2} \frac{\Delta \bar{\epsilon}^p}{{}^\tau \bar{\sigma}}$$

and

$$\Delta \epsilon^c = \frac{3}{2} \frac{\Delta \bar{\epsilon}^c}{{}^\tau \bar{\sigma}} {}^\tau S \quad (4.12)$$

where the superscript τ denotes weighted values using the $\bar{\alpha}$ -method. We distinguish $\bar{\alpha}$ in the $\bar{\alpha}$ -method from the α for the thermal expansion coefficient. For example,

$${}^\tau S = (1 - \bar{\alpha}) {}^{i-1} S + \bar{\alpha} {}^i S$$

and so on. For the plastic strain components, the recommended value of $\bar{\alpha}$ is 1, and for the creep strain components, the recommended value is $\bar{\alpha} \geq \frac{1}{2}$.

Solving equations 4.8, 4.11, 4.12 yields ${}^i S$.

The basic idea in the development of the ESF algorithm is to iterate on a single unknown variable, the effective stress, rather than on the six unknown components in solving ${}^i S$. The governing equation is obtained by taking the scalar product of both sides of equation 4.8, which gives

$$({}^i \bar{\sigma})^2 = 9({}^i G)^2 ({}^i \bar{\epsilon}^e)^2$$

where

$${}^i G = \frac{{}^i E}{2(1 + {}^i \nu)}$$

and $\bar{\epsilon}^e$ denotes the elastic deviatoric effective strain at point i , see equation 4.7.

$${}^i\bar{\epsilon}^e = \sqrt{\frac{2}{3}} {}^i\epsilon^e \bullet {}^i\epsilon^e \quad (4.13)$$

Since the right hand side of equation 4.13 depends only on the effective stress ${}^i\bar{\sigma}$, the problem has been reduced to finding the effective stress which results in a zero value for the effective stress function,

$$f = ({}^i\bar{\sigma})^2 - 9({}^iG)^2 ({}^i\bar{\epsilon}^e)^2$$

During iteration, 1,2,3,...,n, convergence is reached if

$$|f({}^i\bar{\sigma}^n)| \leq \text{tolerance}$$

Typically we use 1% of σ_y as the tolerance.

4.5 Deformation

By introducing a reference configuration in the deformation equations, any one configuration in the deformation process can be expressed in that reference configuration. Figure 4.1 shows the displacement of a particle from its initial position ${}^{i-1}\mathbf{x}$ to the current position ${}^i\mathbf{x}$, defined by the deformation equations

$$\mathbf{x} = \mathbf{X}({}^r\mathbf{x}, t)$$

The deformation gradient tensor is the simplest to define in terms of the deformation equations. This tensor also includes more information than some strain measurements. It describes both the rotation and stretching experienced during the deformation.

The deformation gradient with one end in the reference configuration is denoted here by ${}^i\mathbf{F}$. Hence, in this context ${}^i\mathbf{F}$ is defined as the tensor whose rectangular Cartesian components are the partial derivatives $\partial^i x_k / \partial^r x_m$. The tensor ${}^i\mathbf{F}$ operates on an arbitrary infinitesimal material vector $d^r\mathbf{x}$ at ${}^r\mathbf{x}$. It associates the vectors $d^i\mathbf{x}$ and $d^r\mathbf{x}$ as

$$d^i\mathbf{x} = {}^i\mathbf{F} \bullet d^r\mathbf{x}$$

In indicial form

$$d^i x_k = \frac{\partial^i x_k}{\partial^r x_m} d^r x_m$$

Figure 4.1 Displacement, stretch, and rotation of a vector $d^{i-1}x$ at position $i-1$ to d^ix at new position i . Both of them have unique mappings to reference configuration.

One advantage of the Lagrangian formulation is that it traces the changes of mechanical properties in the deformed material naturally. In the updated Lagrangian formulation the mechanical properties are updated in every time step. In every current step, all history results are treated as initial conditions. The formulation deals with the same material in the final and initial configurations. Without deformation, a local coordinate system will remain unchanged in two configurations. An infinitesimal vector is computed in the local coordinate system. When deformation occurs between the two configurations, the local coordinate system changes its scale and direction. So does the infinitesimal vector. In general, this local coordinate system differs from one point to another in a curvilinear coordinate system. For the steady state formulation, the mesh has the features of both the Lagrangian formulation and the Eulerian formulation. Each element would no longer contain the same set of material points. The stress or strain history of a deformed material particle can only be found from an upstream position of a streamline. The position is currently taken by another material point and the local coordinate system at that position is

unlikely to be the same one as that of the current point, even without deformation. Strategic mapping is necessary.

Figure 4.2 indicates the relationships between the two deformed configurations and the undeformed configuration (reference configuration). Note here that all configurations are defined in a global Cartesian coordinate system. This coordinate system describes the Lagrangian part of the problem, while the material moving against this system is the Eulerian part. Applied to a steady state welding problem, this Cartesian system moves at a constant speed with the welding source.

By choosing an undeformed reference configuration properly and by mapping material points in any of the other configurations to the reference configuration, it is possible to obtain the deformation gradient tensor between any two deformed configurations. A few mappings are required to reach this indirectly from the deformed configurations to the reference configuration or in reverse order. The same material point P is located in the reference configuration at ${}^r\mathbf{x}$, in deformed configuration at ${}^{i-1}\mathbf{x}$, and in deformed configuration at ${}^i\mathbf{x}$.

To map the reference configuration in an element (the material set a-b-c-d) to an isoparametric element $i-1$, the Jacobian operator ${}^rJ({}^{i-1}\xi)$ at point P is, in indicial form,

$${}^rJ({}^{i-1}\xi) = \frac{\partial {}^r x_k}{\partial {}^{i-1}\xi_k}$$

To map the $i-1$ deformed configuration in the same element (the same material set) to the same isoparametric element $i-1$, the Jacobian operator ${}^{i-1}J({}^{i-1}\xi)$ at point P is, in indicial form,

$${}^{i-1}J({}^{i-1}\xi) = \frac{\partial {}^{i-1}x_k}{\partial {}^{i-1}\xi_k}$$

When material deforms from the reference configuration to the $i-1$ deformed configuration, the deformation gradient tensor, ${}^{i-1}\mathbf{F}$, at point P is obtained through mapping to and from the isoparametric element $i-1$,

$${}^{i-1}\mathbf{F}(\mathbf{x}) = \frac{\partial {}^{i-1}\mathbf{x}}{\partial {}^r\mathbf{x}} = {}^{i-1}J({}^{i-1}\xi) \bullet {}^rJ^{-1}({}^{i-1}\xi)$$

In indicial form,

$${}^{i-1}F_{mn} = \frac{\partial {}^{i-1}x_m}{\partial {}^r x_n} = \frac{\partial {}^{i-1}x_m}{\partial {}^{i-1}\xi_k} \frac{\partial {}^{i-1}\xi_k}{\partial {}^r x_n}$$

Figure 4.2 Topology of material point P between reference configuration and configurations at i and $i-1$. Note the infinitesimal vectors $d^i x$ and $d^{i-1} x$ locate in two different material groups but both contain point P .

To map the reference configuration in another element (the material set $e-f-g-h$) to another isoparametric element i , the Jacobian operator ${}^r J({}^i \xi)$ at point P is, in indicial form,

$${}^r J({}^i \xi) = \frac{\partial {}^r x_k}{\partial {}^i \xi_k}$$

To map the i deformed configuration in the same element (the material set $e-f-g-h$) to the same isoparametric element i , the Jacobian operator ${}^i J({}^i \xi)$ at point P is, in indicial form,

$${}^iJ({}^i\xi) = \frac{\partial {}^ix_k}{\partial {}^i\xi_k}$$

When material deforms from the reference configuration to the i deformed configuration, the deformation gradient tensor, ${}^iF$, at point P is obtained through mapping to and from the isoparametric element i ,

$${}^iF(x) = \frac{\partial {}^ix}{\partial {}^rx} = {}^iJ({}^i\xi) \bullet {}^rJ^{-1}({}^i\xi)$$

In indicial form,

$${}^iF_{mn} = \frac{\partial {}^ix_m}{\partial {}^rx_n} = \frac{\partial {}^ix_m}{\partial {}^i\xi_k} \frac{\partial {}^i\xi_k}{\partial {}^rx_n}$$

Therefore, a relative deformation gradient tensor, F , between initial configuration $i-1$ and final configuration i , can be defined

$${}^{i-1}F(x) = \frac{\partial {}^ix}{\partial {}^{i-1}x} = \frac{\partial {}^ix}{\partial {}^rx} \bullet \frac{\partial {}^rx}{\partial {}^{i-1}x} = {}^iF \bullet {}^{i-1}F^{-1} \quad (4.14)$$

In indicial form,

$${}^{i-1}F_{mn} = \frac{\partial {}^ix_m}{\partial {}^rx_k} \frac{\partial {}^rx_k}{\partial {}^{i-1}x_n}$$

4.6 Strain Increment Measurement

Any constitutive model requires that stresses and strains must match each other, i.e., the measurements of stresses and strains must be in same configuration. Their inner product should equal the strain energy density. This is also true of the stress and strain increments. Once the type of stress or stress increment has been chosen, the type of strain or strain increment used is defined, and *vice versa*. In the following, when the stress rate is specified, the corresponding strain is implied.

When the displacement-gradient components of a strain tensor are not small compared to unity, the problem of characterizing the strain from the initial state is more difficult than in the small-strain case. For a weld, in some local area within the heat affected zone, the

displacement-gradient components can be of the order of unity. Thus, regions far from the heat affected zone may have large displacements and large rigid body rotations but small strains. Looking at a weldment, a large rigid body rotation from the original shape can often be seen with the naked eye. Infinitesimal strain measures can cause large errors in the residual stress analysis for welds [38]. Finite strain measurements have to be used in the stress and deformation analysis for welds.

There are two total strain measurements referring to initial and final configurations respectively. The measurement based on the initial configuration, or material coordinates, is called the Green-Lagrangian strain. The measurement based on the final configuration, or spatial coordinates, is called the Almansi-Eulerian strain. Clearly, both formulations should yield the same numerical results provided the appropriate transformations corresponding to the constitutive relations are applied. When a deformation has a plastic component, the deformation is path dependent. Nonlinearity can be severe over a finite time step by using either the Green-Lagrangian strain or the Almansi-Eulerian strain. The solution could diverge.

An accepted way of tracing the deformation history is to use the strain rate and to integrate the strain rate and the constitutive equations over the finite deformation interval, i.e., to integrate the stress rate over the interval. Indeed, many research papers have exploited various stress rates. The advantages and disadvantages of different stress rate formulations are described in references [38][49][50][51][52][53]. Among these formulations, the most attractive are the Jaumann stress rate formulation and Green-Naghdi stress rate formulation, because they directly relate the Cauchy stresses and velocity strains. However, these formulations present some numerical difficulties. Large rigid body rotations are the most difficult problem for these formulations.

The difficulty in using the Jaumann stress rate is encountered when applying the rate equation to finite increments [54]. Consider an initial stress state of

$${}^0\sigma = 10 \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

When either the forward or the backward Euler integration is applied, 100 solution steps are required to rotate this stress state ninety degrees with an acceptable error. The error is introduced because the incremental Jaumann stress equation is a very low order

approximation to a rotational transformation. An immediate improvement in performance can be obtained by explicitly performing a rotational transformation

$${}^{t+\Delta t}\sigma = {}^{t+\Delta t}\mathbf{R} {}^t\sigma {}^{t+\Delta t}\mathbf{R}^T$$

Hughes and Winget [55] have proposed a scheme to calculate an approximation to the matrix ${}^{t+\Delta t}\mathbf{R}$. They considered it crucial to the accuracy to evaluate all variables in ${}^{t+\Delta t}$ midpoint, or average, configuration. The midpoint scheme has been reported to work well [38] until the rigid body rotation reaches 180° , which means a collapsed midpoint configuration as pointed by Hughes [49] in Figure 4.3.

Figure 4.3 Behavior of the midpoint, or average, configuration as a function of rotation.

The logarithmic strain, or Hencky strain, fits best the experiment result [49]. Along a streamline, the incremental logarithmic strain at point i is

$$\Delta \boldsymbol{\varepsilon} = {}_{i-1}\mathbf{R} \ln({}_{i-1}\mathbf{U}) {}_{i-1}\mathbf{R}^T$$

where $\mathbf{R}$ is a rotation tensor rotating the stress or strain in the orientation of point $i-1$ to that of the point i , and $\mathbf{U}$ is a stretch tensor describing the stretch from $i-1$ to i in the orientation of stress (or strain) at $i-1$. $\mathbf{R}$ and $\mathbf{U}$ can be obtained by a polar decomposition of a relative deformation gradient tensor [56][57]. The method of decomposition is described in [58].

$${}_{i-1}\mathbf{F} = {}_{i-1}\mathbf{R} {}_{i-1}\mathbf{U}$$

Physically this decomposes a continuous deformation process into 3 successive steps; a stretch in the initial orientation by the operator $\mathbf{U}$; a rigid-body rotation by the operator $\mathbf{R}$ to rotate the stretched body to the current orientation; and finally a translation to point i .

The logarithmic strain, named as the updated Lagrangian Hencky formulation, has been advocated in [46][54] for large strain, large rigid body rotation and large displacement. A comparison [46] of the traditional Jaumann formulation and the updated Lagrangian Hencky formulation shows the following:

- In simple stretching (or compression) the two formulations yield identical results.
- In simple (rigid body) rotation, the updated Lagrangian Hencky formulation yields the correct solution for very large rotations in a single incremental step, whereas the Jaumann formulation is restricted to small incremental rotations per step.

The updated Lagrangian Hencky formulation is used in this thesis.

With the formulae in the section 4.5, a summary of current formulation to calculate incremental stress from point $i-1$ to i along a streamline is as follows:

Step 1: Decompose the relative deformation gradient at point i , equation 4.14

$${}_{i-1}\mathbf{F} = {}_{i-1}\mathbf{R} {}_{i-1}\mathbf{U}$$

Step 2: Calculate the incremental logarithmic strains at the strain orientation of point $i-1$,

$$\Delta \boldsymbol{\varepsilon}' = \ln({}_{i-1}\mathbf{U})$$

$$\Delta \epsilon_m = \frac{\text{tr}(\Delta \epsilon)}{3}$$

$$\Delta \epsilon = \Delta \epsilon' - \Delta \epsilon_m$$

Step 3: Calculate the total Cauchy stresses at the stress orientation of point $i-1$,

$${}^{i-1}({}^i \sigma) = {}^{i-1} \sigma + \int_{i-1}^i D d\epsilon$$

$${}^i S = \frac{{}^i E}{1 + {}^i \nu} ({}^i \epsilon'' - \Delta \epsilon^p - \Delta \epsilon^c - \Delta \epsilon^{\text{TrP}})$$

$$= \frac{{}^i E}{1 + {}^i \nu} \frac{1 + {}^{i-1} \nu}{{}^{i-1} E} {}^{i-1} S + \frac{{}^i E}{1 + {}^i \nu} (\Delta \epsilon - \Delta \epsilon^p - \Delta \epsilon^c - \Delta \epsilon^{\text{TrP}})$$

$${}^i \sigma_m = \frac{{}^i E}{1 - 2 {}^i \nu} ({}^i \epsilon_m - {}^i \epsilon^{\text{th}} - {}^i \epsilon^{\text{TrP}})$$

Step 4: Rotate the Cauchy stresses to the current orientation

$${}^i \sigma = {}_{i-1} R {}^{i-1}({}^i \sigma) {}_{i-1} R^T$$

4.7 Implementation Technique

4.7.1 Stiffness Matrix and Residual Vector

For the updated Lagrangian formulation, the usual procedure in a time step is to calculate the stiffness matrix and residual vector element by element. In each element, the Gauss quadrature points are visited in turn. Stresses and strains are recorded at each Gauss point, for both the initial and final states.

The steady state formulation uses streamlines to trace the history. Before welding, the mesh has no distortion, and the elements of the mesh are regular. The Gauss points in elements are aligned to form streamlines by the methods and data structure described in the chapter 3.

The Gauss points are aligned to form straight lines in the undeformed state. Since the mesh deforms with respect to a Lagrangian frame, these straight lines distort continuously

with the deformation process. They are exactly the streamlines for the current state when the convergence is reached. The whole non-linear approach is to build up streamlines.

The steady state analysis differs from the usual Lagrangian formulation for calculating the stiffness matrix and residual vector in that the modified formulation loops over all Gauss points directly. Every Gauss point knows the element it resides in, which makes it easier for Gauss point to make contributions to the element, or to the nodes of the element. Since the Gauss points are object-oriented, giving the pointers from Gauss points to elements is simple and natural.

The streamlines are calculated one after another in the order of *upstream first*. The Gauss points on one streamline are taken in order, so that upstream points are always evaluated first. The rule of *upstream first* has two aspects in this implementation. First, the streamline with its head point at a relatively upstream position will be treated first. This guarantees that all start points of lines can get an updated initial state. Second, within one streamline, a Gauss point at a relatively upstream position will be calculated first. With the rule *upstream first*, the initial data is ready to be fetched when the current point is calculated. It is analogous to the integration of the strains from t_{i-1} to t_i in time space.

Since the history of strains or stresses comes from the upstream, which is all within the same observed space, every Gauss point need only store its current (or final) stresses and current strains. Savings can be half the storage space of a Gauss point used in the usual updated Lagrangian formulation. The previous upstream point stores the initial data for the current point. For an 8-node brick element, there usually are 8 Gauss points. If each Gauss point stores 32 values in double precision in the Lagrangian formulation, the steady-state formulation saves about 1 KB in every 8-node brick element.

4.7.2 Consistent Fields

The FEM implementation must be done in such a way to permit the analysis of incompressible strain fields. Unrealistic results have resulted from the normal integration of the stiffness matrix and residual vector using the Gaussian quadrature rules. For a linear eight-node brick element in a thermo-elasto-plastic problem, locking can occur due to the variation of the thermal strain within the element [41] [33], which results in a higher order in the dilatation components of the strain than the basis functions of the element can support. When the analysis involves a phase transformation, a similar problem has been

observed [41] since the volume change in a phase transformation and the material properties are often a function of temperature.

The locking problem can also occur due to inconsistent histories. For a Lagrangian formulation, this is not a problem, since there is no material moving relative to an element. An element at the current step can receive a complete consistent strain field from the last step as long as it was consistent in the last step and the element contains the same set of material points. When material enters and/or leaves an element, as occurs in the Eulerian formulation, consistency can not always be maintained without special measures. Inter-element variation may cause variations in the strain history received by different points in one element. Unlike the inconsistency in the incremental strains or the incremental stresses caused by temperature and/or phase transformation as described above, the inconsistency here exists in the total strains or stresses.

For isotropic materials, methods of selective reduced integration are often applied to alleviate the inconsistency within an element. The reduced integration on the dilatation components of strains reduces the order of the volumetric strain distribution. Thus the consistency is obtained by a compulsory mean. For eight-node brick elements it is obtained by using a single, mean value, calculated at the element centroid. Following the procedure suggested by Hughes [59] the strain-displacement matrix B is modified. This results in a combination of full integration of the distortion terms and reduced integration of the dilatation terms.

When the thermal strain in an eight-node brick element is integrated by a single point integration, some accuracy in temperature field has been sacrificed. The element is treated as a constant temperature element. Therefore, in areas with large temperature gradients, the mesh should be fine enough to include all phase changes in the material. For example, in the edge weld, shown in Figure 4.8, the temperature in the longitudinal direction behind weld pool drops from 900 °C to 560 °C over a distance of about 9.5 mm. If only one element spans this distance, then the plastic and transformation strains will cause a very inaccurate result. To keep the temperature changes between two elements to under 50 °C, there must be at least 6 elements within this distance, if the temperature gradient is constant. In other words, the element length in the longitudinal direction should not exceed 1.5 mm. If the problem is done in a Lagrangian formulation, this means that in order to keep a complete history, the lengths in the longitudinal direction of all elements along the weld path should be less than 1.5 mm. This places a heavy burden on the current capacity.

Several possible ways may help to solve the problem caused by inter-element inconsistency. Clermont, et al., [60] used a stream tube method in fluid mechanics. It was a geometrical method which mapped the physical domain D into a computational domain D_1 . The field data and boundary conditions in D were mapped to D_1 by a known or an unknown transformation. After the transformation, a complex flow domain was changed to a simpler computational domain and the transformed lines of the physical streamlines were defined as straight lines or circles. However, the transformation was not always available, so that the method was restricted to plane or axisymmetric flows without vortices and purely circulatory flows or vortex flows.

Agrawal and Dawson [61] compared two methods for integrating the strains for the Eulerian velocity fields associated with large strain material forming processes. In the Galerkin formulation, partial differential equations 4.15 for the deformation gradient were solved, in the weak sense, over the entire domain based on a weighted residual formula.

$$\frac{DF_{ij}}{Dt} = L_{ij} F_{ij} \quad (4.15)$$

where,

$$F_{ij} = \frac{\partial x_i}{\partial X_j}$$

$$L_{ij} = \frac{\partial u_i}{\partial x_j}$$

$$u_i = \frac{\partial x_i}{\partial t}$$

with X_j as the previous coordinates and x_i as the current coordinates. The other method they used was a streamline integration. With this technique, the equations 4.15 were integrated along characteristic lines that were defined by the method of characteristics. Applications with this streamline integration were reported by Dawson [34]. It seems promising that the Galerkin formulation can be applied to solve the inter-element inconsistency considered here, if the approximating functions used are of the same order as the ones used in deformation analysis. However, no test cases were given to either method for locking caused by inconsistent inter-element strain histories.

In this thesis, the domain changes its shape continuously during deformation. Therefore the streamlines are updated from straight lines. If the elements are not graded in the streamline direction, a consistent history can be convected downstream. Then a set of elements will contain the same group of streamlines, and form a material stream tube. The inconsistent history only occurs when the mesh changes from the finer one to the coarser one. This is because the streamlines in the coarser element would get their historical data from different small elements. Therefore, grading in down-streamline direction behind the weld pool is not allowed in this thesis. However, grading from a coarser mesh to a finer mesh does not cause problems. Before the base metal enters the frontier of the heat source, the temperature in the metal would not rise significantly in most cases. The length of the HAZ in front of the weld pool is usually 10 to 20 mm. Hence, the mesh in front of this 10 to 20 mm region can be graded to a very coarse mesh. This is demonstrated in the examples of tests.

4.7.3 Starting a Streamline

Most streamlines start in the undeformed upstream region. This region is assumed to be at room temperature, and the initial stress and strain is assumed to be zero. When the temperature in the material gets high enough, recrystallization may occur and the yield stress may soften. Recrystallization erases the previous plastic strain. Softening reduces the inherited stresses. For streamlines starting at a high-temperature free surface such as the wall of the weld pool, the origins of the streamlines are fully austenitic and recrystallized. The initial stress and strain are zero.

When there is grading from coarse to fine in the downstream direction, the graded element initiates new streamlines. Since the data structure ensures that the upstream element is computed first, the initial values of new streamlines can be interpolated from the internal values of the upstream element. The interpolation procedure is done first to project the values of the Gaussian points of an element to its corner nodes. This uses Patel's *Least Square Stress Projection Schemes* [44]. Then the initial values of a new streamline can be interpolated from those corner nodes with element basis function.

4.8 Test Cases

The code has been tested in several ways. For elastic deformation, a uniaxial stretch test has been performed on a two-element mesh. A thermal expansion test has been performed on a five-element mesh.

Figure 4.4 Stresses in an uniaxial stretching test with a two element bar.

Figure 4.5 (a) (b)

Figure 4.5 (c) (d)

The two-element mesh has the size: $2 \times 1 \times 1$ m. Iso-contour graphs were drawn with the TAURUS graphical software. The nodal values used to plot iso-contours are the average values picked from the nearest Gauss Points in the elements containing the node. Although all values at Gauss Points are stored in double precision, the nodal values of stresses and strains are stored in single precision. For these nodal values are not for computing. They are just for supporting the graphical software, which reads data only in single precision.

Figure 4.5 (e) Thermal expansion of a middle element in a 5 element bar. The two ends are fixed in x direction. Deformation scale factor is 50. Contours are 6 stress components.

Since, in elastic deformation, the deformed body can return to its original shape after unloading, the formulation is equivalent to a single step in a Lagrangian formulation. The differences are only in the integration procedures. The load case used had one end fixed in the x-direction and a prescribed x-displacement of 0.1 mm applied at the other end. Numerical results are shown in Figure 4.4. There is a uniform longitudinal stress, σ_{xx} . Round-off damage has created other stresses that are within 0.005% of the longitudinal stress. Since graphically presented data had only 6 digit precision, the damage could be enlarged during interpolations. If computed data are all large enough this damage would not be seen graphically.

Thermal expansion and contraction were also tested within the elastic range. The mesh size was $15.8 \times 3.2 \times 3$ mm, divided evenly along the x-direction into 5 elements. Results are shown in Figure 4.5. The mid element, element 3, had a temperature increment of 30°C . Although either a Lagrangian formulation or a steady state formulation reach the same results in this case, the meanings are different for the two formulations. All elements but element 3 were kept at constant room temperature in the Lagrangian formulation. While a thermal expansion occurred in element 3, there was no thermal expansion or shrinkage in any other elements. In the steady state formulation, the material in element 4 and element 5 had experienced a complete thermal cycle, heated up from 20°C to 50°C and then cooled down to 20°C again. A corresponding cycle of expansion and contraction occurred in these two elements. When thermal expansion occurred in element 3, there was a corresponding shrinkage in element 4 and element 5.

In this test, all 6 components of stresses have obtained values great enough to expel the round-off damage as seen in test 1. In Figure 4.5, disturbances can not be presented in contours. This test shows the algorithm behaved well when there is an elastic recovery.

When the deformation is large enough to cause plastic flow, it is necessary to follow the streamlines to provide the history of plastic deformation. Any comparisons of the results, between the computed by current codes and the quoted from the other analyses, or between the computed and the quoted from experimental measurements, can only be true under one presumed condition: the results are valid only for the steady state deformation. Simple load cases, like uniaxial stretch or compression, do not serve this purpose well.

The next test case is an edge weld on a long plate. The results are compared with those computed in the Lagrangian formulation and measured in an experiment, provided by Oddy [41].

4.8.1 Edge Weld

An edge weld has been performed on a thin strip. This example has been analyzed with a Lagrangian formulation [38][41]. The mesh in Figure 4.6 was created on a piece of material cut from the long strip, which was assumed to have a steady-state temperature field. The mesh size is $543 \times 50.8 \times 6.35$ mm. Although this domain has the same size as the one used for the Lagrangian formulation in previous computations, the previous one was not designed for long welds. It was assumed to be a short weld on a short plate, so that it

Figure 4.6 FEM mesh designed for simulating the edge weld.

Figure 4.7 Distribution of temperature, °C, in full view. At the rear end, the highest temperature is around 160 degree, and the distribution tends to be even.

Figure 4.8 Contours of Temperature, °C, around the weld pool area. Top: symmetry plane; Bottom: outer surface.

Figure 4.9 Distortion of the mesh after an edge weld. All displacements are enlarged 30 times. The undeformed mesh before welding is shown in grey lines.

Figure 4.10 Contours of stress, σ_x (MPa), in full view.

Figure 4.11 Contours of stress, σ_{xx} (MPa), around the weld pool area. The phase transformation causes negative stress in the marked area.

Figure 4.12 Contours of stress, σ_{xx} (MPa), near the rear end. Open ends affect apparently the stress only in the last two x-layers of elements.

Figure 4.13 Contours of stress, σ_y (MPa), around the weld pool area.

Figure 4.14 Contours of stress, σ_x (MPa), around the weld pool area.

Figure 4.15 Contours of shear stress, σ_{xy} , (MPa), around the weld pool area.

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Figure 4.16 Contours of shear stress, σ_{xy} (MPa), around the weld pool area.

Figure 4.17 Contours of shear stress, σ_{xy} (MPa), around the weld pool area.

had the starting transient. In order to compare the results for a more similar circumstance around weld pool, the currently used temperature field has been directly interpolated from one of the temperature fields in the Lagrangian formulation. In transient analysis, this temperature distribution was the one at 100.5 seconds after welding started. With medium resolution in space and time, it costs 65 steps in the Lagrangian formulation to reach this state for temperatures and stresses.

The x-y plane ($z=0$) is assumed to be a plane of symmetry. The heat source moves in the positive x-direction. Only half ($z>0$) of the temperature and stress fields are computed and displayed. In the stress analysis no displacement is allowed normal to this x-y symmetry plane.

Figure 4.7 shows the temperature field on the full domain. A more detailed distribution around the weld pool is displayed in Figure 4.8. The length of the element in the finest part of the mesh in weld path direction is 1.6 mm. Looking at the temperature distribution on the symmetry plane and outer surface of the weldment, one can see the through-thickness changes of the temperature field around the weld pool area. These changes affect the distribution of residual stresses after weld. High temperatures also affect metallurgical processes, which in turn affect the formation of stresses. The fineness of the mesh in the thickness direction determines the resolution with which we can resolve the detail in the metallurgical changes.

The thermal distortion bends the bar into the expected "S" shape in Figure 4.9. The displacements in Figure 4.9 have been magnified 30 times. In a welded structure, the residual stresses are highly localized, so is the distortion around the weld path. Missing the restraint caused by the material cut-off from the front and rear of the domain misses some bending moments. Ignoring these bending moments causes errors near the ends. However, they won't significantly alter the results, because the stresses due to these bending moments have only a small effect on the stresses some distance away from the ends. It can be seen that the effects are limited to only a few millimeters to the end of the domain, Figure 4.12 and Figure 4.18.

A full view of longitudinal stress (x-direction) over the domain is shown in Figure 4.10. The more detailed pictures of the stress around the weld pool and at the rear end are given in Figure 4.11 and Figure 4.12, respectively. For this weld Figure 4.13 to Figure 4.17 show that the longitudinal stress is the most significant one; with an average value 3

times larger than the other 5 stress components. It is the longitudinal stress that causes the distortion most apparently in Figure 4.9. Considering the relative importance and the availability of existing data, only the computed and measured longitudinal stresses will be compared.

Figure 4.18 The through-thickness average of longitudinal stress σ_L versus distance from welded edge. For the Lagrangian formulation, sampling data is from the mid-length of the weld path; For the current formulation, the data from the near end of the path.

Figure 4.18 shows the computed values of the through-thickness average longitudinal stresses, comparing to the measured stresses and the stresses computed in the Lagrangian formulation [41][62]. Both computations, the current and the Lagrangian formulation, use the same constitutive relation. The computational results fit in the range of the measured data. However, the steady-state formulation has the higher average stress near the weld center line. A possible reason for the difference, as discussed in the first chapter, is that the coarse mesh results in incomplete thermal cycles. When the finer mesh concentrates in a small range around the observed point, the heat source is not properly applied outside of this small range. In other words, the nodes in the coarse mesh before and after observed point could miss the melting temperature in weld pool. In these lower peak temperature

areas, there would be less plastic flow than that exists in reality. As a result, there would be lower tensile residual stresses when the material cools down. Figure 4.19 supports this explanation. In Figure 4.19 comparisons have been made in 4 locations from weld center outward gradually. With x as the weld path direction and x - y plane as the symmetric plane, z coordinate indicates the distance from x - y plane. The effect of the incomplete thermal cycle is most apparent in the place where the temperature has steep gradients and material points have more constraints from surrounding material. At material points close to a corner with external free surfaces, the differences between two computations are small. In the vicinity of weld center, the constraints due to the symmetric plane are the same in both computations and the volume expansion due to phase transformations compensates for the shrinkage during cooling down. Thus, the results show less difference. For those internal nodes of the weldment, more interactions exist between the nodes and the surrounding material. Thermal expansion and contraction are affected more by the plastic flow in the front and rear materials. In material further away from the weld center, where temperatures tend to be uniform and thermal effects are less important, the stresses between two computations become very similar. This tendency is clear in Figure 4.19d, where the distribution of σ_{xx} is at 4.8 mm from the welded edge and the peak temperature never goes higher than 450 °C, see Figure 4.8.

Several reasons can possibly explain why the longitudinal stress at the center of welded line tends to be lower than the measured values in Figure 4.18. The mathematical model assumes that material in the weld center experiences solidification and recrystallization, which ideally release all stresses and plastic strain in the material. However, the mechanical and metallurgical phenomena are much more complicated than that assumed. Leaving aside any inaccuracy involved in the stress measurement, there are mechanical and metallurgical aspects that affect the result. For the thermal cycle experienced, material might cool down to lower and more uniform temperature past the rear edge of the domain. A coarse grain structure, as predicted in Chapter 3 on **Steady State Microstructure**, could increase hardness and brittleness in the HAZ. Diffusion of chemical elements, e.g., hydrogen, is easier in weld pool area. These harmful elements change the mechanical properties of the welded material. Also, material properties used in computations may not be accurate, especially the properties at high temperature and in phases other than the original phase of the base metal.

Figure 4.19 The through-thickness distribution of stress σ_{xx} . The x-y plane is the symmetric plane. The weld is on the top edge of the plane.

Lower peak temperatures due to the coarse mesh in the transient analysis result in the lower temperature in the front HAZ of the weld pool, as described in Chapter 1. This lower temperature reduces less the stiffness of the material. Material in this zone has a strong resistance to the compression due to thermal expansion. This is shown in Figure 4.20. Figure 4.20 is the longitudinal stress cycle versus thermal cycle undergone by a point on the weld path. When the observed material point cools down from peak temperature after the heat source, the stress changes similarly in both analyses. However, a larger compressive stress is observed in the material ahead of the weld pool in the transient analysis. There possibly are two aspects that influence the results in the area.

Figure 4.20 The evolution of stress σ_{xx} at a material point on the weld path of an edge weld. In the Lagrangian formulation, the observed point is a node at the middle of the weld path. In this formulation, it is a streamline, or the edge for the weld path.

First, the sampling points are fewer in the steady-state analysis than that in the transient analysis, which has small time steps. The mesh ahead of the weld pool is too coarse in the current analysis. There is only one layer of elements to describe the temperature changes that occur from 150 °C up to the peak temperature. This results in low resolution of the stress history when the area is converted to time space. Second, the collapse of the material in the weld pool releases the stresses in the material just ahead of the weld pool. Temperatures jump from 200 °C to the melting temperature, 1450 °C for low-alloy carbon steel, within 2 mm in this analysis. Since the distance is so small between the weld pool and the low temperature material, little resistance to the compression from the expansion material is expected. If the temperature gradients were not so steep, the compressive stress would be higher. This is shown in Figure 4.21. The observed point goes under the weld pool in Figure 4.21, so that the peak temperature of the point never goes higher than 750 °C. There is a cut-off temperature for the material to simulate the

softening that occurs at very high temperatures where the material can not resist any force. When the peak temperature does not reach the cut-off temperature, stresses can keep rising with plastic deformation. It should be noted that, for material which goes through the weld pool in a thermal cycle, differences of the compressive stresses created during heating up don't have a large effect on residual stresses after cooling down.

4.8.2 Butt Weld with Filler Material

As a comprehensive analysis, the simulation of distortion and residual stresses has been carried out on a butt weld with added filler material. The butt weld has many practical applications. Many shell or vessel constructions use this process to connect sheet metal. Thorough investigations have been made of how various welding procedure parameters affect distortion in butt welds [62]. Many empirical formulas are available to estimate distortion in butt welds.

Figure 4.21 The evolution of stress σ_{xx} at a material point. In the Lagrangian formulation, the point is a node at the middle of the weld path. In current formulation, it is a streamline that is parallel to the weld path and does not go through the weld pool, or it is the bottom edge in Figure 4.7.

In this numerical investigation, the designed mesh contains about 10,000 elements. Steady state temperature distribution and the welding parameters have been given in Chapter 2 (Figure 2.5). The coordinates are x: the longitudinal direction; y: the thickness direction; and z: the lateral direction. The weld line is along x direction. Filler material is added behind the weld pool. The x-y plane is defined as the symmetrical plane through the weld pool, so that no material is allowed to move across the x-y plane after the weld pool.

Under the mathematical assumptions made above, the computational results predicted the distortion quite well, Figure 4.22. The shrinkage in longitudinal direction, x, and in the lateral direction, z, is small compared to the angular distortion, although it is still visible in Figure 4.22. Comparing the gray-line mesh (undeformed) and the solid-line mesh (deformed), the distortion is clear after it is enlarged 5 times. The longitudinal shrinkage makes the two meshes different lengths at weld center. The angular distortion changes the cross-section of weldment to a V shape. Figure 4.24 is the sectional distortion at the rear end of the domain. It is notable that considerable rigid body rotation occurs in most elements. It can be clearly seen without scaling up the displacements.

Kihara and Masubuchi examined the effect of the shapes of grooves on the angular change [63]. They concluded that an approximate ratio 0.6 of (top groove depth + 0.5 middle groove-free depth) to the thickness could minimize the angular change. The mesh used for FEM analysis here has the groove depth 5 mm, middle groove-free depth 9 mm, and the plate thickness 19 mm. Hence, the ratio is 0.5. Okerblom [64] gave a simple formula.

$$\beta = 0.13 \frac{IV}{vt^2}$$

where β = angular distortion, °.

I = current, A

V = voltage, V

v = weld velocity, mm/sec

t = plate thickness, mm.

The formula is based on the consideration of the elastic equilibrium shape of the deformation zone, under the action of the solidification and cooling of the weld pool.

Figure 4.22 Distortion of the structure after butt weld. The deformation scaling factor is 5. Greyed mesh is the mesh before welding.

Figure 4.23 Contours of residual stress, σ_x (MPa), after butt weld. For a thick plate, the maximum longitudinal stress is not on top surface.

Figure 4.24 Distorted section of a butt welded plate. Note the rigid body motion of elements remote from the weld center. The grey lines are the original mesh.

Figure 4.25 Contours of residual stress, σ_x (MPa), at a section after butt weld. Note the maximum stress is not located on the surface. The grey lines are the deformed mesh.

Leggatt and White [65] obtained a similar empirical formula, which took into account the weld penetration.

$$\beta = \frac{IV}{vt^2} \frac{6p(t-p)}{t^2}$$

where p is the weld penetration, mm. The angular distortion predicted by Okerblom's relation for the current case, with $IV/v = 1.5$ KJ/mm, is 0.54° . According to Leggatt and White, it is 6.08° , with the weld penetration depth 8 mm. The angular rotation of top face in Figure 4.24 is about 1.97° . Thus the numerical prediction agrees well with the predictions of Okerblom and Leggatt and White.

Figure 4.23 is the longitudinal stress distribution in the steady state. Figure 4.25 is the distribution in the section near the rear end. Since the weldment has been prepared with double bevel, the maximum stresses, compressive or tensile, do not appear on the surfaces. A stress concentration exists at the root of the bottom bevel. It occurs possibly due to the singularity caused by sharp angle at the symmetric plane. The concentration might not be so serious at that place if the symmetric constraints were not applicable to the angle tip.

Chapter 5 Computational Heat Transfer in Welds with Complex Weld Pool Shapes*

5.0 Introduction

The current computational capability for solving the energy equation coupled to weld pool physics cannot predict the weld pool shape in real welds with sufficient accuracy. However, it has been shown that the transient temperature field in many welds could be computed accurately by modelling the weld pool as a distributed power density and flux function [66] and solving the energy equation uncoupled to the weld pool physics. Nonlinear transient 3D FEM analysis is often used. Unfortunately, this method has not worked well for welds with complex weld pool shapes. In particular, Barlow's experimental results revealed that a second weld pool existed in some welds [67], e.g., a submerged arc weld, which is not easily modelled with only a distributed power density and flux distribution. The thicker the weldment and the larger the heat input, the more complex is the weld pool.

In order to investigate the thermal effects outside the weld pool region, either the thermal flux or power density distribution can be specified, i.e., natural boundary conditions, or the temperature of the weld pool can be prescribed, i.e., essential boundary conditions. The question concerns the functional form of these boundary conditions, i.e., what is the distribution function that can model the heat input as closely as possible to a real weld pool? Since an exact temperature field and an exact power density and flux distribution exist for the real weld, both methods should be able to provide the exact solution. The choice depends on which one can be measured more accurately and conveniently. There is also the question of which is more convenient and efficient to use.

The most popular model for welding heat input is due to Goldak et al [66]. They found that a Gaussian distribution of power density inside a double ellipsoid moving along the weld path was convenient, accurate and efficient for most realistic welds with simple shapes. Since the model reflects the depth and shape of a weld, it has proved to be more realistic and flexible in application than previous models.

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* Much of the material in this Chapter has been published in reference [70]

Unfortunately, when the shape of a weld pool is more complicated than the shape of a double ellipsoid, e.g., the double pool in a submerged arc weld as described by Barlow [67], researchers have not been able to find a power density distribution function that accurately computes the transient temperature field.

In this chapter a model with prescribed temperature distribution in the weld pool is presented, which demonstrates that the prescribed temperature field can model complex weld pools accurately. The advantages of using prescribed temperature distribution are as follows,

- The temperature distribution can be measured more accurately through experiment [68] than the power density distribution.
- At the liquid - solid interface the temperature can be set to the melting point of the base metal.
- The cross-section of the prescribed volume can be measured from a metallograph as Barlow [67], and Glickstein and Friedman [69] have demonstrated.
- The effects of radiation and convection on the surface of the weld pool are already incorporated in the prescribed temperature field and need not be included in the weld model.
- The computing time is reduced because the prescribed degrees of freedom need not be evaluated.

5.1 Power Input

If the prescribed temperature model is accurate, the net power input for the weld, ηVA (efficiency η , volt V , ampere A), will equal the total thermal load or reaction at the nodes in the prescribed temperature field of the weld pool. This is a consistency check and a redundant measure of correctness. Since the total heat input is determined only by the temperature field at the liquid-solid boundary, i.e., $q = -k T_n$, equivalence can be achieved by adjusting the weld pool size. The power input does not depend on the temperature of the interior of the weld pool even if the weld pool is a cavity. In a weld with a double pool, the metal in the leading pool is usually blown away in a real weld. In this model, the absence of molten metal in the cavity can be ignored without penalty.

The weld pool shape and size is formed progressively. If the prescribed temperature field has constant size and shape, can it represent the heat input from a real weld pool? It is apparently not a problem in a steady state. However, to an analysis of the starting

transient, it is time dependent. Methods for minimizing this problem are shortly described in section 5.3. When the constant size is applied the power input is unrealistically higher, as shown in Figure 5.4. But it decreases quickly to a stable constant. It exists usually 5 to 10 seconds after starting. It can be expected that the prescribed temperature field, or the weld pool, will become stable in the same time length.

5.2 Implementation of Prescribed Temperature Model

Superposition of a group of small weld pools can approximate a complex weld pool. Each small weld pool has its mathematically defined geometry.

Three-dimensional finite elements make up the analyzed domain. The welding path is assumed given as any valid geometric curve on the surface of the domain, on which a local coordinate system moves. From the local coordinate system, a tangential vector and a principal normal can be computed at any point on the curve.

Typically, a point is calculated according to the velocity and the time as the leading weld pool travels on the path. Such a point serves as the centre of the leading weld pool. The locations of other weld pools on the path are specified relative to the centre of the leading weld pool.

At the centre of each weld pool, an outward normal is calculated. This can be computed as the average of the outward normals of all external surfaces of the elements containing the centre. The techniques to locate the elements have been described in Chapter 3.

For each weld pool, unit vectors for the outward normal and tangential direction define a local coordinate system. The distribution function in a weld pool has a standard form, e.g., a double ellipsoid, when it is defined in the local coordinate system. A point consists of (x', y', z') in the local coordinates. The transformation matrix from global to local coordinates is

$$[H] = \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} x'_x & x'_y & x'_z \\ y'_x & y'_y & y'_z \\ z'_x & z'_y & z'_z \end{bmatrix}$$

To identify the small subset of nodes in the vicinity of the weld pool, from the total set of nodes in the mesh, which usually are enormous, a kdTree (k-dimensional binary-search tree) provides an $O(\log N)$ algorithm. N is the total number searched. A kdTree is a tree data structure, which organizes nodes according to the node position in space [71].

A transformation from global to local coordinates is done on the small set of nodes selected by the kdTree.

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = [\mathbf{H}] \begin{bmatrix} x - x_0 \\ y - y_0 \\ z - z_0 \end{bmatrix}$$

where x , y , and z are global coordinates and x_0 , y_0 , and z_0 define the origin of a local coordinate system (x', y', z') .

For any distribution function, including a double ellipsoid, all nodes can then be tested to determine if they are in the domain of the distribution function. For example, a node is in the front part of an ellipsoid if and only if

$$x' > 0$$

and

$$\frac{(x')^2}{a_1^2} + \frac{(y')^2}{b_1^2} + \frac{(z')^2}{c_1^2} \leq 1.0$$

If this is true, the node is prescribed with a temperature

$$T = T_0 \exp \left\{ A \left(\frac{(x')^2}{a_1^2} + \frac{(y')^2}{b_1^2} + \frac{(z')^2}{c_1^2} \right) \right\} \leq 1.0 \quad (5.1)$$

where T_0 is the temperature at the origin, which is the maximum temperature, and A is a constant, which has to be evaluated so that $T = T_m$, the melting point temperature at the boundary of the fusion zone (FZ) and HAZ. If

$$\frac{(x')^2}{a_1^2} + \frac{(y')^2}{b_1^2} + \frac{(z')^2}{c_1^2} = 1.0$$

and

$$T_m = T_0 e^A$$

$$A = \ln\left(\frac{T_m}{T_0}\right)$$

Substituting A into equation 5.1

$$T = T_0 \left(\frac{T_m}{T_0} \right)^{\left(\frac{(x')^2}{a_1^2} + \frac{(y')^2}{b_1^2} + \frac{(z')^2}{c_1^2} \right)}$$

The nodes inside any distribution function can be identified and assigned temperatures in a loop containing above equations.

5.3 Starting Transient

When a real weld is started, the weld pool is not formed instantly. First, a Gaussian flux distribution heats the surface of the solid to the melting point. Then a thin layer of molten metal forms. This grows in width and depth with time. With increasing depth, the weld pool surface is depressed and stirring is induced by electro-magnetic, buoyancy, arc pressure and surface tension forces.

Modelling this starting transient is much more complex than modelling the steady state weld pool. A simple technique is to prescribe the temperature of the steady state weld pool until the temperature in HAZ reaches the steady state. Then the power density and flux distribution for the steady state are evaluated. The analysis is restarted using the prescribed power density and flux until the weld pool reaches steady state. Then switch to the prescribed temperature model. However, this starting method has not been implemented yet.

Figure 5.1 FEM mesh for weld simulation. The heat source is applied on the finest mesh in the middle part.

A simpler technique is to hold the weld pool stationary for a few seconds. In practice, welders usually do this -- keeping the electrode at the starting point until a full weld pool forms. The total energy input for the prescribed temperature heat source for time $[0, t_1]$ will equal to the energy input for a constant power heat source for a time $[0, t_2]$, where $t_1 < t_2$. Using the shorter time, t_1 , the prescribed temperature heat source satisfies the energy input in a weak sense, so that it reduces errors in the whole domain.

There is also a second order error in the starting transient temperature field because of time dependent diffusion.

Figure 5.2 Cross section of the deep penetration Barlow weld containing a “bay” region. The section is divided into three areas, fusion zone (FZ), heat-affected zone (HAZ) and base metal.

5.4 Computational Results

5.4.1 Weld Condition

Computational results are presented for the experiments described by Barlow. It is a weld deposited on a low carbon steel plate of thickness 19 mm. The weld length is about 250 mm. In order to minimize end effects, the length and width of the plate are chosen to be 1224 mm and 500 mm, respectively. This is consistent with Barlow's experiment where the plate is considered infinite in length and width.

The temperature-dependent thermal conductivity and volumetric heat capacity are taken from [66].

Figure 5.1 shows the mesh used. The element length in the finest part is 16 times smaller than the length in the coarse part far away from heat source, which results graphically in a black area. In this test case, the updated Lagrangian formulation is used. The total number of elements is 12,092, and the total number of nodes is 15,323. Most elements are concentrated along the weld path for high resolution in the HAZ, where the temperature gradient changes rapidly during welding. Several levels of grading elements are used [72] to allow a coarse mesh in the far weld area. The ratio of element sizes, the largest to the smallest, is 16. This reduces greatly the computing cost without losing significant accuracy.

The size of the weld pool, see Figure 5.3, was determined from the experimental results in Reference [67]. The same weld parameters as condition 1, in Reference [67], were applied in order to compare the computed results with the results of experiment. They are: the current is 700 ampere; the voltage 30 Volt; the nominal power input 3.2 KJ/mm, the weld speed 6.67 mm/sec, the electrode extension 30 mm, and the wire diameter 5 mm.

Figure 5.3 Frame of weld pool, the compound ellipsoid model. The top is a cutaway view of the frame along weld path. The bottom is the bird's-eye view. The temperatures at nodes inside the pool are prescribed by equation 5.1. For this frame, two local coordinate systems are required. Each local coordinate system contains one double ellipsoid. The smaller deep ellipsoid is the leading pool, and the larger shallow ellipsoid is the rear pool.

As mentioned earlier, the prescribed temperature model used as the heat source is correct only in the steady state, i.e., when the heat input to the base metal does not change with time. The results presented here are those at about 24 seconds from the beginning.

According to the node reaction to power input (Figure 5.4), it can be seen that a relatively steady state is formed as early as 5 seconds after striking the arc. Since the electrode is usually held still for a few seconds after the arc is struck, the total energy input per unit length (KJ/mm) is greater than the nominal value in the steady state. This total energy input is matched by adjusting the time length the prescribed temperature weld pool is held stationary, Figure 5.4.

Figure 5.4 Decay of power input for constantly prescribed temperature field. The power input simulates the heat input from the weld pool in the Barlow weld. The power input is the summation of node reactions.

5.4.2 Temperature Field

Figure 5.5 shows the contours of the temperature field. The region near the weld pool is magnified in Figure 5.6. The deep leading pool directly under the welding arc can be seen. It is suspected to be a concave puddle in the real weld because the liquid metal is blown out into the shallower rear pool. The rear pool is formed to accumulate this ejected liquid metal. It is shallower and wider, so that the temperature gradient is relatively small within the rear pool. Between the front and the rear pools, there is only a thin layer of molten metal.

Contour Values ($^{\circ}\text{C}$): A = 197; B = 375; C = 553;
D = 730; E = 908; F = 1090

Figure 5.5 The temperature field 24 seconds after striking the arc. Temperature is in $^{\circ}\text{C}$. The minimum temperature = 20; the maximum temperature = 1800.

Contour Values ($^{\circ}\text{C}$): A = 197; B = 375; C = 553; D = 730; E = 908;
F = 1090; G = 1260; H = 1440; I = 1620

Figure 5.6 A closer look at the weld pool and surrounding area. Temperature is in $^{\circ}\text{C}$. The minimum temperature = 20; the maximum temperature = 1800.

Contour Values ($^{\circ}\text{C}$): A = 197; B = 376; C = 555; D = 734; E = 914;
F = 1090; G = 1270; H = 1450; I = 1630

Figure 5.7 Temperature contours for the corresponding single weld pool model. The minimum temperature = 20; the maximum temperature = 2000.

Contour Values ($^{\circ}\text{C}$): A = 553; B = 709; C = 865; D = 1020;
E = 1180; F = 1330; G = 1490; H = 1640

Figure 5.8 The envelope temperature contours on a section on which the temperature field projects. The numbers shown on the mesh are FEM node numbers.

The temperature contours outside the HAZ are approximately elliptical in shape. A similar result could be obtained using a single weld pool (Figure 5.7). Glickstein and Friedman [69] used a two-dimensional model to simulate the temperature field in a section along the weld path. Their model gave similar contours outside of the HAZ although it did not predict transient temperatures accurately inside the HAZ.

Figure 5.9 The thermal cycles of the nodes directly under the weld path. The node numbers are shown in Figure 5.8.

Figure 5.8 is the envelope of maximum temperatures in a section, through which the weld pool has passed completely. Note an envelope temperature contour is the locus of maximum temperatures projected on the plane perpendicular to the weld line. It is not the temperature contours on a cross-section at some instant of time. Note the melting point temperature is between contour G and contour F. The contour representing the melting

temperature envelope is superimposed on the weld pool. There is good agreement with data from experiments.

5.4.3 Thermal Cycle

Corresponding to the node numbers in Figure 5.8, a set of thermal cycle (time vs. temperature) curves are given in Figure 5.9 to Figure 5.11. The computed thermal cycle within one FEM element (nodes 183, 184, 192, and 193) is obtained by interpolating the curves at corner nodes. It is found that the shape of the thermal cycle is very sensitive to the position selected.

Figure 5.10 The thermal cycles of the nodes along the widest side of the double weld pool. The node numbers are shown in Figure 5.8. These show thermal cycles are similar to those obtained from single weld pool.

For nodes 170 and 171, i.e., for the region directly under the weld pool, the thermal cycles are simple. The HAZ is thin and basically the same as those obtained from the simulation of the double ellipsoid heat source. Similarly the thermal cycle of nodes 199, 201, and 217 at the widest part of the weld pool are not unusual.

The effect of the second weld pool is most apparent in the "bay area". The thermal cycles at nodes 183, 184, 192, and 193 suggest a second temperature peak. Therefore this area is held at high temperature ($> 1100^{\circ}\text{C}$) longer than other areas in the HAZ. Because of these quite different thermal cycles, temperature history dependent phenomena are expected to be quite different from other areas of the HAZ.

Figure 5.11 The thermal cycles of selected nodes within the "bay area". Note the temperature arrest due to the second weld pool in the model. The node numbers are shown in Figure 5.8.

5.4.4 Predicting Microstructure

Figure 5.12 compares computed results and Barlow's experimental results in the "bay area". Note that the agreement is excellent, which supports the analysis. To the author's knowledge, this is the first bay area thermal cycle analysis that is realistic.

Figure 5.12 Comparison of the thermal cycles between computed result and Barlow's experimental result in the "bay area". Note that the triggering times are set differently for ease of presentation.

Since the thermal cycle under the second weld pool is different, the microstructure is expected to be different. From the method of Khoral [22], the thermal analysis is coupled to the microstructure analysis. Note this is done in the Lagrangian formulation rather than the Eulerian formulation described in Chapter 3. The results are shown in Figures 5.13 and 5.14. Since the method is valid only in the HAZ, those contours inside the weld pool (contour G, Figure 5.8) have no meanings. Along the weld pool, there is a very thin layer of large grains. As expected, this thin layer becomes much thicker in the "bay area". As a result, the hardenability rises in the "bay area". More important, the fast cooling rate and the large grain size in the "bay area", causes more bainite to form, which causes the area to be harder and possibly more brittle.

Contour Values: A = 2.42%; B = 4.83%; C = 7.25%;
D = 9.66%; E = 12.1%; F = 14.5%

Figure 5.13 Bainite contours in a cross section, where the austenite transformation is complete.

Figure 5.14 Grain size contours in a cross-section, where the temperature has cooled to under 200 °C in the HAZ. The grain size is sensitive to the time the austenite phase persists above the dissolution temperature for NbC and VC precipitates.

Chapter 6 Mixing Thermal Shell and Brick Elements*

6.0 Introduction

In welds, many three dimensional elements are needed to analyze accurately a localized heat source and its surrounding field. Since most welds are made with the arc on one side of a pipe, a temperature difference between two surfaces is expected. Ignoring the three-dimensional distribution around the weld pool, no matter how small, can cause improper estimates of HAZ, particularly if the HAZ is small compared to weldment.

In most weld structures far away from the weld pool, it can be assumed that the top and bottom of a shell structure have the same temperature. In thin walled structures, this assumption can be true close to the weld pool. The thinner the wall, the smaller the three-dimensional area around the heat source. Since the assumption is fundamental for a thermal shell, the use of thermal shell elements is adequate and reasonable.

As mentioned in Chapter 1, **Introduction**, using shell elements not only reduces the computing cost but also improves numerical-conditioning of large elements. Since relatively thin-walled structures are popular in industry and the application of shell assumption is attractive, shell elements have been hot topics for a long time in the FEM analysis. Many studies on the formulation and the application of shells in FEM have been published [74 - 83].

In the far weld region, there is little doubt that shell elements are more efficient and accurate. Although there are exceptions for electron beam and laser welding and for welding thin sheet, the temperature field around most weld pools is truly three-dimensional. Neglecting the variation of temperature in the thickness direction can result in considerable error. Hence it is important to use bricks for accuracy in the area near the weld pool.

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* Much of the material in this chapter has been published in reference [73]

Mixing shell and brick elements can provide a more efficient mesh for analyzing transient problems with localized loads such as welds. However, since the nodal degrees-of-freedom in these two types of elements are different, the connection of shell elements to three-dimensional elements presents considerable difficulty. Not many publications can be found about the combination of three-dimensional elements and shell elements. Surana [84] gives a transition element to join a three-dimensional element and a shell element. In his model, a brick-shell transition element has been created by combining the basis functions of the three-dimensional element and the shell element. He constructs the transition element with its own basis function. As a result, a special set of elements has to be coded to deal with the transition, which is difficult for commercially available FEM packages that produce effective stiffness matrix and load vector. Also it reduces the flexibility in automatic FEM.

In this chapter, we present a method to connect a three-dimensional element to the shell element. The element is called a Shell - Brick transition element. It is not really a new element but a brick with constraints according to the shell assumption. It has more flexibility and can be added to other FEM packages without altering the original code.

6.1 Thermal Shell

In the region that thermal shell elements are accurate, the temperature gradient tends to lie in a plane tangent to the mid-layer of the shell. The heat flow normal to the mid-plane, which is often due to convection and radiation, can be treated as a distributed source or sink.

6.1.1 Defining a Shell

A shell can be defined completely in its curvilinear coordinate system (r, s) . $\mathbf{r}$ and $\mathbf{s}$ are two tangential vectors of the shell at a point (r, s) . Assuming there is no deformation of the shell during thermal computation, the outward normal of the shell is $\mathbf{t} = \mathbf{n}$, where

$$\mathbf{n} = \frac{\mathbf{r} \times \mathbf{s}}{\|\mathbf{r} \times \mathbf{s}\|}$$

A position vector in the global Cartesian coordinate system can be expressed in curvilinear coordinates

$$\mathbf{x} = \mathbf{X}(r, s)$$

The tangential vectors $\mathbf{r}$ and $\mathbf{s}$ at a point (r, s) of the curvilinear system can be expressed in Jacobian components

$$\mathbf{r} = \frac{\partial \mathbf{x}}{\partial r}$$

$$\mathbf{s} = \frac{\partial \mathbf{x}}{\partial s}$$

Note all vectors, $\mathbf{x}$, $\mathbf{r}$ and $\mathbf{s}$, are defined in the global Cartesian coordinate system.

The propagation of temperature in a thermal shell is restricted within the shell. Flux in the normal direction is much smaller than that in tangential direction. But the temperature gradients (or fluxes) are two-dimensional only in a local coordinate system sitting on a tangent plane of the shell. When observed in a global Cartesian coordinate system, they are three-dimensional in general, since the shell has arbitrary orientation. While the evaluation of temperature gradients is convenient in a local coordinate system on the shell, the whole problem has to be solved globally. Therefore, a local coordinate system and its mapping to and from the global system are necessary.

6.1.2 Laminar Coordinate System

A laminar coordinate system $(\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3)$ is convenient for presenting the temperature gradients and the thermal properties in shell elements. It is erected on a plane tangent to the middle layer of the shell [78]. Figure 6.1 shows the relationships among the global Cartesian, the curvilinear, and the local laminar coordinate systems.

The basis vectors, $\mathbf{e}'_i$ ($i = 1, 2, 3$), are orthonormal to each other. $\mathbf{e}'_3$ is perpendicular to the tangent plane, so that $\mathbf{e}'_3 = \mathbf{n}$. $\mathbf{e}'_1$ and $\mathbf{e}'_2$ are constructed such that they are offset at the same angle from the unit natural basis vectors $\mathbf{e}_r$ and $\mathbf{e}_s$ respectively, where

$$\mathbf{e}_r = \frac{\mathbf{r}}{\|\mathbf{r}\|}$$

$$\mathbf{e}_s = \frac{\mathbf{s}}{\|\mathbf{s}\|}$$

Figure 6.1 Curvilinear Coordinate System (r, s, t) and Local Laminar Cartesian Coordinate System $(\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3)$ on Shells.

Let

$$\mathbf{A} = \frac{\mathbf{r} + \mathbf{s}}{\|\mathbf{r} + \mathbf{s}\|}$$

$$\mathbf{B} = \mathbf{e}'_3 \times \mathbf{A}$$

We have

$$\mathbf{e}'_1 = \frac{\mathbf{A} - \mathbf{B}}{\|\mathbf{A} - \mathbf{B}\|}$$

$$\mathbf{e}_2' = \frac{\mathbf{A} + \mathbf{B}}{\|\mathbf{A} + \mathbf{B}\|}$$

6.1.3 Temperature Field of Shells

Temperature at a point in space is a scalar quantity. It is invariant to coordinate transformations. By this property, the local element stiffness matrix and load vector, in which every contribution to a node is a scalar, can be assembled directly into the global stiffness matrix and load vector. By doing so, the formulae are greatly simplified and the computing time for the coordinate rotation is avoided.

Because of C^0 continuity, the temperature is continuous across the element boundary. It is

$$T = N_i(r, s) T_i$$

And the temperature derivative is continuous within elements.

$$\begin{bmatrix} \frac{\partial T}{\partial x'} \\ \frac{\partial T}{\partial y'} \end{bmatrix} = [\mathbf{J}^*]^{-1} \begin{bmatrix} \frac{\partial T}{\partial r} \\ \frac{\partial T}{\partial s} \end{bmatrix}$$

where

$$[\mathbf{J}^*] = \begin{bmatrix} \frac{\partial x'}{\partial r} & \frac{\partial y'}{\partial r} \\ \frac{\partial x'}{\partial s} & \frac{\partial y'}{\partial s} \end{bmatrix}$$

Two mappings have been applied to obtain $\mathbf{J}^*$.

The first mapping of derivatives, with the Jacobian $\mathbf{J}_1$, is between the global coordinate system and the local curvilinear coordinate system.

$$\begin{bmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial s} \end{bmatrix} = [\mathbf{J}_1] \begin{bmatrix} \frac{\partial}{\partial X} \\ \frac{\partial}{\partial Y} \\ \frac{\partial}{\partial Z} \end{bmatrix}$$

where

$$[\mathbf{J}_1]^{-1} = \begin{bmatrix} \frac{\partial X}{\partial r} & \frac{\partial Y}{\partial r} & \frac{\partial Z}{\partial r} \\ \frac{\partial X}{\partial s} & \frac{\partial Y}{\partial s} & \frac{\partial Z}{\partial s} \end{bmatrix} = \begin{bmatrix} \mathbf{r} \\ \mathbf{s} \end{bmatrix}$$

The second mapping of derivatives, with Jacobian $\mathbf{J}_2$, is from the laminar coordinate system to the global coordinate system

$$\begin{bmatrix} \frac{\partial}{\partial X} \\ \frac{\partial}{\partial Y} \\ \frac{\partial}{\partial Z} \end{bmatrix} = [\mathbf{J}_2]^T \begin{bmatrix} \frac{\partial}{\partial x'} \\ \frac{\partial}{\partial y'} \end{bmatrix}$$

where

$$[\mathbf{J}_2] = \begin{bmatrix} \frac{\partial x'}{\partial X} & \frac{\partial x'}{\partial Y} & \frac{\partial x'}{\partial Z} \\ \frac{\partial y'}{\partial X} & \frac{\partial y'}{\partial Y} & \frac{\partial y'}{\partial Z} \end{bmatrix} = \begin{bmatrix} \mathbf{e}'_1 \\ \mathbf{e}'_2 \end{bmatrix}$$

The mapping of derivatives, with Jacobian $\mathbf{J}^*$, from the laminar coordinate system to the curvilinear coordinate system is then

$$\begin{bmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial s} \end{bmatrix} = [\mathbf{J}_1] [\mathbf{J}_2]^T \begin{bmatrix} \frac{\partial}{\partial x'} \\ \frac{\partial}{\partial y'} \end{bmatrix} = [\mathbf{J}^*] \begin{bmatrix} \frac{\partial}{\partial x'} \\ \frac{\partial}{\partial y'} \end{bmatrix}$$

The natural boundary conditions applied to the surfaces of the shell affect the temperature field through their equivalent -- the function $P(\xi, \eta)$ of the distributed heat source. In an isoparametric element, the power contribution of an element to its node i is

$$q_i = \int_{-1}^{+1} \int_{-1}^{+1} P(r, s) \det[J^*] \text{thickness}(r, s) dr ds$$

6.2 Shell - Brick Transition Element

The method presented here is general. It can provide the transition from shells to other solid elements besides bricks, such as wedge-shaped elements. However, only the 8-node brick element is treated in this section because of its popularity and availability in our FEM package.

The transition element between a three-dimensional brick element and a shell element begins as a brick element. Under assumptions similar to that of the shell elements, some degrees of freedom in the brick element are constrained, forcing the element to be compatible at the boundary with the connected shell element. In Figure 6.2, one side of the brick element is collapsed. In practice, any pair of nodes can collapse to conform with the neighboring shell node.

Suppose we have a brick element with 6 nodes, shown in Figure 6.2, on which the corner nodes connect other brick elements and the mid-edge nodes (transition nodes) connect shell elements. For transition node j , the same assumption as shell node is applied, i.e., the temperature is constant through the thickness of the shell. Thus, the temperature field in the element can be expressed as

$$T = N_j(r, s) T_j + N_k(r, s, t) T_k$$

- k ---- brick nodes, 1 to m .
- j ---- shell nodes, $m+1$ to n .

m is 4 in a 6 node transition element, in Figure 6.2.

If T_t is the temperature at the top surface and T_b is the temperature at the bottom surface, then for transition nodes

$$T_i = T_b = T_j \quad (6.1)$$

Figure 6.2 The transformation of a brick element to a transition element is shown. In particular, the relation between the transition node j and its top and bottom nodes is shown.

Whether the engineering problems are, linear or nonlinear, the assembled equations for solver in the FEM are usually a set of linear equations. The linear equations for a pure brick element in matrix form are

$$[K] [T] = [R] \quad (6.2)$$

where

$$[K] = \begin{bmatrix} k_{11} & k_{12} & - & k_{1i} & - & k_{1j} & k_{1b} & - & - & k_{1n} \\ k_{21} & k_{22} & - & k_{2i} & - & k_{2j} & k_{2b} & - & - & k_{2n} \\ - & - & - & - & - & - & - & - & - & - \\ k_{i1} & k_{i2} & - & k_{ii} & - & k_{ij} & k_{ib} & - & - & k_{in} \\ - & - & - & - & - & - & - & - & - & - \\ k_{j1} & k_{j2} & - & k_{ji} & - & k_{jj} & k_{jb} & - & - & k_{jn} \\ k_{b1} & k_{b2} & - & k_{bi} & - & k_{bj} & k_{bb} & - & - & k_{bn} \\ - & - & - & - & - & - & - & - & - & - \\ - & - & - & - & - & - & - & - & - & - \\ k_{n1} & k_{n2} & - & k_{ni} & - & k_{nj} & k_{nb} & - & - & k_{nn} \end{bmatrix}$$

$$[T] = [T_1 \ T_2 \ \dots \ T_i \ \dots \ T_j \ T_b \ \dots \ T_n]^T$$

$$[R] = [R_1 \ R_2 \ \dots \ R_i \ \dots \ R_j \ R_b \ \dots \ R_n]^T$$

R_i is the element contribution to the nodal load at node i of the element. It is power in the thermal analysis. Therefore, the power of the nodal load at node j should be the summation of the power at the top node and the bottom node.

$$R_j = R_i + R_b \quad (6.3)$$

By putting equation 6.1 into equation 6.2,

$$k_u T_i + k_{ib} T_b = k_u T_j + k_{ib} T_j = (k_u + k_{ib}) T_j,$$

such that

$$k_{ij} = k_u + k_{ib}$$

Putting equation 6.3 into equation 6.2 results in

$$k_{ji} = k_u + k_{ib}$$

After applying the constraint, equation 6.2 has the components

$$[K] = \begin{bmatrix} k_{11} & k_{12} & \dots & k_{1i} & \dots & k_{1j} & \dots & \dots & k_{1n} \\ k_{21} & k_{22} & \dots & k_{2i} & \dots & k_{2j} & \dots & \dots & k_{2n} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \ddots & \vdots \\ k_{i1} & k_{i2} & \dots & k_{ii} & \dots & k_{ij} & \dots & \dots & k_{in} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \ddots & \vdots \\ k_{j1} & k_{j2} & \dots & k_{ji} & \dots & k_{jj} & \dots & \dots & k_{jn} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \ddots & \vdots \\ k_{n1} & k_{n2} & \dots & k_{ni} & \dots & k_{nj} & \dots & \dots & k_{nn} \end{bmatrix}$$

$$[T] = [T_1 \ T_2 \ \dots \ T_i \ \dots \ T_j \ \dots \ T_n]^T$$

$$[\mathbf{R}] = [R_1 \ R_2 \ - \ R_1 \ - \ R_1 \ - \ - \ R_n]^T$$

This constraining operation is repeated on all transition nodes.

6.3 Implementation

As discussed in previous chapters, a very fine mesh is required to accommodate the steep gradients of temperature along the weld path. For a simple geometry, such as prisms, it is easy to create a locally condensed mesh in a mesh generator like INGRID. But, for a complicated geometry, like the tee-joint shown in Figure 6.3, mesh density ought to be evenly distributed at the time it is created in the mesh generator. Where the shell elements will be, there should not be more than one layer of bricks in the thickness direction. As a result, the mesh for the tee-joint is initially one layer everywhere. To implement successfully this mixed shell and brick model for the tee-joint, two steps are needed. First, specify the weld path and refine the elements along the weld path. Multi-layer elements through the thickness exist after this refinement, which enables the three-dimensional weld pool to be accurately analyzed. Next, make the shell elements automatically from those bricks that are far away from the weld path and have only one layer in thickness.

With these two steps, the initial mesh needs only the minimum number of brick elements required to define the geometry of the domain. Smalltalk, an Object Oriented Programming environment, has again been used to manipulate all geometry. The initial mesh is the input into Smalltalk. A geometry database that can answer the topology of the geometry is created in Smalltalk. Nodes, elements, edges, inter-element faces and outer surfaces, and the relationship between these geometrical components are frequently asked during refining, shelling and moving the heat source.

Figure 6.3 illustrates the results after the first two steps. The left is the initial mesh with 1120 brick elements to define the geometry. On the right the mesh is shown after refining and shelling. It has 3136 elements, including 896 shells and 64 shell-brick transition elements. The cutaway view on the up-right shows the transition from the dense three-dimensional mesh to a very coarse shell. A fine mesh along the weld path has been formed to guarantee adequate resolution and accuracy. In the weld zone, the element size is more than 5 times smaller than the element size far away from the weld. Refining is done along the weld path using a splitting technique similar to that of McDill, et al. [14].

Figure 6.3 Refining and Shelling on a pipe tee-joint (left) The finished mesh (right) is ready for weld analysis. The top-right is a cutaway view of the finished mesh.

6.3.1 Weld Path and Refining

The weld path can be defined by either a formula for any space curve or a set of element edges. In the current implementation, the element edges are chosen to form the weld path. On the basic mesh, free element surfaces are picked out in the collection of element faces. By looking up the node face dictionary in Smalltalk, the element surfaces are separated to make up several pieces of surfaces for the whole geometry. A weld path is defined by choosing an outer edge on one of pieces and giving start and end points on the outer edge.

A local coordinate system is created at the point on the weld path occupied by the weld heat source at time t . This local coordinate system describes the orientation of the heat source in a standard form, as described in the previous chapter. The local x-direction contains the tangent of the path, indicating the direction the weld pool is travelling. The local z-direction is the direction of the depth of the heat source. It is the average of the outward normals on the surfaces of the elements at the current position of the heat source.

Refinement is done by splitting elements according to both the weld path and the size of the heat source. Several passes of splitting can be applied, each pushing the finer mesh one layer out from the weld path. Two passes of refinement have been performed in Figure 6.3.

6.3.2 Shelling

Shelling is defined here to mean collapsing a brick element into a shell element. In the context of this thesis, hopefully, it would not be confused with the definition in dictionaries. Locating the transition elements between shell elements and brick elements after shelling and finding the topological relation in the element are the tasks in shelling.

Shelling is done automatically with the support of the geometry database in Smalltalk. The rule for shelling is that the element for conversion to a shell element should have top and bottom surfaces free and not contain any heat source nodes. Any potential shell element has to become a shell-brick transition element if it is adjacent to any element that cannot be shelled.

Shelling proceeds in two steps. First, all candidates for conversion to shells are selected by walking through all surfaces. Element changes are then performed by judging the candidate. If the candidate can not be converted it remains a brick. If the candidate can be converted and the neighbors of the candidate permit, a shell element or shell-brick transition element is formed. The new element replaces the old element in the mesh for solving. The old element serves as the parent of the new element, so that the old mesh can easily be recovered for other arrangements or analysis, e. g., stress analysis.

6.4 Computational Results

The test problem is a weld joining two pipes at a right angle. This kind of tee-joint weld is common in industry. The complexity of the tee-joint geometry is an ideal test for shelling codes, since it needs all the features described in this chapter. The diameters of the pipes are 100 mm and 50 mm respectively and the wall thickness is 3.125 mm. The speed of the weld is 2 mm per second. The power input is 1.5 kJ/mm, measured in the way described in chapter 5.

Isothermal contours, 65 seconds after starting the weld, are shown in Figure 6.4.

To illustrate the advantages of the mixed thermal shell and brick elements, a comparative analysis is done on the joint using the same welding conditions. Using a uniform mesh restricts the size of the observed domain. Only a small portion around the joint can enter the solver because of computer capacity. The boundaries between this portion and the rest of the pipes are assumed to be insulated. The total number of the elements in the comparative mesh is 5120. The element size in the comparative mesh is about the same as that in the refined mesh in Figure 6.4. The time for solving is almost twice that of the shelled mesh. Contours are shown in Figure 6.5. Not only does this mesh cost more time for solving but it also could not keep the assumed boundary condition during welding. As the temperature rise becomes significant at the boundary of the mesh, notable heat flow, which should actually pass to the rest of the pipe, is reflected. This incorrect boundary condition results in temperatures that are too high.

Two cutaway-view meshes with isothermal contours at 40 seconds are shown for comparison in Figure 6.6. The temperature difference in the thickness of the pipes is limited to the region near the weld. The contours close to the weld centre through the

Figure 6.4 Temperature contours of tee-joint weld 65 seconds after starting welding. The mesh is a mixture of shells, bricks, graded bricks and shell-brick transition elements.

Figure 6.5 Comparative analysis with same weld parameters as that used in Figure 6.4. Only a piece cut from the tee joint is meshed. The mesh contains 5120 brick elements.

Figure 6.6 Cutaway view of the mesh in Figure 6.4 (bottom) and Figure 6.5 (top). The isothermal contours show the temperature field at time 40 seconds. The assumption the temperature is constant through the thickness in the region converted shell elements is seen to be satisfied.

thickness of pipes are similar to each other mesh. It is clear from Figure 6.6 that the shell assumption is satisfied in the rest of the pipes.

Conclusions

Methods have been developed for computational weld mechanics under steady state conditions. Detailed analyses of several welds have been performed. Temperature, microstructure and stress fields are presented in graphs.

- Thermal analysis has been implemented in a transformed Eulerian formulation.
  - The model accounts naturally for addition of filler material.
  - The test cases indicate that a reasonable accuracy could be achieved with the assumed boundary conditions.
  - The model gives the thermal history of a material point by traversing geometry space along a streamline and mapping values into the time dimension.
- Microstructures in a steady state weld evolve along the streamlines.
  - A data structure has been created to support this model. The data structure provides streamlines, which in turn provide the temperature history for every material point.
  - The data structure can also be used to find the elements that determine the starting condition of each streamline.
- Stresses and distortions are analyzed in the Lagrangian formulation or an Eulerian frame.
  - The kinematics model is uniquely developed, which is different from the usual Lagrangian or Eulerian models.
  - History-related quantities at a material point are obtained from streamlines in a reference frame after some mappings.
  - The solution includes elastic and plastic effects. It includes also the strain caused by phase transformation.
  - Tests have been done on edge and butt welds. The distortions shown in the

pictures are easily measured.

- Satisfactory results are obtained. Stresses at a material point evolving along a streamline can be presented. Computed longitudinal stresses have been compared with the data calculated in the Lagrangian formulation and measured in experiments.

- Significant savings on computing time have been achieved on all calculations with the steady state formulation.

A heat source model prescribed with temperatures was developed. It was able to analyze the dual weld pool observed by Barlow. Results demonstrated that this model enables the transient temperature field to be computed accurately for weld pools with complex shapes.

- The computed results agreed well with experimental results published by Barlow. In addition, the input data can be measured more accurately and conveniently than the power density distribution.
- The model is computationally more efficient than the prescribed power density distribution model.
- The model presented here resolves the details of the transient temperature field and microstructure in the "bay area". These details are believed to be important to the evaluation of the weld.

Thermal shell and shell-brick transition elements have been developed to make the analysis more efficient.

- Tests have been performed on a tee-joint pipe weld. Compared to a full three-dimensional mesh, results are very accurate. For the same number of elements, using the mixed shell and brick elements can cover more geometry, thus, the error due to false boundary conditions was eliminated.

Future Work

To have analysis software more widely used in industry, it is important to integrate them systematically. This can range from mesh creation, material property selection to presentation of results and feedback to the designer. A user friendly environment is useful for welding engineers to do FEM analyses when they are not familiar with codes.

The current software has no ability to predict behavior in the weld pool or in the arc. Fluid flow analyses are important for predicting the shape of a weld pool. Solidification analyses are required to predict correctly microstructures in the fusion zone behind the weld pool. Since microstructures affect also residual stresses, the results of stress analysis can be improved by coupling the results of both thermal and microstructure analyses to stress analysis.

Constitutive models in stress analysis can be improved. Currently, most constitutive models are based on macroscopic stresses and strains. It has been reported that evaluations of material hardening based on microstructural models are in good accord with experiments. Such models can include an equation for the evolution of slip system deformation resistance.

Stress analysis with shell elements, buckling of welds and fracture mechanics of welds should be studied.

Nonlinear analysis should be applied to the thermal analysis, when the non-symmetric solver is available. Many experiments and computational experiences show that material properties are nonlinear.

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