A Holistic Micro-Macro Model of an Arc Weld Pool with Microstructure Evolution in the Fusion and Heat-Affected Zones

by

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The undersigned recommend to
the Faculty of Graduate and Postdoctoral Affairs
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Abstract

The research describes a micro-macro computer model that captures most of the physics of a weld pool, the fusion zone and the heat-affected zone in a low-alloy steel weld.

The macro-model uses either FEM or Smoothed Particle Hydrodynamic (SPH) methodology for the weld pool geometry. The SPH model solves the transient 3D non-linear energy equation for temperature and fraction solid and the Navier-Stokes equations for velocity and pressure. This predicts the transient weld pool size, shape and oscillations including transient temperature, fraction solid, velocity, composition including mixing and dilution and macro-scale solidification. The number of particles ranges from 50K to 500K with particle spacings of roughly 0.2 mm. Time steps are usually $0.2 \mu s$ and the number of time steps is about 1 to 2M for 1 s physical time.

A micro-model for the evolution of microstructure in the FZ includes a model for dendrite growth during the weld pool solidification of a Fe-C-Mn alloy system. A 3D cellular approach is used for the dendrite growth simulation in the micro scale where the solid phase growth is controlled by the constitutional and capillary under-cooling at the liquid-solid interface. This micro model is coupled to a macro-model of the weld in a welded structure.

Another micro-model describes the dissolution of ferrite and homogenization of austenite in a low-alloy steel weld. A synthetic microstructure is introduced containing a representation of individual grains. The process is driven by the thermal cycle and

carbon diffusion.

Holistic frameworks are finally introduced for the HAZ and fusion zone to establish correlations between the weld process parameters in the macro model such as weld process type, weld current, voltage, weld heat input, weld speed, base metal and filler metal composition and the solidification microstructure as well as the solid state microstructure transformations and mechanical properties in the neighborhood of a spatial point in macro-model.

To my parents, Mohammad and Zahra,
For their love and support

And to Shokoofeh,
Her presence and love gave me courage and hope to carry on

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List of Symbols

General symbols and definitions.

Symbol	Definition
$\mathbf{a}_a$	Acceleration vector of particle a (m/s^2)
A_b	Function value for particle b at $\mathbf{r}_b$
$A(\mathbf{r}_b)$	Field interpolated at particle b at $\mathbf{r}_b$
$\mathbf{B}_a$	Second order correction tensor for particle a
c_0	Nominal carbon composition of an alloy ($wt.\%$)
c_0^α	Carbon concentration in ferrite at T_e ($wt.\%$)
c_0^γ	Carbon concentration in austenite at T_e ($wt.\%$)
$\bar{c}_n$	Average carbon concentration in a two-phase cell ($wt.\%$)
c_n^α	Carbon concentration in ferrite at transformation step n ($wt.\%$)
c_n^γ	Carbon concentration in austenite at transformation step n ($wt.\%$)
$c_e^\alpha(T)$	Equilibrium carbon composition in ferrite at temperature T ($wt.\%$)
$c_e^\gamma(T)$	Equilibrium carbon composition in austenite at temperature T ($wt.\%$)
Δc_n^α	Concentration change in ferrite at transformation step n ($wt.\%$)
Δc_n^γ	Concentration change in austenite at transformation step n ($wt.\%$)
c_0^C	Initial carbon concentration in the liquid alloy ($wt.\%$)
c_0^{Mn}	Initial manganese concentration in the liquid alloy ($wt.\%$)
c_p	Specific heat ($J/kg\ K$)
C	Concentration of solute
C_{ps}	Specific heat solid ($J/kg^\circ K$)
C_{pl}	Specific heat liquid ($J/kg^\circ K$)
C_{ijkl}^l	Forth order tensor maps strain rate tensor to stress tensor

c_s	Speed of sound (m/s)
d_d	Droplet diameter (mm)
d_e	Wire diameter(mm)
dt	Differential time increment (s)
dT/dt	Cooling rate ($^{\circ}K/s$)
$\frac{dW}{dr}$	Scalar derivative of the kernel function
D_l^C	Diffusion coefficient of carbon in the liquid alloy (m^2/s)
D_l^{Mn}	Diffusion coefficient of manganese in the liquid alloy (m^2/s)
D_{ij}	Deformation rate tensor (or strain rate tensor) (m/s)
$D(T)$	Temperature dependent solute diffusivity
f_0^{γ}	Fraction of austenite in the domain at T_e
f_d	Droplet frequency (s)
f_l	Fraction liquid
f_n^{γ}	Fraction austenite in a cell at transformation step n
h_0	Convection coefficient ($W/(m^2 K)$)
h	Enthalpy per unit volume (J/m^3)
$\mathbf{F}_a^{internal}$	Equivalent internal forces acting on particle a (N)
$\mathbf{F}_a^{external}$	Sum of external forces on particle a (N)
$\mathbf{f}_a^{external}$	External Force vector per unit mass on particle a (m/s^2)
F_0	Boundary force constant
G	Temperature gradient ($^{\circ}K/m$)
h	Smoothing length or characteristic width of the kernel
H	Enthalpy (J/kg)
H_s	Enthalpy solid (J/kg)
H_l	Enthalpy liquid (J/kg)
H_v	Enthalpy vapor (J/kg)
I	Current (A)
k^C	Distribution coefficient of carbon in the liquid alloy
k^{Mn}	Distribution coefficient of manganese in the liquid alloy
m_b	Mass of particle b (kg)
m_l^C	Liquidus line slope (Carbon) ($K/wt.\%$)

m_l^{Mn}	Liquidus line slope (Manganese) ($K/wt.\%$)
N	Number of nearby particles
p	Scalar pressure field (Pa)
P	Input power (W)
$q(x, y)$	Heat flux function (W/m_2)
Q	Heat generation per unit mass (W/kg)
Q_v	Heat generation per unit volume (W/m^3)
$\mathbf{r}_b$	Position vector of particle b
R	Ratio of particle distance to supporting length (chapter 2)
R	Growth rate (chapter 3) (m/s)
T	Temperature ($^{\circ}K$)
T_d	Droplet temperature ($^{\circ}K$)
T_s	Solidus temperature ($^{\circ}K$)
T_l	Liquids temperature ($^{\circ}K$)
T_v	Vaporization temperature ($^{\circ}K$)
T_0^{γ}	A_3 temperature at 0 $wt.\%$ carbon ($^{\circ}K$)
$T_{c_0}^{\gamma}$	A_3 temperature (austenization temperature) at c_0 ($^{\circ}K$)
T_e	Eutectoid temperature ($^{\circ}K$)
T_a	Local actual temperature ($^{\circ}K$)
T_{amb}	Ambient temperature ($^{\circ}K$)
T_{Ref}	Reference temperature ($^{\circ}K$)
T^*	Melting temperature of the pure metal ($^{\circ}K$)
ΔT_c	Constitutional undercooling ($^{\circ}K$)
$\Delta T_{capillary}$	Capillary undercooling ($^{\circ}K$)
ΔT_k	Kinetic undercooling ($^{\circ}K$)
ΔT_t	Thermal undercooling ($^{\circ}K$)
$\mathbf{v}$	Velocity field (m/s)
$\mathbf{v}_a$	Velocity of particle a (m/s)
$\mathbf{v}_b$	Velocity of particle b (m/s)
$\mathbf{v}_d$	Droplet initial velocity (m/s)
v_e	Wire speed (m/s)

v_w	Weld speed (m/s)
V	Voltage (Volt)
V_{int}	Liquid-solid interface velocity (m/s)
W	Weighting function or kernel
∇P	Gradient of a scalar field
$(\nabla \mathbf{A})_a$	Gradient of a vector or tensor field at a
$(\nabla \mathbf{v})_a$	Velocity gradient at particle a
$(\nabla \cdot \mathbf{A})_a$	Divergence of a vector or a tensor field $\mathbf{A}$ at a
$(\nabla^2 A)_a$	Laplacian of a scalar field at a
$\nabla \mathbf{v}$	Velocity gradient tensor
$\nabla W(\mathbf{r}_a - \mathbf{r}_b, h)$	Directional kernel gradient from particle a to b
Δx	Particle Spacing (m)
η	Arc efficiency
κ_{int}	Local curvature at the liquid-solid interface ($1/m$)
κ	Thermal conductivity ($W/m K$)
γ	Constitutive Constant value
Γ	Gibbs-Thompson coefficient ($m K$)
μ_k	Kinetic coefficient ($m/s^\circ K$)
μ	Shear viscosity ($Pa.s$)
ν	Number of dimensions
Ω_{ij}	Rate of rotation tensor
Φ	Any differentiable function
ρ_b	Interpolated density of particle b ($kg m^{-3}$)
ρ_0	Reference density ($kg m^{-3}$)
σ_0	Kernel constant
σ_{ij}	Total stress tensor (Pa)
σ_a	Total stress tensor for a
σ_b	Total stress tensor for b
τ_d	Droplet period (s)
τ_{ij}	Viscous stress tensor (Pa)
ζ	Coefficient of bulk viscosity (Ns/m^2)

Chapter 1

Introduction

1.1 Welding Process

The primary purpose of doing a welding process is to join separated metallic parts to make a unified permanent bond between them. This is done by applying a source of energy which causes a local melting and re-solidification of the parts. Welding can also be used in a local repair process of a structure. The type of energy source specifies the type of welding process such as arc, laser, electron beam. The heat input from the energy source brings the temperature of the alloys to a value above the melting point and up to the vaporization depending on the process. The intensity of the source ranges from 10^6 w/m^2 in a gas metal arc welding to 10^9 w/m^2 in laser or electron beam welding process where vaporization can occur. As the trailing edge of the weld pool solidifies, the weld is made. This solidification usually takes place in about millisecond. Fig. 1.1 schematically illustrates the processes happening during gas metal arc welding (GMAW).

Figure 1.1: Schematic of an arc welding process with a consumable electrode.

1.2 Weld Problems

It's not only the matter of joining the welded parts by making a weld. The quality of the final weld must be assured as an essential part since some concerns are always associated with any welding process. From the point of view of industries, the main concerns with the weld are cracking, distortion and buckling. In addition, post-weld problems such as crack propagation, fracture under cyclic loads and stress corrosion cracking and failure under tensile loads are potential problems.

The question is *how can we prevent, predict or control these kinds of problems?* Usually, it is thought that by optimizing the input parameters available in a weld procedure such as power input (voltage $\times$ current), weld speed, filler and base metal materials, wire speed, wire diameter and joint designs, one can avoid such problems but because a weld is a complex optimization process requires running too many experiments which would be very costly.

Figure 1.2: Coupling in a weld and associated physics. Modified from [1].

1.3 Welding Model Through the Simulation

Looking deeper into a weld, more control parameters can be identified. Welding is a multi-physics problem involving complex interactions between different fields namely thermal, mechanical and metallurgical.

Fig. 1.2 illustrates the coupling between different fields and major phenomena within them. The dominant couplings are shown in bold lines. Without an integrated computer model, it is difficult to understand or investigate such complexity.

1.3.1 Computational Weld Mechanics (CWM)

Progress in computer technology and ease of accessibility to the computing machine since 1980s pushed weld researchers to think about developing computer models in the area of weld technology as an alternative way to understand unknown aspects of a welding process. New powerful computers also accelerated development of new mathematical models for welding problems that could be solved numerically. A wide variety of models have been developed, starting with simple 2D models, i.e., conductive heat transfer of a weld to very focused studies on one aspect, i.e., effect of cathode sheath on heat transfer to the weld pool, which requires a deep understanding of plasma physics [14]. However few models have been developed which focused on the weld as a multi-physics problem. As an example, the idea, aims and methods of computational weld mechanics (CWM) were well overviewed by Goldak et.al [15] which might be considered as a basis for a coupled holistic multi-physics, multi-scale CWM software package.

See Fig. 1.2 again. Thermal, microstructural, mechanical are defined as three main *components* of a CWM package. One can define a long list of *phenomena* for each component. Note that some phenomena are crucial in a weld while some others can be ignored or simplified. Then the significant *physics* involved in each phenomena

should be identified and understood. Mathematical *models* should be developed and numerical *methods* should be implemented.

To make it more clear, suppose one chooses thermal as a component to focus on. Then one focuses on fluid flow phenomena since convective heat transfer involves flow of molten metal. Forces involved in the weld pool fluid flow could be gravity, buoyancy, electromagnetic force, surface tension gradient, etc. If one chooses the surface tension effect as physics then this includes finding the curvature at the liquid-plasma interface. As a final step curvature can be computed by adopting a numerical algorithm as a method to find the curvature numerically.

A CWM package can be designed in a top to bottom fashion. Three components can be coupled together primarily by incorporating few physics and simple models. For instance, only conduction can be considered for the heat transfer model. Microstructure component may ignore all phase transformations and only take thermal expansion into account and finally plastic deformation can be ignored for the mechanical. Such a strategy makes it possible for a developer to add new phenomena, physics, models and methods in order to improve the modeling capabilities without disturbing the functionality of the primary package. When the results for a new feature are acceptable, they can be integrated into the package as an option or upgrade.

The strategy mentioned above includes describing the new physics, mathematical models, developing numerical algorithm for solving equations, ODEs and PDEs, coding, testing the machinery, verification, validation and production process. These steps already revealed some hidden tasks needed for the CWM package development. Additionally, it requires system and resource management in order to achieve the goals in reasonable CPU time.

1.3.2 Current State of CWM and Objective of This Research

The latest CWM tools are able to do a coupled full 3D transient thermal, microstructure evolutions and transient stress-strain analysis. Multi-pass welds with different filler metal added for each pass can be analyzed. Transient displacement and residual stress fields can be predicted with a considerable accuracy. However, there are still several limitations. As an example, to predict a weld pool geometry, a heat source model is required to predict the geometry of the weld pool for a certain weld procedure. Usually heat source parameters should be adjusted in advance using data from real welds. This limitation could be removed by development of a predictive weld pool model. If no experimental data is available, i.e., a micrograph of a cross section of a multi-pass weld, a weld joint is usually made in the simulation tool with a user defined geometry and patterns. A predictive tool which deposits filler metals for multi pass-weld joints would be helpful. Microstructure analysis usually assumes a homogeneous alloy composition and there is no notion of grains and non-equilibrium effect during the phase transformation.

The major goals of the thesis is to do the following tasks that could not be done or had not been been done before and in this way overcome several major limitations in the current state of the art.

The research targets the two components shown in Fig. 1.2, thermal and microstructural, and could extend current CWM tools by adding new physics and modeling methods.

- Predict weld pool shape, size, penetration, width, reinforcement and to predict mixing and dilution between base metal and filler metal for a weld pass in a multi-pass weld joint.
- Create an FEM mesh of a multi-pass weld joint that resolves the filler metal added in each weld pass.

To accomplish the two objectives mention above, a new method called smoothed particle hydrodynamic, SPH, was implemented for the weld pool model due to the robustness of the method for fluid dynamics problems. It solves coupled energy and momentum equations to compute the 3D transient temperature field in the domain. The SPH method can handle different materials, mixing and dilution in the weld pool. The development procedure included mathematical modeling, numerical algorithms, software development, verification and possibly validation, production and testing. The current version of the SPH weld pool model can be simply extended to any welding process such as arc and laser and hybrid arc-laser welding process by adding the corresponding physics. This 3D Lagrangian model also captures the dynamic behavior of the weld pool for a longer period of time that is difficult to attain using other numerical algorithms.

- Compute the solidification microstructure that forms on the trailing edge of the weld pool in low-alloy steel welds with at least three alloying components in a multi-physics, multi-scale holistic model for welds and weld joints.
- Create synthetic microstructure models for the heat-affected zone of low-alloy steel welds that represent individual crystals or grains with realistic compositions and with non-displacive transformations controlled by carbon diffusion.

To do these tasks, new models were implemented for the microstructure evolution during weld pool solidification and microstructure evolution in the heat-affected zone. Micro-scale solidification model in the micro domain captured the dendrite growth and segregation of alloying components for the Fe-C-X system. The solid state phase transformations during heating and cool down where fully or partially austenization occurs was modeled as well. The thermal cycle and carbon diffusion controls the grain growth and solid state phase transformations. The coupled mechanical field, is naturally influenced by the temperature and phase change.

- Develop the capability to do stress analysis with transformation plasticity at the micro-scale in the fusion zone and heat-affected zone of low-alloy steel welds.
- Create workflows that can be automated for each of the above tasks.

Two frame works were developed for the HAZ and fusion zone in which the welding parameters are related to the final microstructure and hardness as well as stress-strain curve of a spatial point in the fusion and heat affected zone.

It is believed that the completion of the above tasks would be a significant step towards the goal of automated computational weld mechanics for welds and welded structures. Note that the term holistic used above does not indicate the completeness of the model but tries to demonstrate the integrated nature of the model addressing thermal, mechanical and microstructure fields. In other words it is more complete than most models for welding technology.

1.4 Contributions

The present research was accomplished in a group work research atmosphere under the leadership of Prof. John Goldak.

To establish SPH Weld pool model from step one, a tight collaboration and hours of discussions were done. Prof. Goldak assisted with the selection and planning of SPH method for the weld pool. I, as a candidate, brought the SPH concept to the initial testing environment. SPH momentum and energy equations were coded in Mathematica. The transient solution using an explicit scheme was tested. The Mathematica code were translated into *C* by Dr. Sylvain Pitre, Post Doctoral Fellow, in computer science. He also coded the CUDA version of the SPH code to run on a GPU. Dr. Jinaguo Zhou, from Goldak Technology Inc., developed the *C++* code in the VrSuite framework. As also he implemented the combined FEM Energy-SPH

Navier-Stokes solvers. Stanislav Tchernov, from Goldak Technology Inc., provided GUI support for all solver and process parameters, data flows, etc.

This development procedure required testing the machinery, testing the code correctness and verification of the model to provide appropriate feedback that I made as candidate.

The original codes for the dendrite model and austenite-ferrite transformation were developed by Prof. Andrei Artemev, Professor in the Department of Mechanical and Aerospace engineering. He also provided valuable guidance. The codes were re-written in VrSuite by Dr. Jianguo Zhou and GUI support provided by Stanislav Tchernov. As a candidate, I tested the code for the machinery, verification, and further extension by providing feedbacks.

During all steps mention above, unlimited guidance, providing ideas, thoughts, and constructive feedbacks were provided by Prof. Goldak through discussions.

1.5 Outline of the Thesis

This research is organized in the following chapters and appendices:

Chapter 2 This chapter present an implementation of the developed weld pool model using the SPH method. The mathematical description, and modeling steps, and verification procedure are discussed first. Simulation results are presented as well to show the capability of the model.

Chapter 3 This chapter is organized in this way. The synthetic microstructure is introduced first. Second, the algorithm for the austenite-ferrite transformation in a low-alloy steel weld is discussed. The model incorporates the synthetic microstructure introduced in the previous part. Bench mark tests for verification are presented as well. Finally, the HAZ microstructure framework and simulation results are discussed.

Chapter 4 The first part of the chapter describes the computer model for dendrite growth during the weld pool solidification. The results give dendrite structure and solute segregation in the weld fusion zone. In the final part, the fusion zone microstructure framework is discussed where the macro weld model is linked to micro models for the solidification, microstructure and transient stress-strain evolution.

Chapter 5 The chapter provides a conclusion, some on-going model developments, and suggests work for future development.

Appendix 1

SPH numerical solution steps

Appendix 2

Verification tests

Chapter 2

Weld Pool Simulation Using SPH

2.1 Introduction

A weld pool model with high spatial and temporal resolution is described. It is based on a Smoothed Particle Hydrodynamics (SPH) formulation in which the coupled Navier-Stokes and energy equations are solved. The advantages of SPH are that it deals gracefully with free surfaces, droplets from an electrode falling into a weld pool, mixing and dilution and solidification in a weld pool. The model allows detailed information about complicated transport phenomena in the weld pool which are typically difficult to model using other numerical methods such as FEM and FDM. Particle spacings of roughly 0.1 mm to 1 mm can be used depending on a trade off between speed and accuracy. The theory and modeling procedures are described first in this chapter. In the second stage, the GMAW process is modeled as a stream of droplets emitted from an electrode tip. Experimental studies are reviewed in order to calculate input data for the droplets in the SPH weld pool model. Some simulation results are presented at the end of the chapter.

2.2 Smoothed Particle Hydrodynamics (SPH)

Smoothed particle hydrodynamics (SPH) gives approximate numerical solutions of the equations of fluid dynamics by representing the fluid with a set of particles [16]. It was independently developed by Gingold and Monaghan [17] and Lucy [18] in 1977. The method was originally applied to astrophysics problem but gradually many other areas in science and engineering took advantage of this method.

The idea is to replace a continuum with a finite number of particles. The method does not need any grid to approximate a field or spatial derivatives. A field value at any point in space is interpolated using the weighted value of a function at the nearby particles. Also a field derivative at any point is simply related to the analytical derivative of a kernel function and the value weights in the set of adjacent particles. Problems involving free surface flows, large deformation, shock waves, moving interfaces, mixing, etc., are handled easily with the SPH method. Due to its unique capabilities, it has been adopted as an efficient computational method in simulating various problems in applied mechanics.

2.3 Definitions

In the standard approach, the following integral interpolant can be used to approximate any function $A(\mathbf{r})$ defined and continues in Ω . [16]

$$A(\mathbf{r}) = \int_{\Omega} A(\mathbf{r}') W(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}' \quad (2.1)$$

where W is the weighting function or kernel which is normalized to unity and approximates a Dirac δ - function as $h \rightarrow 0$. h is called the smoothing length or characteristic width of the kernel which is typically close to the particle spacing. In a discrete

approximation Eq. 2.1 has the following form:

$$A(\mathbf{r}) = \sum_{b=1}^N \frac{m_b}{\rho_b} A_b W(\mathbf{r} - \mathbf{r}_b, h) \quad (2.2)$$

In which a differential volume element $d\mathbf{r}'$ is replaced by the finite volume of the particle $\Delta V_b = m_b/\rho_b$. b denotes the nearby particle label. Particle b has mass m_b , position $\mathbf{r}_b$, and interpolated density ρ_b .

Note that $A(\mathbf{r})$ and A_b are different functions. A_b denotes the function value computed for particle b at $\mathbf{r}_b$ and $A(\mathbf{r})$ is the field computed at position $\mathbf{r}$ using the sum of weighted value of A_b . This means that A_b is not identical to the field value $A(\mathbf{r}_b)$ approximated at b . The summation is over all particles but in practice, it is over the N neighboring particles labeled by b ($b = 1, 2, \dots, N$) which fall inside a fictitious sphere (Circle in 2D) surrounding the point at $\mathbf{r}$. (See Fig. 2.1) A cut-off distance of κh is typically used for the kernel function definition. In other words, the kernel function becomes zero when $|\mathbf{r} - \mathbf{r}_b| > \kappa h$. This reduces the computation cost since summation is done over on nearby particles.

The field value of the function A at the position of particle a is interpolated as

$$A(\mathbf{r}_a) = \sum_{b=1}^N \frac{m_b}{\rho_b} A_b W(\mathbf{r}_a - \mathbf{r}_b, h) \quad (2.3)$$

Again note that a function value computed at a is different from the field interpolated at a . As an example, by replacing A with density on the either side of Eq. 2.3, the density on particle a is interpolated from the mass of surrounding particles in terms of the kernel function W as

$$\rho(\mathbf{r}_a) = \sum_{b=1}^N m_b W(\mathbf{r}_a - \mathbf{r}_b, h). \quad (2.4)$$

Figure 2.1: 2D SPH interpolation.

Eq. 2.4 denotes the summation density method which has been used extensively for the density approximation. The main advantage of using this method is that it conserves mass exactly. However, the approximation to the density field is poor near boundaries since a part of the supporting domain falls outside the problem domain.

2.3.1 Conventions.

In the SPH formulation presented here, we will denote $\mathbf{r}_a - \mathbf{r}_b$, $\mathbf{v}_a - \mathbf{v}_b$, as $\mathbf{r}_{ab}$ and $\mathbf{v}_{ab}$ respectively. In literature usually $W(\mathbf{r}_a - \mathbf{r}_b, h)$ is shown as W_{ab} for simplicity.

2.3.2 Kernel Functions.

The interpolating kernel W is analogous to the shape or basis functions in FEM and in a similar way, different types of kernels can be used in SPH. The lowest order one that can be used in SPH is called M4 (cubic) spline with continuous first and second derivatives as a minimum requirement. For example, the following kernel function is

Figure 2.2: The smoothing function used in [2], solid line: function, Dash line: first derivative.

given in [2]

$$W(\mathbf{r}, h) = \frac{\sigma_0}{h^\nu} \begin{cases} 1 - \frac{3}{2}R^2 + \frac{3}{4}R^3 & 0 \leq R \leq 1 \\ \frac{1}{4}(2 - R)^3 & 1 \leq R \leq 2 \\ 0 & R > 2 \end{cases}$$

If we call $w = \frac{\sigma_0}{h^\nu}$ and $R = \frac{|\mathbf{r} - \mathbf{r}_0|}{h}$ is the relative distance between two points, Fig. 2.2 displays the plot for the kernel function described above and its derivative where ν is the number of dimensions and σ_0 is a normalization constant with the values of $\frac{2}{3}$, $\frac{10}{7\pi}$, $\frac{1}{\pi}$ for 1D, 2D and 3D dimensions respectively [2].

2.3.3 SPH Approximation of the Derivatives.

The key idea in any computational fluid dynamics algorithm is to approximate the derivatives in the governing equations using information from a finite number of points. In a standard SPH approximation for the hydrodynamics equations, the spacial

derivative of a function is replaced with the derivative of the kernel function [19].

Having Eq. 2.3, the derivative of function A at particle a is given by

$$\nabla A(\mathbf{r}_a) = (\nabla A)_a = \sum_b \frac{m_b}{\rho_b} A_b \nabla W(\mathbf{r}_a - \mathbf{r}_b, h) \quad (2.5)$$

In the above equation, the derivative of the kernel function in the direction from particle a to particle b is given by

$$\nabla W(\mathbf{r}_a - \mathbf{r}_b, h) = \frac{dW}{dr} \frac{1}{|\mathbf{r}_a - \mathbf{r}_b|} (\mathbf{r}_a - \mathbf{r}_b) \quad (2.6)$$

For this form of the equation, the derivative does not vanish when A is constant [16]. Here is the Monaghan recipe for solving this problem [16].

Method 1:

Multiply A by any differentiable function Φ and take the gradient

$$\nabla(\Phi A) = \Phi \nabla A + A \nabla \Phi \quad (2.7)$$

We can rearrange for ∇A

$$\nabla A = \frac{1}{\Phi} [\nabla(\Phi A) - A \nabla \Phi] \quad (2.8)$$

$\nabla(\Phi A)$ and $\nabla \Phi$ are calculated using Eq. 2.5 at particle a as $(\nabla(\Phi A))_a = \sum_b \frac{m_b}{\rho_b} \Phi_b A_b \nabla W(\mathbf{r}_a - \mathbf{r}_b, h)$ and $(\nabla \Phi)_a = \sum_b \frac{m_b}{\rho_b} \Phi_b \nabla W(\mathbf{r}_a - \mathbf{r}_b, h)$

The SPH form of Eq. 2.8 for particle a is given by the following expression:

$$\begin{aligned} (\nabla A)_a &= \frac{1}{\Phi_a} \left[\sum_b \frac{m_b}{\rho_b} \Phi_b A_b \nabla W(\mathbf{r}_a - \mathbf{r}_b, h) - A_a \sum_b \frac{m_b}{\rho_b} \Phi_b \nabla W(\mathbf{r}_a - \mathbf{r}_b, h) \right] \\ &= \sum_b \frac{m_b}{\rho_b} \frac{\Phi_b}{\Phi_a} (A_b - A_a) \nabla W(\mathbf{r}_a - \mathbf{r}_b, h) \end{aligned} \quad (2.9)$$

Method 2:

An alternative way to obtain the SPH derivative is to start with the following equation

$$\nabla \left(\frac{A}{\Phi} \right) = \frac{1}{\Phi^2} (\Phi \nabla A - A \nabla \Phi) \quad (2.10)$$

Rearrange the derivative of A , to the following form

$$\nabla A = \Phi \left[\nabla \left(\frac{A}{\Phi} \right) + \frac{A}{\Phi^2} \nabla \Phi \right] \quad (2.11)$$

$\nabla(\frac{A}{\Phi})$ and $\nabla\Phi$ are calculated using Eq. 2.5 at particle a as $(\nabla(\frac{A}{\Phi}))_a = \sum_b \frac{m_b}{\rho_b} \frac{A_b}{\Phi_b} \nabla W(\mathbf{r}_a - \mathbf{r}_b, h)$ and $(\nabla\Phi)_a = \sum_b \frac{m_b}{\rho_b} \Phi_b \nabla W(\mathbf{r}_a - \mathbf{r}_b, h)$ Using Eq. 2.5, the SPH form of the above equation for particle a is written as [16, 20]:

$$(\nabla A)_a = \sum_b \frac{m_b}{\rho_b} \left[\frac{\Phi_a}{\Phi_b} A_a + \frac{\Phi_b}{\Phi_a} A_b \right] \nabla W(\mathbf{r}_a - \mathbf{r}_b, h) \quad (2.12)$$

2.3.4 Application to the Governing Equation.

Equations 2.9 and 2.12 give the general SPH expression for the gradient, where different choices of function Φ give different versions of derivatives. Note that the quantity A can be a scalar, a vector or a tensor. Next consider some examples.

2.3.4.1 Gradient of a Scalar Field.

Define A as pressure P . By substituting $\Phi = \rho$ in Eq. 2.12 and multiplying both sides by $\frac{1}{\rho_a}$ we find the following SPH form.

$$\left(\frac{1}{\rho} \nabla p \right)_a = \sum_b m_b \left[\frac{p_b}{\rho_b^2} + \frac{p_a}{\rho_a^2} \right] \nabla W(\mathbf{r}_a - \mathbf{r}_b, h) \quad (2.13)$$

This is the most popular SPH form of the pressure gradient used in the literature [16]. In a similar way, using $\Phi = 1$, Eq. 2.12 results in another form

$$\left(\frac{1}{\rho}\nabla p\right)_a = \sum_b \frac{m_b}{\rho_b \rho_a} (p_b + p_a) \nabla W(\mathbf{r}_a - \mathbf{r}_b, h) \quad (2.14)$$

Bonet uses this form in his work (See Eq. 25 in [21]).

To approximate the gradient of scalar quantities such as temperature, concentration or voltage, Eq. 2.9 is used where by substituting $\Phi = 1$, one gets

$$(\nabla A)_a = \sum_b \frac{m_b}{\rho_b} (A_b - A_a) \nabla W(\mathbf{r}_a - \mathbf{r}_b, h) \quad (2.15)$$

2.3.4.2 Gradient and Divergence of a Vector Field.

Eqs. 2.9 and 2.12 can be simply applied to a vector or tensor field $\mathbf{A}$ [20,21]. Gradient of a vector field is given by

$$(\nabla \mathbf{A})_a = \sum_b \frac{m_b}{\rho_b} \frac{\Phi_b}{\Phi_a} (\mathbf{A}_b - \mathbf{A}_a) \otimes \nabla W(\mathbf{r}_a - \mathbf{r}_b, h) \quad (2.16)$$

For example, for $\mathbf{A} = \mathbf{v}$ and $\Phi = 1$, the velocity gradient is computed as

$$(\nabla \mathbf{v})_a = \sum_b \frac{m_b}{\rho_b} (\mathbf{v}_b - \mathbf{v}_a) \otimes \nabla W(\mathbf{r}_a - \mathbf{r}_b, h) \quad (2.17)$$

This equation will be use to compute the strain rate tensor (See Eq. 22 in [21]). The divergence of a vector or a tensor field $\mathbf{A}$ is given by

$$(\nabla \cdot \mathbf{A})_a = \sum_b \frac{m_b}{\rho_b} \frac{\Phi_b}{\Phi_a} (\mathbf{A}_b - \mathbf{A}_a) \cdot \nabla W(\mathbf{r}_a - \mathbf{r}_b, h) \quad (2.18)$$

or

$$(\nabla \cdot A)_a = \sum_b \frac{m_b}{\rho_b} \left[\frac{\Phi_a}{\Phi_b} A_a + \frac{\Phi_b}{\Phi_a} A_b \right] \cdot \nabla W(\mathbf{r}_a - \mathbf{r}_b, h) \quad (2.19)$$

where $\cdot$ represents dot product.

2.3.5 Second Derivative.

The derivation of the second derivative is not discussed here. An expression for the second derivative of temperature in the energy equation is given by [19, 22, 23] which is adopted as a SPH form of the second derivative of a scalar field.

$$\nabla^2 A(\mathbf{r}_a) = \nabla \cdot (\nabla A(\mathbf{r}_a)) = -2 \sum_b \frac{m_b}{\rho_a \rho_b} (A_a - A_b) \nabla W(\mathbf{r}_a - \mathbf{r}_b, h) \cdot \frac{(\mathbf{r}_a - \mathbf{r}_b)}{|\mathbf{r}_a - \mathbf{r}_b|^2} \quad (2.20)$$

where $\nabla W(\mathbf{r}_{ab}, h)$ is computed by Eq. 2.6.

2.3.6 Summary of SPH Equations

1. The density at particle a is given by

$$\rho_a = \sum_b m_b W(\mathbf{r}_a - \mathbf{r}_b, h)$$

2. The field A is approximated at particle a as

$$A_a = \sum_b \frac{m_b}{\rho_b} A_b W(\mathbf{r}_a - \mathbf{r}_b, h)$$

3. The derivative of the kernel function in the direction from particle a to particle b is given by

$$\nabla W(\mathbf{r}_a - \mathbf{r}_b, h) = \nabla W(\mathbf{r}_{ab}, h) = \frac{dW}{dr} \frac{(\mathbf{r}_a - \mathbf{r}_b)}{|\mathbf{r}_a - \mathbf{r}_b|}$$

4. The gradient of a scalar field A at particle a is given by

$$(\nabla A)_a = \sum_b \frac{m_b}{\rho_b} \frac{\Phi_b}{\Phi_a} (A_b - A_a) \nabla W(\mathbf{r}_a - \mathbf{r}_b, h)$$

or

$$(\nabla A)_a = \sum_b \frac{m_b}{\rho_b} \left[\frac{\Phi_a}{\Phi_b} A_a + \frac{\Phi_b}{\Phi_a} A_b \right] \nabla W(\mathbf{r}_a - \mathbf{r}_b, h)$$

5. The gradient of a vector or tensor field A at particle a is defined as

$$(\nabla A)_a = \sum_b \frac{m_b}{\rho_b} \frac{\Phi_b}{\Phi_a} (A_b - A_a) \otimes \nabla W(\mathbf{r}_a - \mathbf{r}_b, h)$$

where $\otimes$ represents the outer product.

6. The divergence of a vector field $\mathbf{A}$ at particle a is given by

$$(\nabla \cdot \mathbf{A})_a = \sum_b \frac{m_b}{\rho_b} \frac{\Phi_b}{\Phi_a} (A_b - A_a) \cdot \nabla W(\mathbf{r}_a - \mathbf{r}_b, h)$$

where $\cdot$ represents the dot product.

7. The curl of a velocity field is given by

$$(\nabla \times \mathbf{v})_a = \sum_b \frac{m_b}{\rho_b} (\mathbf{v}_b - \mathbf{v}_a) \times \nabla W(\mathbf{r}_a - \mathbf{r}_b, h)$$

where $\times$ represents the cross product.

2.4 SPH Stress Tensors For a Newtonian Fluid

2.4.1 Force Balance Equation

For particle a , interacting with other particles, the acceleration vector $\mathbf{a}_a$ is given by Newton's law as

$$m_a \mathbf{a}_a = m_a \frac{d\mathbf{v}_a}{dt} = \mathbf{F}_a^{external} - \mathbf{F}_a^{internal}. \quad (2.21)$$

$\mathbf{F}_a^{internal}$ represents the equivalent internal forces acting on particle $\mathbf{a}$ due to the state of stress inside the material and $\mathbf{F}_a^{external}$ accounts for sum of external forces on particle a [21]. The time integration of the above equation describes the motion of the particle. The total internal force on particle a is related to the total state of stress for particle a which allows one to write Eq. 2.21 as

$$\frac{d\mathbf{v}_a}{dt} = \frac{1}{\rho_a} (\mathbf{Div} \sigma_a) + \mathbf{f}_a^{external} \quad (2.22)$$

where $\mathbf{f}_a^{external}$ is the force vector per unit mass due to all the external forces acting on particle a at time t .

Eq. 2.22 can be applied to any medium. However, to specify a well posed problem, additional BCs, ICs and constraints are needed that relate the stress to the velocity or displacement as well as an equation of state. This will be discussed in the following sections.

2.4.2 Constitutive Equation for Viscous Fluids

2.4.3 Definitions

Assume that a fluid has a velocity field $\mathbf{v}$, then the velocity gradient tensor at a point is written as

$$\nabla \mathbf{v} = \frac{\partial \mathbf{v}_i}{\partial \mathbf{x}_j} \equiv \begin{pmatrix} \frac{\partial \mathbf{v}_1}{\partial x} & \frac{\partial \mathbf{v}_1}{\partial y} & \frac{\partial \mathbf{v}_1}{\partial z} \\ \frac{\partial \mathbf{v}_2}{\partial x} & \frac{\partial \mathbf{v}_2}{\partial y} & \frac{\partial \mathbf{v}_2}{\partial z} \\ \frac{\partial \mathbf{v}_3}{\partial x} & \frac{\partial \mathbf{v}_3}{\partial y} & \frac{\partial \mathbf{v}_3}{\partial z} \end{pmatrix} \equiv \begin{pmatrix} \mathbf{v}_{1,x} & \mathbf{v}_{1,y} & \mathbf{v}_{1,z} \\ \mathbf{v}_{2,x} & \mathbf{v}_{2,y} & \mathbf{v}_{2,z} \\ \mathbf{v}_{3,x} & \mathbf{v}_{3,y} & \mathbf{v}_{3,z} \end{pmatrix}. \quad (2.23)$$

Any matrix can be decomposed into the sum of a symmetric and an anti-symmetric matrix. Applying that decomposition to the above matrix, we define the symmetric

part of the velocity gradient tensor (Eq. 2.23) as the deformation rate tensor (or strain rate tensor) given by $D = \frac{1}{2} (\nabla \mathbf{v} + \nabla \mathbf{v}^T)$ or equally as $D_{ij} = \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right)$.

Similar to the deformation rate tensor, the rate of rotation tensor is defined as $\Omega = \frac{1}{2} (\nabla \mathbf{v} - \nabla \mathbf{v}^T)$ or equally as $\Omega_{ij} = \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} - \frac{\partial v_j}{\partial x_i} \right)$

Note that $\nabla \mathbf{v} = \mathbf{D} + \mathbf{\Omega}$ and also note that trace of $\nabla \mathbf{v}$ is $\nabla \cdot \mathbf{v}$. For incompressible flow, the trace becomes zero.

2.4.4 Stress-Strain Rate Relationship for a Newtonian Fluid

The total stress tensor can be always split into two parts. The first term is called *hydrostatic stress or pressure tensor* and the second term is the *deviatoric stress or viscous stress tensor*.

$$\sigma_{ij} = -p\delta_{ij} + \tau_{ij} \quad (2.24)$$

To establish this constitutive equation which relates the viscous stress to the deformation rate, we make these assumptions:

1. The viscous stress tensor, σ_{ij} , is related to the rate of deformation tensor D_{ij} through a linear function.
2. The fluid is isotropic which means that there is no preferred direction;
3. The fluid is homogenous which means that fluid properties do not depend on position;
4. During a rigid body rotation no strain acts on the fluid;
5. When a perfect fluid is at rest, the stress is hydrostatic [24].

Assumption 1 suggest the most general linear relation as

$$\tau_{ij} = C_{ijkl}^l D_{kl}. \quad (2.25)$$

C_{ijkl}^l is a fourth order tensor with 81 components relating viscous stress to the strain rate tensor, under the above constraints, this general relationship is simplified to the following linear form.

$$\tau_{ij} = \lambda \delta_{ij} D_{kk} + 2\mu D_{ij} \quad (2.26)$$

or equally is written as

$$\boldsymbol{\tau} = \lambda (\text{Div } \mathbf{v}) \mathbf{I} + 2\mu \mathbf{D} \quad (2.27)$$

where μ is called the first coefficient of viscosity or coefficient of shear viscosity of a fluid and λ is the second coefficient of viscosity. They are measured by experiment, for example, the dynamic viscosity μ , can be obtained by doing a *simple shear* test, like a Couette flow test. Substituting Eq. 2.26 into Eq. 2.24 we can write the total stress as

$$\sigma_{ij} = -p \delta_{ij} + \tau_{ij} = -p \delta_{ij} + 2\mu D_{ij} + \lambda \delta_{ij} D_{kk} \quad (2.28)$$

or

$$\sigma_{ij} = -p \delta_{ij} + 2\mu \left(D_{ij} - \frac{1}{3} \delta_{ij} D_{kk} \right) + \left(\lambda + \frac{2}{3} \mu \right) \delta_{ij} D_{kk}. \quad (2.29)$$

or identically as

$$\boldsymbol{\sigma} = -p \mathbf{I} + \mu \left(\nabla \mathbf{v} + \nabla \mathbf{v}^T - \frac{2}{3} \nabla \cdot \mathbf{v} \right) + \zeta (\nabla \cdot \mathbf{v}) \mathbf{I}. \quad (2.30)$$

$\zeta = \lambda + \frac{2}{3}\mu$ is often called the coefficient of bulk viscosity. For an incompressible fluid, $D_{kk} = \nabla \cdot \mathbf{v} = \mathbf{0}$, therefore the full stress tensor takes the following simple form

$$\sigma_{ij} = -p\delta_{ij} + 2\mu D_{ij}. \quad (2.31)$$

Since in SPH, the fluid is often assumed to be slightly compressible, $D_{kk} = \nabla \cdot \mathbf{v} \neq \mathbf{0}$, Eq. 2.29 is used as total stress tensor in the fluid. Substituting σ (Eq. 2.30) into Eq. 2.22, the force balance equation for particle a for a compressible Newtonian fluid can be written as

$$\rho_a \frac{D\mathbf{v}_a}{Dt} = -\nabla p_a + \mu \nabla^2 \mathbf{v}_a + \left(\zeta + \frac{1}{3}\mu\right) \nabla(\nabla \cdot \mathbf{v}_a) + \mathbf{F}_a^{external} \quad (2.32)$$

The SPH form of Eq. 2.32 is solved for velocity and pressure. This will be explained in the next section.

2.5 SPH Formulation for Stress Tensor for a Newtonian Fluid

2.5.1 Pressure Tensor

The fluid is treated as a weakly compressible fluid in the formulation given in [16]. (Weakly compressible means that the fluid is almost incompressible. This is a good assumption for liquid water at atmospheric pressure. It is not a good assumption for a perfect gas.) This makes it easier to determine the fluid pressure using an equation of state which is basically much faster than solving the Poisson pressure equation. For weakly compressible fluids, the relationship between pressure and density can be given by the following equation of state.

$$p = B \left[\left(\frac{\rho}{\rho_0} \right)^\gamma - 1 \right] \quad (2.33)$$

where γ is a constant that can be prescribed a value between 1 and 7, ρ_0 ($kg\ m^{-3}$) the reference density. B is a constant related to the bulk modulus of elasticity of the fluid given by $B = c_s^2 \rho_0 / \gamma$, where c_s is the speed of sound. Eq. 2.33 is used to compute the pressure term in Eq. 2.32.

2.5.2 Deviatoric Stress Tensor

Eq. 2.26 relates the deviatoric stress tensor to the deformation rate tensor. Computing the deformation rate tensor, D_{ij} , consists of computing the velocity gradient given by Eq. 2.23 which has the following form in an SPH formulation [21]

$$\nabla \mathbf{v}_a = \sum_b \frac{m_b}{\rho_b} (\mathbf{v}_b - \mathbf{v}_a) \otimes \nabla W(\mathbf{r}_a - \mathbf{r}_b, h) \quad (2.34)$$

with the derivative of the kernel function in the direction from particle a to particle b given by $\nabla W(\mathbf{r}_a - \mathbf{r}_b, h) = \frac{dW}{dr} \frac{1}{|r_{ab}|} (\mathbf{r}_a - \mathbf{r}_b)$

So in the **first step**, for a given velocity field, the velocity gradient tensor is computed using Eq. 2.34. In the **second step**, the deformation rate tensor is computed by $D = \frac{1}{2} (\nabla \mathbf{v} + \nabla \mathbf{v}^T)$. In the **third step**, the stress tensor is computed using the constitutive equations given in Eq. 2.29 or 2.31. Note that Bonet uses the first two terms in the RHS of Eq. 2.29. In the **last step**, the divergence operator is applied to the stress field to compute the equivalent internal force per unit volume. The most general SPH expressions for the internal force (N) in the literature are given

by

$$\mathbf{F}_a^{internal} = \left(\frac{m_a}{\rho_a} \right) \nabla \cdot \sigma_a = \sum_b m_a m_b \left(\frac{\sigma_b}{\rho_b^2} + \frac{\sigma_a}{\rho_a^2} \right) \cdot \nabla W_{ab} \quad (2.35)$$

or

$$\mathbf{F}_a^{internal} = \left(\frac{m_a}{\rho_a} \right) \nabla \cdot \sigma_a = \sum_b \frac{m_a m_b}{\rho_a \rho_b} (\sigma_b \pm \sigma_a) \cdot \nabla W_{ab}. \quad (2.36)$$

These are easy to obtain. Using $\Phi = \rho$ in Eq. 2.19 gives Eq. 2.35 and using $\Phi = 1$ in Eq. 2.19 results in Eq. 2.36 with $+$ sign in the brackets. Using $\Phi = 1$ in Eq. 2.18 results in Eq. 2.36 with $-$ sign in the brackets. In the code used for the weld pool model, Eq. 2.35 was used to compute the equivalent internal forces for the RHS of the force balance equation.

2.5.3 Correction to Gradient and Divergence Operators

Simple verification tests turned out that the velocity gradient operator given by Eq. 2.34 does not provide precise results for the velocity gradient. The following correction term given by [21, 25] is used to correct the velocity gradient computed using Eq. 2.34.

$$\mathbf{B}_a = \left(\sum_b \frac{m_b}{\rho_b} (\mathbf{r}_b - \mathbf{r}_a) \otimes \nabla W_{ab} \right)^{-1} \quad (2.37)$$

For particle a , $\mathbf{B}_a$ would be a second order correction tensor. Two different methods are discussed in [25] and [21] to derive the correction tensor. For every time step, the correction term is computed for every particle and applied to the Eqs. 2.34, 2.35 and 2.36.

The final equation for the corrected velocity gradient and internal force will take

the following forms.

$$\nabla \mathbf{v}_a = \left(\sum_b \frac{m_b}{\rho_b} (\mathbf{v}_b - \mathbf{v}_a) \otimes \nabla W_{ab} \right) \cdot \mathbf{B}_a \quad (2.38)$$

$$\nabla \mathbf{u}_a = \left(\sum_b \frac{m_b}{\rho_b} (\mathbf{u}_b - \mathbf{u}_a) \otimes \nabla W_{ab} \right) \cdot \mathbf{B}_a \quad (2.39)$$

$$\nabla \cdot \sigma_a = \mathbf{F}_a^{internal} = \left(\sum_b m_a m_b \left(\frac{\sigma_b}{\rho_b^2} + \frac{\sigma_a}{\rho_a^2} \right) \nabla W_{ab} \right) : \mathbf{B}_a \quad (2.40)$$

or

$$\nabla \cdot \sigma_a = \mathbf{F}_a^{internal} = \left(\sum_b \frac{m_a m_b}{\rho_a \rho_b} (\sigma_b \pm \sigma_a) \nabla W_{ab} \right) : \mathbf{B}_a. \quad (2.41)$$

where $:$ denotes the double contraction of two tensors as $\mathbf{A}:\mathbf{B} = A_{ij}B_{ij}$

2.5.4 Summary of SPH Stress-Strain Rate

For a given or computed velocity vector for particle a:

1. Compute velocity gradient tensor (see 2.23) using Eq. 2.34

$$\nabla \mathbf{v}_a = \sum_b \frac{m_b}{\rho_b} (\mathbf{v}_b - \mathbf{v}_a) \otimes \nabla W_{ab}$$

2. Compute the correction tensor given in Eq. 2.37

$$\mathbf{B}_a = \left(\sum_b \frac{m_b}{\rho_b} (\mathbf{r}_b - \mathbf{r}_a) \otimes \nabla W_{ab} \right)^{-1}$$

3. Compute the corrected velocity gradient by Eq. 2.38

$$\nabla \mathbf{v}_a = \left(\sum_b \frac{m_b}{\rho_b} (\mathbf{v}_b - \mathbf{v}_a) \otimes \nabla W_{ab} \right) \cdot \mathbf{B}_a.$$

4. Compute the deformation rate tensor D_{ij}

$$D = \frac{1}{2} (\nabla \mathbf{v} + \nabla \mathbf{v}^T)$$

5. Compute the viscous stress tensor using Eq. 2.26

$$\tau_{ij} = \lambda \delta_{ij} D_{kk} + 2\mu D_{ij}$$

6. Compute the hydrostatic stress tensor $p\delta_{ij}$ using Eq. 2.33

7. Compute the total stress tensor as

$$\sigma_{ij} = p\delta_{ij} + \lambda \delta_{ij} D_{kk} + 2\mu D_{ij}$$

8. Compute the internal force using Eq. 2.40 or 2.41.

2.6 SPH Form of Heat Equation

For an incompressible fluid, the rate of change in internal energy for particle a is given by

$$\frac{dH_a}{dt} = \frac{1}{\rho_a} \nabla \cdot (\kappa_a \nabla T_a) + Q_a \quad (2.42)$$

where H is the enthalpy per unit mass, ρ the density, κ the thermal conductivity, T temperature, and Q the internal heat generation per unit mass. In the above equation, the viscous dissipation has been neglected.

Give the label a to particle i , the SPH form of Eq. 3.5.1 is given by [16, 22]

$$\frac{dh}{dt} = \frac{1}{\rho_a} \sum_b \frac{m_b}{\rho_b} (\kappa_a + \kappa_b) \frac{(T_b - T_a)}{|\mathbf{r}_{ab}|^2} \mathbf{r}_{ab} \nabla W_{ab} + Q_a \quad (2.43)$$

where label b accounts for the nearby particles surrounding particle a and the gradient of the kernel is defined as

$$\nabla W_{ab} = \frac{dW}{dr} \frac{1}{r_{ab}} (\mathbf{r}_a - \mathbf{r}_b) \quad (2.44)$$

Cleary and Monaghan [22] showed that to get a continuous heat flux, Eq. 2.43 should be solved by replacing $\kappa_a + \kappa_b$ in Eq. 2.43 with

$$\frac{4\kappa_a\kappa_b}{\kappa_a + \kappa_b} \quad (2.45)$$

Taking the above modification into account, Eq. 2.43 can be written in terms of temperature as

$$c_p \frac{dT_a}{dt} = \frac{1}{\rho_a} \sum_b \frac{m_b}{\rho_b} \left(\frac{4\kappa_a\kappa_b}{\kappa_a + \kappa_b} \right) \frac{(T_b - T_a)}{|\mathbf{r}_{ab}|^2} \mathbf{r}_{ab} \nabla W_{ab} + Q_a \quad (2.46)$$

2.7 Modeling Procedure

2.7.1 Creating Particles

The goal is to replace a continuum with the finite number of particles. Typically, in a simplest case particles are positioned in a cubic grid. Imagine a grid with cubic cells in which the length of the cube is Δx . A particle is positioned at the centroid of each cell. This can be done by making a cubic mesh of a domain in any mesh generator

tools and positioning a particle at the centroid of each element (see Fig. 2.3)

Figure 2.3: Example of a particle mesh of a continuum.

2.7.2 Assigning Particle Type

To apply boundary conditions, deal with inlet and outlet problems, particle activation and deactivation, and assign an specific functionality to a particle, different particle types are specified such that solver can distinguish between particle types. As an example, for a set of particles available to solve a heat transfer problem, all particles with unknown temperature are called "domain particle" and are assigned type 0 and the subset of particles with an assigned temperature are assigned particle type 1. In a similar way, inactive, Crespo, boundary, inlet, periodic inlet and outlet particles are assigned their type. Also specific attributes may be defined for each particle type. Fig. 2.4 illustrates a particle mesh with different particles types.

2.7.3 Assigning Particle Attributes and Material Properties

In a general case, in order to deal with multiple materials, each individual particle carries its own attributes. The attributes are listed in the Table. 2.1. Note that some of these attributes are material properties such as thermal conductivity and viscosity. Some of them should be calculated or solved such mass, velocity, temperature, etc. Depending on the solver each particle takes the required material properties from a library.

Figure 2.4: Example of an SPH particle mesh with different particle types.

Attribute	Symbole	Unit (SI)
Mass	m	kg
Reference density	ρ_0	kg/m^3
Position	$\mathbf{r}$	m
Velocity	$\mathbf{v}$	m/s
Viscosity	ν	Ns/m^2
Speed of sound	c_s	m/s
Specific heat	c	$J/kg\ K$
Thermal conductivity	κ	$W/m\ K$
Temperature	T	K
Enthalpy	H	J/kg
Pressure	P	N/m^2
Fraction solid	F_s	—

Table 2.1: Particle attributes.

2.7.4 Finding the Neighboring Particles

All quantities related to a particle are interpolated from its neighboring particles contained in the supporting domain of the kernel (see Fig. 2.1). The length of this supporting domain is typically κh and the kernel value is zero for distances greater than κh . Another cubic grid with the length of κh is considered. The function of this grid is to find the neighboring particles. Note that computing particle adjacency lists is more efficient using a fixed background mesh. The background mesh is not used directly in the SPH theory, e.g.; there is no solution to the equation on the background mesh nodes. In a simplest case it is only necessary to look for particles in 26 neighboring cells and a cell which is occupied by the target particle. This is due to the fact that the kernel function goes to zero for a distance bigger than $2h$.

2.7.5 Positioning the Particles and Computing Particle Mass

The mass of particle a is computed using the reference density of that particle as $m_a = \rho_{0a}(\Delta x)^\nu$ where ν is 1, 2, and 3 for 1D, 2D, and 3D problems respectively.

2.8 Solution Procedure and Verification Tests

This solution procedure for the energy equation, momentum equation, and coupled energy and momentum equations are discussed in Appendix A. The verification test procedures are described in Appendix B.

2.9 Boundary Treatment in SPH

Different methods have been proposed to enforce boundary conditions in SPH NS. One treats the force applied to the domain particle by the boundary particle as an internal force and the other treats the force applied to the domain particle as an external force.

In no case the motion of the boundary particle affected or altered by any force that might be applied by the domain particle on the boundary particle. When two particles are interacting with each other in SPH, the symmetric internal force is generated between particles as $\nabla \cdot \sigma$. The total stress tensor σ includes thermodynamic pressure, deviatoric and volumetric stress tensors. For particle a the acceleration $\mathbf{a}_a$ is given by:

$$\mathbf{a}_a = \frac{1}{m_a} (\underbrace{\mathbf{F}_{pressure} + \mathbf{F}_{shear\ viscous} + \mathbf{F}_{volumetric\ viscous}}_{\mathbf{F}_{internal} = \frac{1}{\rho} \nabla \cdot \sigma} - \mathbf{F}_{external}) \quad (2.47)$$

2.9.1 Dynamic Boundary Condition

In the treatment described by Crespo et al [3], boundary particles are constrained to satisfy the same equations as domain (fluid) particles. This is the reason that the force applied to the domain particle by the boundary particle is treated as an internal force. Thus, they follow the summation density equation, equation of state and momentum equation. However their positions are not updated during the time integration and their positions are either fixed or they move with a prescribed velocity. This case is found to be useful when a sticking boundary condition is required to simulate the condition where $\mathbf{v} = 0$ on the boundary.

Assume that a fluid particle is approaching the boundary and it comes inside the kernel support domain of boundary particles. In this case, the density of the boundary particle (which has fixed mass) increases resulting in a pressure increase. A repulsive force is produced and exerted on the fluid particle due to a pressure term which is an internal force acting on the domain particle. Note that this force is symmetric.

2.9.1.1 Switch between Active to Crespo Particles

As mentioned, Crespo particles are Dirichlet particles with either prescribed displacement or velocity. Note that some of Crespo particles in the adjacency list of active particles contribute in density calculation. The switch between the Crespo and Active particles is based on the particle temperature. A user defines a switching temperature which is slightly below the solidus temperature of the alloy. Note that inactive particles set are reserved or ghost particles that do not physically exist. They are simply used to allocate memory and $F = ma$ added to the domain in the form of either Crespo or active through periodic inlet and inlet.

2.9.2 Repulsive Boundary Particles

This method was proposed by Monaghan [4] and is similar to the force due to a inter-molecular Lennard-Jones potential. Monaghan used ghost or virtual particles located right on the solid boundary to produce such a high repulsive force to the fluid particles near the boundary to prevent fluid particles crossing the boundary. The force acting on the domain particle by this boundary particle is considered an external force in the current SPH code.

If $\mathbf{r}_{ab}$ is defined as the distance between particle a and boundary particle b the force per unit mass has the following form:

$$F(\mathbf{r}_{ab}) = F_0 \left[\left(\frac{\Delta x}{|\mathbf{r}_{ab}|} \right)^4 - \left(\frac{\Delta x}{|\mathbf{r}_{ab}|} \right)^2 \right] \frac{\mathbf{r}_{ab}}{|\mathbf{r}_{ab}|^2} \quad (2.48)$$

where Δx is the initial particle spacing.

Note that these particles are just virtual particles and do not satisfy the momentum equation. They are used just to compute the distance of approaching fluid particles to the virtual boundary particles. The equation shows that the force value depends only

on the relative distance and only particles are affected that have their relative distance less than spacing. This force is added to the momentum equation for those particle that experience this force. This boundary type works well when a slip boundary condition is required to simulate the condition where $\mathbf{v} \cdot \mathbf{n} = 0$ on the boundary.

Figure 2.5: Boundary Treatment, left: Crespo's dynamic boundary particle [3]; right: Monaghan's repulsive boundary particle [4]

2.9.3 Inlet-Outlet

When inactive particles are inserted into the inlet with a prescribed velocity and temperature (or enthalpy) they exert force on active particles. The force is the same as the force between active particles. The force type is identical to the one described by Crespo. The force from the inlet particle acting on the domain particle is treated as an internal force.

Figure 2.6: Inlet implementation, a: before activation; b: immediately after activation.

Figure 2.7: Some examples of enthalpy-temperature curves [5].

2.10 Phase Change Problems

There are few analytical methods to solve phase change problems. The most well known method is a 1D phase change problem in semi-infinite domain solved by Stefan where he used constant thermodynamical properties in liquid and solid phases. In the context of numerical methods, there are several approaches to deal with the heat transfer problems with a phase change involved. Hu [26] reviews some of these methods such as fixed grid method, variable grid methods, latent heat evolution method, apparent heat capacity method, effective capacity method, heat integration method, source based method and enthalpy method.

Adopted by many researchers, the enthalpy method is used in the present work in which the latent heat is considered by the enthalpy and enthalpy-temperature relation. This method is discussed by Voller [5]. Fig. 2.7 shows three different enthalpy-temperature curve. Curve A shows the isothermal solidification of a pure material or an alloy of eutectic composition. Curve B shows the evolution of latent heat over a range, T_s and T_l and curve C represents the nonlinear evolution of latent heat over the solidification range $T_s - T_l$.

Figure 2.8: Enthalpy as function temperature for 16Mn Cr5 Steel [6].

2.10.1 Enthalpy-Temperature Relationship

The general expression of the temperature dependency of the enthalpy of a material may be expressed as

$$H(T) = \int_{T_{Ref}}^{T_l} C_{ps}(T) dT + f_l(T)L_l + \int_{T_l}^{T_v} C_{pl}(T) dT + f_v(T)L_v \quad (2.49)$$

In the above equation given in [27] two phase changes, from solid to liquid and from liquid to vapor are involved. Fraction liquid and fraction vapor are assumed to vary linearly from solidus temperature to liquidus temperature and liquidus temperature to vapor temperature. The liquid and vapor fraction are given by $f_l(T) = \frac{T-T_l}{T_l-T_s}$ and $f_v(T) = \frac{T-T_v}{T_l-T_v}$. Fig. 2.8 shows the obtained enthalpy-temperature relation for 16Mn Cr5 Steel by integrating the measured specific heat. There has been 3 % uncertainty in specific heat for $T \leq 1200$ and larger uncertainties for $T \geq 1200$ [6] due to the fact that there is less confidence in the data for elevated temperatures. More discussion on the affect of uncertainties in thermo-physical data on the validation procedure of a computerized weld model is available in [6].

Table 2.2: Parameters required to make enthalpy-temperature function.

Name	Symbol	Units	16MnCr5 Steel [6]	Steel 304 [28]
Solidus temperature	T_s	$^{\circ}K$	1750	1697
Liquids temperature	T_l	$^{\circ}K$	1800	1727
Vaporization temperature	T_v	$^{\circ}K$	2500	—
Enthalpy solid	H_s	J/kg	1.0×10^6	1.20×10^6
Enthalpy liquid	H_l	J/kg	1.4×10^6	1.26×10^6
Enthalpy vapor	H_v	J/kg	2×10^6	—
Specific heat solid	C_{ps}	$J/kg^{\circ}K$	655.17	711.8
Specific heat liquid	C_{pl}	$J/kg^{\circ}K$	1100	837.4

2.10.2 Simplified Enthalpy Method

Keeping the sources of uncertainties in mind, assume that there is only solid into liquid phase transformation, thus we only need to consider the first three terms in Eq. 2.49. For most welding simulations one may only need to consider the solid into liquid phase change. Having Eq. 2.49 and the experimental data displayed in Fig. 2.8, we may consider another level of simplification which is the assumption of constant specific heats for each solid and liquid phases.

Fig 2.8 confirms that a piecewise linear function can be considered to establish the enthalpy and temperature relation for steel. With this simplification the enthalpy-temperature relation can be described by the few parameters listed in Table 2.2.

We make the following piecewise functions for the solid, mushy and liquid regions:

$$H(T) = \begin{cases} C_{ps}(T - T_s) + H_s & \longrightarrow T_{ref} \leq T < T_s \\ H_s + f_l(T) L_l & \longrightarrow T_s \leq T < T_l \\ C_{pl}(T - T_l) + H_l & \longrightarrow T_l \leq T \leq T_v \end{cases}$$

In the above function, $L_l = H_l - H_s$ is the latent heat of melting, $C_{ps} = \frac{H_s - H_{ref}}{T_s - T_{ref}}$ is the constant heat capacity of the solid phase, $C_{pl} = \frac{H_v - H_l}{T_v - T_l}$ is the constant heat

capacity of the liquid phase and the fraction liquid is given by [29].

$$f_l = \begin{cases} 0 & \longrightarrow T_{ref} \leq T < T_s \\ \frac{T-T_s}{T_l-T_s} & \longrightarrow T_s \leq T < T_l \\ 1 & \longrightarrow T_l \leq T \leq T_v \end{cases}$$

2.10.3 Solve the Energy Equation in Terms of Enthalpy and Phase Fraction

To deal with the effects of latent heat during the phase change, the SPH form of the energy equation is solved in terms of temperature. To proceed to the next time step a correction is done to the temperature based on the enthalpy-temperature relation (See. Fig. 2.8)

For each time step

1. Compute the temperature increment dT using Eq 2.46.
2. Compute the enthalpy change per unit mass by $dH = c_p dT$.
3. At the end of the time step compute the enthalpy per unit mass by $H_3 = H_1 + dH$.
4. Compute the corrected temperature based on the enthalpy-temperature relationship.

2.11 SPH Weld Pool Simulation

The welding torch moves wrt to the welded structure. However, the weld pool usually reaches quasi-steady state in about 3 weld lengths. For this reason, it is useful to view the weld pool as a spatial or Eulerian sub-domain moving through a Lagrangian welded structure. This Eulerian sub-domain has inlet and outlet BCs and possibly Dirichlet or Neumann BCs on side boundaries that are mapped from the Lagrangian

welded structure. However, the SPH model in this Eulerian sub-domain is Lagrangian. Therefore this SPH Lagrangian formulation is contained in a spatial or Eulerian sub-domain that moves through a weld structure formulated as a Lagrangian or material formulation.

The following sections describes steps in modeling the SPH weld pool as well as several applications of the SPH weld pool model namely, 2D SPH weld joint, 2D and 3D Eulerian weld pool model in which welding torch is fixed and the part is moving and a Lagrangian weld pool in which torch is moving along a weld joint path. Experimental studies of the filler metal added to the weld pool are reviewed first. This is required for the present SPH weld pool model in which filler metal is added to the molten puddle periodically through a droplet with a specified size, periodicity and velocity.

2.11.1 Droplet Formation and Detachment in GMAW

Mass flow from a consumable electrode is an essential feature of most arc welding processes. How the metal is transferred to the weld pool, has been the subject of research [30]. Droplet formation is governed by a combination of several factors such as the balance of forces on the droplet, heat transfer from resistive heating of the wire and the plasma to the droplet, and current density distribution in the molten droplet [14].

In order to model the droplet formation and detachment, a unified model which includes the electrode, the plasma in the arc region, the liquid pool and the solid work piece is needed. This requires a mathematical model in which conservation of mass, energy and momentum along with Maxwell equations for the solid, liquid and the plasma regions are solved simultaneously to obtain temperature, position, velocity, acceleration, pressure, magnetic field and the current density. The most well known of such models has been done by Haidar and Lowke [14], Fan [31] and Lowke [32]

Consider a GMAW welding process. In such a process, the electrode plays the role of the electrode and consumable wire at the same time. The wire electrode is heated mainly by two sources, volumetric resistive heating and the heat flux from the plasma at the tip of the electrode. After the electrode tip melts and a droplet forms, several forces result in the droplet's detachment. These forces are thought to include the electro-magnetic pinch effect, surface tension, gravity, and drag force from the shielding gas.

The transfer mode is another feature in GMAW. Depending on the welding parameters, the droplets can flow to the weld pool with different sizes, shapes and rates [30]. For instance in GMAW welding there is a transition current where below the transition current, large droplets are formed and detached by gravity which is known as a *globular* mode. Above that transition current, smaller droplets form and flow towards the weld pool in a *projected*, *spray* or *streaming* mode. This behavior has been studied experimentally [8, 9, 33, 34] and using mathematical models [32, 35].

Figure 2.9: Schematic of droplet transfer modes. Left: streaming mode; Right: globular mode.

2.11.2 Effect of Shielding Gas

During GMAW using argon shielding gas, small droplets are formed due to the tapered electrode tip at a current above 230 A. For carbon dioxide and helium, larger droplets

are formed due to the absence of the taper [7]. Fig. 2.10 shows the droplet size with three different shielding gases. So addition of carbon dioxide and helium can suppress the taper formation and the weld process can be easily controlled.

Figure 2.10: Effect of type of shielding gas on the droplet size for GMAW [7].

2.12 Experimental Data for the Liquid Droplet

2.12.1 Introduction

In the current development stage of the SPH model, assume that there is no plasma region and a droplet has already formed with a certain size falling into the weld pool with a certain feed rate and velocity. Therefore, droplet formation rate, droplet size, droplet temperature and initial velocity are the essential input parameters for the current SPH weld pool model. Droplets are also accelerated when they detach from the electrode [30]. However only an initial velocity is considered for the droplet after detachment and the acceleration is only due to gravity.

Figure 2.11: Schematic of droplets falling to the weld pool in GMAW welding.

2.12.2 The Droplet Temperature

According to [30], experimental studies indicate that above 200 A the surface temperature of the droplet is at the boiling temperature of steel and the average temperature is between 2000°C and 2700°C . More accurate temperature measurements have shown that the average temperature of 2400° varies slightly with the current in the range of 100-200 A.

2.12.3 The Droplet Size

Given in [8,9], the droplet size as a function of welding current for GMAW using a 1.6 mm mild steel wire diameter is shown in Fig. 2.12

Figure 2.12: Droplet size as function current [8,9].

2.12.4 Effect of the Wire Diameter on the Droplet Size

Soderstorm and Mendez [10] conducted experimental studies on the effects of welding current and binary $Ar - CO_2$ shielding gas mixture on the average droplet diameter detached from the electrode tip in the GMAW process. They used electrodes with 0.41, 0.89, 0.59, and 1.59 mm diameters in their research. Their results confirm the general trend for the variation of the droplet size vs current. However the transition current from globular to spray mode depends on the wire diameter.

Fig. 2.13 the average droplet size as a function of current and wire diameter in 90 $Ar - 10\% CO_2$ shielding gas mixture. Experiments suggest that as the wire diameter decreases, the transition current drops as well. Also for smaller wire diameter, the minimum droplet size is slightly bigger than wire diameter in the spray mode.

2.12.5 The Droplet Initial Velocity

The experimental data presented in references [30] can be used for the initial velocity for a steel electrode.

Figure 2.13: Droplet size as function current [10].

2.12.6 The Droplet Frequency

Experimental data provides the droplet feed rate into the weld pool as a function of current, polarity and wire diameter. Fig. 2.14 gives such data from [8,9] that can be parametrized to specify a droplet frequency.

Figure 2.14: Droplet frequency as function current [8,9].

Another possibility is to calculate the droplet frequency f_d , (1/s) based on the droplet size, d_d (mm) and wire speed v_e (mm/s) and wire diameter d_e (mm). The

wire speed is a parameter that is sometimes easy to measure. The mass balance suggests that $\pi \frac{d_d^3}{6} \times f_d = v_e \pi \frac{d_e^2}{4}$ and

$$f_d = 1.5 v_e \frac{d_e^2}{d_d^3}. \quad (2.50)$$

In the above equation, d_e and v_e are usually given in the weld procedure data sheet and d_d is approximated using data provided in Figs. 2.12 and 2.13.

2.12.7 Heat Source

Several methods that can be considered for this purpose are outlined below.

2.12.7.1 All Input Power Embedded in Droplets

The simplest way to account for the power delivered to the weld pool is to assign the total weld input power to the droplet. This can be done simply by assigning a high fictitious temperature to the droplet. This method was only used for preliminary development tests. Note that it may be physically non-sense but energy is conserved.

The power delivery is continuous and each droplet must accumulate the input power during the delay time until the next droplet appears. This increase in temperature can be calculated using

$$Q = \eta P \Delta t = \eta V I \tau_d = m_d c_p (T_d - T_0) \quad (2.51)$$

where m_d is the droplet mass (particle mass $\times$ number of particles in a droplet), P or VI is the input power, the heat source efficiency is η , c_p is the heat capacity and $\tau_d = 1/f_d$ is the period between droplet detachments. The droplet temperature is

then computed as

$$T_d = \frac{\eta V I \tau_d}{m_d c_p} + T_0. \quad (2.52)$$

As an example assume that there are 250 SPH particles in a droplet. With a particle spacing of 0.00025 m and with a droplet density of 7800 kg/m^3 , the mass of this liquid droplet is computed to be $3.047 \times 10^{-5} \text{ kg}$. If the specific heat is 600 J/kgK and the droplet period is 0.04 s, then a power input of 7500 W with the efficiency of 0.7 will raise the temperature of the droplet from 300 K to 10000 K during this period. This is not realistic but it would apply the correct total power to the weld pool. If a fraction of the total power was applied to the weld pool by the arc, the energy in the droplet should be reduced to more realistic levels.

2.12.7.2 Surface Thermal Flux with Gaussian Distribution

A heat flux BC from the arc acts on the molten pool surface. In this case the droplet temperature would be 300 to 500 K above the melting temperature of the alloy. Typically, the input power is considered to have a Gaussian distribution over the weld pool surface. A general function can be considered for the thermal flux as:

$$q(x, y) = \frac{P}{\pi \sigma_0^2} \exp\left(\frac{-(x^2 + y^2)}{2\sigma_0^2}\right) \quad (2.53)$$

where P is the input power, σ_0 is the measure of the width of flux distribution.

2.13 Simulation Results

2.13.1 Demonstration Example 1: 2D SPH Weld Joint Model

The first application of the SPH weld pool model described in this section enables a general user to set up a SPH weld joint analysis. Usually, the geometry of any welded structure can be read from almost all CAD software as an *STL* file. A cut-plane on any cross section of the weld joint is chosen. The cut-plane is normal to the weld path. An example of a welded structure and a cut-plane is shown in Fig. 2.15.

By picking a point (see point O in Fig. 2.16) on the cut plane, one can orient a 2D bounding box in the cut-plane. The axes of the bounding box are oriented by two more points, P_1 and P_2 , in addition to the origin O . The intersection of the STL surfaces with the cut-plane and bounding box in the cut-plane forms a 2D square mesh of the parts and the complement of the parts.

The weld procedure data are introduced in the next step. The data are used to define input power and welding velocity and also position, velocity, size and frequency of the periodic droplet for each weld pass. If a weld pass has multiple electrodes, then more than one droplet is required. The last step is to solve the SPH 2D weld pool problem to add filler metal for each weld pass in this weld joint on this weld joint cross-section.

A 2D square mesh of the cut-plane loops and their complement is shown in 2.17. An example of weld procedure data is shown in Table 2.3. Each droplet represents the tip an electrode and it has its own part number and a unique weld procedure is assigned to it. This suggests that if a user has 3 electrodes or droplets, 3 weld procedure should be created and each individual electrode or droplet could have its own weld procedure and SPH parameters. In Fig. 2.16 one droplet is defined. Therefore one weld procedure is linked to this droplet or electrode.

SPH solver parameters are shown in Table 2.4. Some of them, such as input power,

Figure 2.17: A 2D square mesh of the weld joint, its complement and a droplet to model the filler metal to be added from the wire electrode.

Figure 2.18: Snapshot of the temperature during the single pass weld.

Table 2.3: Example of main welding parameters in a weld procedure.

Welding Process	example: GMAW, GTAW, Sub-Arc, Laser, EB
Type	example: AC Square wave single electrode, pulsed
Shielding gas	example: Ar, Co2, He, Ar-He
Current, I (A)	400
Voltage, V (Volt)	32
Weld speed, v_w (mm/s)	8.5
Wire diameter, d_d (mm)	3.2
Wire speed, v_d (mm/s)	45
Base metal	X70 steel
Filler metal	S3 NiCrMo2.5

can be read directly from a weld procedure and some of them, such as droplet size, should be set properly using experimental data. An example of the solution results of

Table 2.4: Parameters used for SPH simulation.

Current, I (A)	400
Voltage, V (Volt)	28
Weld speed, v_w (mm/s)	22.4
Arc power, P_{Arc} (W)	11200
Arc flux diameter, d_{arc} (mm)	0.005
Arc Pressure, P_{Arc} (Pa)	2000
Arc pressure diameter, d_{ArcP} (mm)	0.003
Droplet diameter, d_d (mm)	3.5
Droplet period, τ_d (s)	100
Droplet temperature, T_d (K)	2100
Droplet initial velocity, v_d (mm/s)	100
Electrode inclination angle, α (degree)	0
Base metal	X70 steel
Filler metal	S3 NiCrMo2.5

the SPH weld pool model which adds filler metal for each weld pass in the weld joint is shown in Fig. 2.18.

2.13.2 Demonstration Example 2: 2D SPH Weld Joint Model with Multi-pass Welds

Multi-pass welds on a weld joint can be simulated by defining more electrodes. Fig. 2.19 shows such a set up with three electrodes, E_1 , E_2 , and E_3 . Each droplet represents

one weld pass with one electrode and has a particular weld procedure, i.e., input power and filler metal material. Each electrode would operate in any time interval by defining the start and end time with a defined weld procedure. Fig. 2.20 shows an snapshot of a weld simulated with three passes.

Figure 2.19: 2D SPH weld joint with 3 electrodes.

Figure 2.20: 2D SPH weld model with multi-pass welds.

2.13.3 Demonstration Example 3: 2D and 3D Eulerian Weld Pool Models

An Eulerian treatment of the weld pool makes it easier to capture the weld pool behavior with the filler metal added in different ways. The first is that the domain does not need to be too long which makes the model computationally efficient. In addition, simulations with smaller particle spacing size would be feasible. In the Eulerian setup, the welded part moves with the weld speed and the arc/electrode are stationary.

Figure 2.21: 2D SPH simulation of a GMAW weld process.

Note that the SPH formulation is purely Lagrangian since we are solving the fields on the moving particle, not on the fixed grid points for the moving particles. The steps are similar in a SPH 2D weld joint with a moving arc except it needs to define inlets and outlets for the particles moving in and out of the domain. The part is defined as a Crespo BC that moves with the welding velocity (see Sec. 2.9.1 for the Crespo BC particles). Fig. 2.21 illustrates such a set up showing all SPH parameters.

2.13.4 2D Eulerian Weld Pool Tests

In the following 2D tests the effects of particle spacing is investigated. The domain size is kept unchanged. Note that for the coarser particles spacing the droplet can not be resolved as well. Part thickness is 12 mm, weld speed is 0.05 m/s .

Figure 2.22: 2D SPH Eulerian weld pool. Obtained temperature fields for 4 levels of SPH particle refinement.

In the first test, coupled SPH NS and SPH Energy solvers were used. No surface heat flux is added to the surface and it assumed that all input power is embedded

in the hot droplets. For all tests, the periodic droplet initial temperature is almost identical. Particle spacings of 0.8, 0.4, 0.2, and 0.1 mm are used. Fig. 2.22 shows the results of the temperature field. As long as there is no concerns about the temperature field close to the weld pool, the temperature field in the down stream are identical suggesting that coarser particle spacing can be used for that region. As is seen, the weld pool length is a bit longer for the top two cases. The reason is that the droplets created by the mesher have a higher mass which means that droplets carry more enthalpy (see Table 2.5). If the droplet enthalpy is adjusted according to the droplet mass such that each droplet carries identical total enthalpy, the temperature field must be almost identical for the down stream region.

Note that the purpose of running coarse spacing analysis is not to study the weld pool dynamics. Obviously coarse spacing can not resolve fluid flow in the weld pool. The purpose of running coarse and fine particle spacing is to show the possibility of using two scale or multi-scale analysis. For example it is not necessary to use fine mesh in those regions far from the weld pool. Temperature results of the coarse analysis can provide boundary conditions for the fine domain (weld pool+ few layers around the weld pool). A fine mesh will handle the heat and fluid flow in the weld pool.

2.13.5 3D Eulerian Weld Pool Tests

In a similar way considered in 2D simulations, domain size is kept unchanged for a 3D simulation. The temperature distribution for the fully developed weld pool is shown in Fig. 2.23. One of the interesting features of the simulation is the number of active particles in every full time steps. The total number of active particles can be a measure of the weld pool mass. Also the time that is required for the weld pool to reach to a quasi-steady state condition can be determined. Fig. 2.24 shows the number of active particles as a function of time. As an example in the plot, time 1.0 s can be considered as a time that the weld pool is fully developed. The initial ramp up

Table 2.5: 2D SPH weld pool in which SPH Energy solver is used instead of FEM solver-Timing profile.

Particle spacing, mm	0.1	0.2	0.4	0.8
Dimension, mm	$50 \times 12 \times 0.1$	$50 \times 12 \times 0.2$	$50 \times 12 \times 0.2$	$50 \times 12 \times 0.2$
Weld Speed, mm/s	50	50	50	50
Power Input, W	0	0	0	0
Droplet radius, mm	0.8	0.8	0.8	0.8
Droplet period, s	0.04	0.04	0.04	0.04
Droplet Temperature, K	5000	5000	5000	5000
Physical time, s	1.0	1.0	1.0	1.0
NbActive Particle	3982	806	412	102
NbNbInactive Particle	41585	5244	2578	697
NbInlet Particle	120	60	30	15
NbOutlet Particle	179	85	44	22
NbPeriodic Particle	208	48	16	4
NbCrespo Particle	60558	15225	3667	919
Droplet mass, kg	0.016	0.151	0.0201	0.021
CPU Time, s	17286	8211	1947 (C ver)	2330 (C ver)
Number of sub steps	2000000	1000000	500000	250000
Time step size, s	5.0e-07	1e-06	2e-06	4e-06

shows the transient part of the solution until the weld pool is fully developed. The initial condition is 300 K before welding starts. This means the particles are Crespo type. As Crespo particles get energy from the arc, their temperature goes up and they change to active particles when their temperature exceeds the transition temperature.

Low frequency modes account for the fluctuation of the weld pool volume and high frequency modes are due to the filler metal droplets splashing into the weld pool which are of the order of droplet frequency. Table. 2.6 shows the timing profile for this test.

2.14 Summary

In computational welding mechanics, prediction of the weld pool geometry, composition and temperature evolution in a welded part is an essential step toward predicting microstructure evolution in the weld fusion and heat-affected zones. Older models

Figure 2.23: 3D Eulerian SPH weld pool. Particle spacing 0.2 mm.

Figure 2.24: Number of active particles as a function time for the simulation test in Fig. 2.23.

Table 2.6: 3D SPH weld pool-Timing profile.

Spacing, mm	0.2
Dimension, mm	$5 \times 20 \times 30$
Weld Speed, mm/s	20
Power Input, W	5000
Droplet radius, mm	0.8
Droplet period, s	0.04
Droplet Temperature, K	2000
Physical time, s	1.5
NbActive Particle	7459
NbNbInactive Particle	369842
NbInlet Particle	2500
NbOutlet Particle	5000
NbPeriodic Particle	268
NbCrespo Particle	370199
CPU Time, s	37915
Number of sub steps	1200000
Time step size, s	1.25e-06

to predict the weld pool sometimes have some limitations. As an example large deformation and mixing in the weld pool may be ignored. A Smoothed Particle Hydrodynamic (SPH) weld pool model was implemented to solve the coupled Navier-Stokes and energy equations in the weld pool. SPH technique can easily manage large deformation, free surface flow, mixing and dilution in a weld pool. By adding more physics, it has the potential to predict realistic weld pool geometry and composition distribution in the fusion zone as a function of weld process parameters. Since the thermal cycle and concentration of alloying components at any spatial point of the fusion zone are required inputs to a microstructure model in a weld fusion zone, these are important.

The SPH Solver development procedure including mathematical and numerical modeling, verification tests (Appendix A) were discussed. In the end, several application of the new weld pool model were demonstrated to show its capabilities. It is believed that the model can be improved by adding additional physics such as surface

tension, Marangoni effect and the magneto-hydrodynamics of the arc.

Computational efficiency can be improved by adopting implicit solvers for the SPH weld pool model. Note that explicit time integration is used for the current model. The time step size in the order of a micro second is restricted by stability. Adopting an implicit solver requires building a global stiffness matrix in each time step that could take time but a much larger time step size that is limited by accuracy, not stability, can be used that can improve the overall computational efficiency.

Chapter 3

Heat-Affected Zone (HAZ)

Microstructure

3.1 Introduction

Microstructure controls most of the important properties of a weld such as strength, hardness and toughness. It is a function of composition and the thermo-mechanical processing history. The capability to predict microstructure in a thermo-mechanical process would be helpful to predict residual stresses and failure mechanisms such as fatigue and resistance to creep and corrosion. In this chapter, an algorithm for computing a synthetic microstructure at any point in the HAZ of a weld in a low-alloy steel is described first. In the second part a model which describes the dissolution and homogenization of austenite-ferrite in a low-alloy steel weld is discussed. The model utilizes a synthetic microstructure and finally, the macro-micro heat affected zone microstructure framework is demonstrated which makes it possible to relate the welding parameters to the microstructure and mechanical properties of a point in a weld HAZ.

3.2 Overview

The microstructure of welds is usually studied experimentally using optical microscopes and various types of electron or atomic probes. Studies of texture and polycrystalline plasticity have representations of microstructures that include individual crystals or grains. Ashby and Easterling [36] developed a simple kinetic model for grain growth integrated over thermal cycle. The thermal cycle was taken from the Rosenthal [37] analytical solution for temperature field produced by a moving point source in thin and thick plates. They assembled and correlated data from simulated and real welds and established diagrams relating welding process parameters (in terms of cooling time from 800 to 500 and peak temperature) to the measured data needed for their model for grain growth, carbide dissolution and martensite formation in several steels.

Ion and Easterling [38] improved the earlier work by Ashby and Easterling and modified the kinetic model of the grain growth to predict the microstructure and hardness. They produced diagrams which explicitly related the heat input from the weld to the grain size and hardness of the HAZ. In the work by Kirkaldy and Venugoplan [39], the evolution of microstructure of low-alloy steels in a Jominy test was simulated. Their goal was to predict the hardenability of low-alloy steels as a function of composition and initial austenite grain size. They used integral equations specialized to the cooling curves in a Jominy test as a function of distance from the chilled end of the Jominy test bar. They computed a density function of phase fractions, i.e., at each point they computed the fraction of each phase.

Watt et al [40] [11] changed Kirkaldy's integral formulation that was limited to a Jominy test specimen to an ordinary differential equation (ODE) formulation that computed the phase fraction as a function of time for a given low-alloy steel composition and initial austenite grain size, for an arbitrary thermal cycle, e.g., the thermal cycle for a point in a weld joint. Their model could take a thermal cycle

from the 3D transient FEM heat transfer model of a weld given in [41] to predict the microstructure evolution of the welds. They added the capability to deal with austenite grain growth developed by Ashby and Easterling, [36], including the effect of the dissolution of precipitates such as vanadium, niobium and titanium carbo-nitrides on the grain growth of austenite. With this computer model the evolution of phase fractions at any point in the HAZ of a low-alloy steel weld could be tracked in time.

However, unlike the work that will be presented in this chapter in which PDEs are solved with a synthetic structure, Kirkaldy and Watt et al solved an ODE at any point in a homogeneous material. They did not resolve each grain in each phase or track the evolution of each crystal grain. Also they did not deal with solute diffusion at the micro-scale and heterogeneous materials. The effect of stress and strain was ignored.

3.3 Approaches to Model Phase Transformation

There are three approaches to model phase transformation in steels. First is a density function method in which a phase transformation at any spatial point is describe by an ODE which is a function of temperature and composition history. This approach has been used in microstructure evolution models by Kirkaldy [39], Watt et.al [40] and Rappaz [42]. There is no notion of a cell or interface in this method and the material is homogeneous.

The phase field method with the sharp interface assumption is a second approach. The main assumption is that the thickness of an interface is much smaller than the size of a domain. The order parameter is not continuous at the interface. Conservation equations are solved in each phase and the phase boundaries are tracked by enforcing a constraint condition at the interface. As an example the Gibbs-Thomson equation can be used to related the interface velocity to the amount of undercooling at the

interface. Such an approach has been modeled numerically Artemev [43].

Phase field with diffuse interface assumption is the third approach which can be derived from the thermodynamics of phase transitions. The phase evolution can be obtained by solving a PDE for the order parameter. The order parameter has a continuous variation across the interface. This method usually needs a cell size of the order of nanometer which might be not feasible to model industrial problems. Solidification with 3D dendrite evolution was simulated by Kobayashi [44]. This method has been also implemented in software tools such as Micress and Thermo-Calc.

3.4 Microstructure Evolution in a Weld HAZ

A typical thermal cycle of a point in a weld HAZ and an iron-carbon phase diagram is shown in Fig. 3.1. When the temperature crosses the eutectoid temperature of 723 C, pearlite transforms to austenite. The diffusion time for carbon to diffuse a distance equal to the pearlite lamellae spacing makes the transformation time for the pearlite to austenite transformation so short that we treat it as instantaneous. The grain boundaries of these austenite grains are in thermal equilibrium with the ferrite grains at the eutectoid temperature. As the temperature rises, the ferrite-austenite grain boundary composition quickly comes to equilibrium defined by the tie-line of the Fe-C binary diagram (see Fig. 3.2). This causes a phase transformation in which austenite grains grow at the expense of the ferrite grains. The kinetics of the ferrite to austenite phase transformation is controlled by the diffusion of carbon. The carbon composition of the austenite and ferrite phases in the grain boundary are in local equilibrium for the current temperature. The centers of the austenite grains can have carbon compositions higher than equilibrium on heating.

If the peak temperature for this point is less than the equilibrium temperature, A_3 , then on cooling, the ferrite grains grow and carbon concentration of the austenite

Figure 3.1: Fe-C phase diagram and thermal cycle for a point in the HAZ of a weld joint with peak temperature 950 C [11].

grain boundary increases as the austenite grains shrink. This permits austenite grains to have higher carbon concentration near the grain boundary and their core to have a lower carbon concentration. When the temperature drops below the eutectoid temperature of 720 C, growth of the ferrite grains stop. Then the transformation of austenite to pearlite, bainite and martensite begins. The algorithm for modeling these transformations is described in [40] and [11]. Note that the ferrite grains do not change as they cool below the eutectoid temperature because they are at equilibrium.

Watt et al [40] compute various temperatures and line segments that describe a pseudo-binary $Fe - C$ phase diagram for the low alloy steel composition. Note that this is a pseudo-binary diagram that considers only equilibrium phase fractions as functions of temperature and the C composition but the binary diagram is adjusted in an attempt to capture the effect of alloying elements Ni, Si, V, Mo, W, Mn, Cr, Cu, P, AL, As, Ti on the binary equilibrium diagram, e.g., the eutectoid temperature and composition is a function of all of the alloying components present in the above list. In effect, this is a para or quasi-equilibrium $Fe - C$ diagram for a given and frozen composition of Ni, Si, V, Mo, W, Mn, Cr, Cu, P, AL, As, Ti, i.e., it assumes that diffusion of the substitutional alloying elements during weld thermal cycles can be

Figure 3.2: Illustration of phase transformations in a low alloy steel during the heating cycle.

ignored because the solute diffusivities are low and the times are short.

3.5 Transient Thermal Cycle

A thermal cycle driving the evolution of the microstructure (Fig. 3.3) is usually obtained by picking a point in macro FEM transient thermal analysis of a weld joint in a welded structure or trusted thermocouple data. One could also import the temperature gradient as a linear polynomial or a higher order polynomials of transient spatial temperature distribution if one desired to include temperature gradients at the micro-scale.

Figure 3.3: An example of a thermal cycle for a point in the HAZ of a weld (Temperatures in Kelvin).

3.5.1 Conservation of Energy or Heat Equation

With enthalpy per unit volume h , thermal flux q and a power density function Q_v , temperature T , temperature gradient ∇T , thermal conductivity tensor κ , specific heat

c_p , the heat equation can be written in the following form:

$$\begin{aligned}\dot{h} + \nabla \cdot \mathbf{q} + Q_v &= 0 \\ q &= -\kappa \nabla T \\ dh &= \rho c_p dT.\end{aligned}$$

This partial differential equation is solved on a domain defined by an FEM mesh with appropriate boundary and initial condition. In the macro-model the domain is usually dynamic in that it changes with each time step as filler metal is added to the weld pass. In the micro-model the domain is fixed in time except for deformation due to thermal stresses. The default initial condition is assumed to be a constant temperature of 300 K. The material properties κ and c_p are usually temperature and microstructure dependent, i.e., the material properties of ferrite and austenite have different values even at the same temperature. The heating effect of the arc is often modelled by a double ellipsoid power density distribution that approximates the weld pool as measured from macro-graphs of the cross-subsection of several weld passes. A convection boundary condition $q = h_0(T - T_{amb})$ is applied to external surfaces where h_0 is the convection coefficient. The FEM formulation of the heat equations leads to a set of ordinary differential equations that are integrated in time using a backward Euler integration scheme. More details on the methodology for computing transient temperature fields in macro-models of welds can be found in [1]. Essentially the same algorithm is used in the micro-model but the length and time scales are shorter.

3.6 Transient Solute Diffusion

Many phase changes, such as the ferrite-austenite phase change, are controlled by the diffusion of carbon. For example, when a pearlite grain is heated above the eutectoid

temperature, it will transform to austenite in a few seconds. This is because the relevant diffusion length is the spacing of the lamellae in the pearlite. As this austenite grain is heated to higher temperatures, the carbon composition of the austenite in contact with ferrite will quickly come to local equilibrium with the composition of equilibrium ferrite-austenite at that temperature. Carbon will flow from the austenite into the ferrite. As it does, the austenite grain will grow limited by the kinetics of carbon diffusion and equilibrium.

The evolution is driven by solute diffusion of the interstitials such as carbon. The solute diffusion in each phase uses the temperature dependent solute diffusivity, $D(T)$, of that phase. The solute diffusion is solved as a transient FEM solution of the conservation of mass for each solute.

$$\frac{\partial C}{\partial t} = \nabla \cdot (D(T)\nabla C) \quad (3.1)$$

3.6.1 Conservation of Momentum Equation

Given the density, ρ , the tensor $\mathbf{D}$ as a 6×6 matrix that maps the strain tensor to stress tensor σ as a 6×1 vector, the body force $\mathbf{b}$ and the Green-Lagrange strain ε , the conservation of momentum equation is solved that can be written in the following form in which inertial forces, $\rho \ddot{\mathbf{x}}$ are ignored.

$$\begin{aligned} \nabla \cdot \sigma + \mathbf{b} &= 0 \\ \sigma &= D\varepsilon \\ \varepsilon &= (\nabla \mathbf{u} + (\nabla \mathbf{u})^T + (\nabla \mathbf{u})^T \nabla \mathbf{u})/2 \end{aligned}$$

This partial differential equation with appropriate boundary and initial condition is

solved for a visco-thermo-elasto-plastic stress-strain relationship using theory and algorithms developed by J.C. Simo and his colleagues [45]. More detailed discussion of the thermal stress analysis of welds can be found in [1] and [46]. The initial state is usually assumed to be stress free. However, if the initial stress state was known, it could be initialized. The Dirichlet boundary conditions constrain the rigid body modes. In the macro-model the system of equations is solved using a time marching scheme with time step lengths of approximately 1 second during welding and usually an exponentially increasing time step length begins when welding stops and the structure cools to ambient temperature. In the micro-model, much shorter time steps are used when they are needed to resolve the phenomena of interest.

3.7 Synthetic Microstructure in the Heat-Affected Zone of Low-alloy Steel Welds

3.7.1 What we gain from synthetic microstructure model?

The most significant outcome of the synthetic microstructure model is that a microstructure model with individual grains simulates real microstructures and can be correlated with the real microstructure data. This is in sharp contrast with the Kirkaldy-Watt algorithm that assumes a homogeneous composition and could only be corrected with average phase fractions. Each grain in a synthetic microstructure can have its phase type/microstructure and its own composition. Synthetic microstructure can be correlated to an observed microstructure directly. This means that each grain can transform in a thermal cycle according to its composition and phase type.

The grains need not be equi-axed. In high strength low-alloy steels, the grains are often pancake shaped, i.e., thin disks possibly elliptical in shape. Also, the microstructure could have texture. Each grain could have a crystal lattice orientation.

Other solvers such as stress solver can use a synthetic microstructure model. For example austenite-ferrite transformation model can use a synthetic microstructure model. (This will be discussed in detail in the next part of this chapter.) Also stress analysis can use this microstructure for mechanical and thermal properties. (This will be discussed in the HAZ microstructure framework where synthetic microstructure is used throughout the frame work.)

3.8 Implementation

One specifies a cubic mesh grid, i.e., $m \times n \times l$ element domain with a cell size of δ . One also specifies the number of grains or crystals in each phase that one wants in this microstructure. Then the algorithms generates (i,j,k) indices for the number of grains specified with one seed for each grain specified. Each value of i, j and k for each seed is obtained from a random number generator multiplied by the number of cells in that direction. Then it grows layers around each seed to get the cells closest to each seed. This makes each grain. Fig. 3.4 (upper left) illustrates generated grains in different color.

Also the number grains of each phase type, e.g., for low-alloy steels one could choose from ferrite, austenite, bainite, martensite phase types, can be specified and is assigned to each grain. Each grain could in principle have a lattice orientation.

Each phase type can also have a different composition. For example one is allowed to assign pearlite a composition of 0.77 % C and ferrite composition of 0.025 % C for a steel with 0.2 % C. Fig. 3.4 shows ferrite and pearlite phase patterns, and initial carbon concentrations in each microstructure. The current microstructure model treats the average over all the phases as having the composition of the alloy.

In the next stage, the grains will grow or shrink with time and temperature. It will have solute diffusion with a solute diffusion solver. In the austenite region, carbon

Figure 3.4: The initial grain structure is shown in the upper left. The initial carbon concentration is shown in upper right. The red in the lower right shows the initial phase fraction pearlite. The lower left shows the initial phase fraction ferrite. when the microstructure (lower right) is heated to just above the eutectoid temperature all pearlite is transformed to austenite. In this case, the austenite carbon is of eutectoid composition.

diffusion would tend to homogenize carbon distribution. This will be discussed in the incoming sections in more detail.

3.9 Dissolution of Ferrite and Homogenization of Austenite in a Low-Alloy Steel Weld

A model is described which computes the dissolution of ferrite in a ferrite-pearlite or ferrite-bainite synthetic microstructure that is heated from below the eutectoid temperature to above the eutectoid temperature. The rate of dissolution of ferrite in the ferrite-austenite region of the equilibrium phase diagram is governed by temperature and the diffusion of carbon in each phase. This describes a thick interface model that assumes that in a cell containing two phases the composition of the phases is given by the lever rule for equilibrium for the average composition of the cell at the current temperature. In other words, the interface cells are assumed to be sufficiently close to equilibrium for the cell size and time steps used in the analysis. The interface is restricted to be one cell thick. In each time step, one solute diffusion equation is solved in the ferrite domain with zero flux boundary conditions and another solute diffusion equation is solved in the austenite domain with zero flux boundary conditions. The reason for using zero flux BC is that carbon in austenite cannot diffuse out of the austenite domain. The same argument applies to the carbon diffusion in the ferrite domain. The ferrite domain contains all cells that have non-zero fraction ferrite. The austenite domain contains all cells that have non-zero fraction austenite. These solvers are independent. They are coupled only by the procedure that changes composition of the phases in the interface cells that enforces local equilibrium in interface cells. Solute is conserved in each time step. This can be viewed as an additive domain decomposition method for a system of Poisson PDEs. In each time step of the solute

diffusion solvers, the composition of the phases in interface cells, i.e., cells containing two phases are updated by applying the lever rule for equilibrium in that cell for the composition and temperature in that cell.

3.10 Related Works

Palmer et al [12] measure austenite growth rate in a 1005 C-Mn steel directly using in-situ synchrotron X-ray diffraction. Lomozik and Zielinska-Lipeiec [47] studied the microstructure and toughness of multi-pass weld metal in P91 steel. They found that heating into the inter-critical region or just above the inter-critical region, the carbides and martensite did not have time to fully transform to austenite. If the austenite that did form had high carbon levels, then it sometimes transformed to twinned martensite on cooling that had lower toughness. Also the martensite-austenite (MA) grains were susceptible to cracking. They attributed this to cause the reduced Charpy toughness that they measured.

Krielaart et al [48] discuss ferrite formation in Fe-C alloys during austenite decomposition under non-equilibrium conditions. They argue that growth of a ferrite grain nucleated on an austenite grain boundary is limited by solute diffusion for thickening growth, i.e., growth normal to the austenite grain boundary. However growth along the austenite interface is controlled by interface mobility, not solute diffusion.

3.11 Algorithm

3.11.1 Initialization Step.

The model could be initialized with a synthetic microstructure described earlier in this chapter for low-alloy steels. When the temperature rises above the eutectoid reaction temperature (T_E) for the first time step, i.e., assume that T_1 is equal to T_E in Fig. 3.5.

1. All cells containing pearlite or bainite are transformed instantaneously into austenite. The fraction of austenite in them (f_0^γ) is assigned the value of 1.0. The carbon concentration in austenite is assigned the value of carbon concentration in pearlite or bainite.

2. All cells containing ferrite and having at least one neighbor cell with austenite in it are assigned the fraction of austenite equal to 10 times the smallest non-zero positive real value. The concentration of carbon in austenite in such cells is assigned the initial value equal to the concentration of carbon in the ferrite in the same cells (c_0^α). This limits the algorithm to dissolution of austenite.

3. If the algorithm is to be generalized to deal with ferrite dissolution, it would need to detect if ferrite was dissolving. If ferrite was dissolving, then in all cells containing only austenite and having at least one neighbor cell with ferrite in it, assign the fraction of ferrite in the austenite cell equal to 10 times the smallest nonzero positive real value. The concentration of carbon in ferrite in such cells is assigned the initial value equal to the concentration of carbon in the austenite in the same cells (c_0^α).

3.11.2 First Transformation Step.

In this step temperature is still at T1.

1. First a diffusion step is calculated in the ferrite domain with zero Neumann boundary conditions, i.e., zero flux boundary conditions. Next a diffusion step is calculated in the austenite domain with zero Neumann boundary conditions, i.e., zero flux boundary conditions in each domain. Note these domains overlap but the solvers are separate independent global solvers. They could be solved in parallel with a sub-domain for each grain of each phase type because there is no coupling between diffusion solvers of the same phase type, e.g., austenite, unless the austenite grains impinge. Corresponding concentration change values due to diffusion for ferrite (Δc_1^α)

Figure 3.5: Austenite-ferrite two-phase region in the Fe-C phase diagram.

and austenite (Δc_1^γ) are obtained for all cells.

2. Concentration fields are updated to:

$$c_1^\alpha = c_0^\alpha + \Delta c_1^\alpha \quad \text{and} \quad c_1^\gamma = c_0^\gamma + \Delta c_1^\gamma \quad (3.2)$$

3. In all two-phase cells the average concentration of carbon in the cell is calculated as

$$\bar{c}_1 = c_1^\alpha (1 - f_0^\gamma) + c_1^\gamma f_0^\gamma \quad (3.3)$$

for every two-phase cell.

4. In all two-phase cells the fraction of austenite is calculated using:

$$f_1^\gamma = \frac{\bar{c}_1 - c_E^\alpha(T_1)}{c_E^\gamma(T_1) - c_E^\alpha(T_1)} \quad (3.4)$$

If $f_1^\gamma > 1.0$, then $f_1^\gamma = 1.0$ and the fraction of ferrite is set to zero in this cell. The

adjacent cells that contain ferrite are assigned the fraction of austenite equal to 10 times the smallest nonzero positive real value. The concentration of carbon in austenite in such cells is assigned an initial value equal to the concentration of carbon in the ferrite in the same cells (c_1^α). Note that this conserves carbon mass.

and in the austenite domain. Corresponding concentration change values for ferrite (Δc_2^α) and austenite (Δc_2^γ) are obtained for all cells.

2. Concentration fields are updated to:

$$\bar{c}_2^\alpha = c_1^\alpha + \Delta c_2^\alpha \quad \text{and} \quad c_2^\gamma = c_1^\gamma + \Delta c_2^\gamma \quad (3.5)$$

3. In all two-phase cells the average concentration of carbon in the cell is calculated as

$$\bar{c}_2 = c_2^\alpha (1 - f_1^\gamma) + c_2^\gamma f_1^\gamma \quad (3.6)$$

for every two-phase cell.

4. In all two-phase cells the fraction of austenite is calculated using:

$$f_2^\gamma = \frac{\bar{c}_2 - c_E^\alpha(T_2)}{c_E^\gamma(T_2) - c_E^\alpha(T_2)} \quad (3.7)$$

If $f_2^\gamma > 1.0$, then $f_2^\gamma = 1.0$ and the fraction of ferrite is set to zero in this cell. The cells adjacent to a cell that only contains austenite and that contain ferrite are assigned the fraction of austenite equal to 10 times the smallest nonzero positive real value. The concentration of carbon in austenite in such cells is assigned the initial value equal to the concentration of carbon in the ferrite in the same cells (c_2^α).

5. The concentration of carbon in the interface cells is set to equilibrium values, i.e., $c_E^\alpha(T_2)$ in ferrite and $c_E^\gamma(T_2)$, corresponding to current temperature.

The third transformation step is similar to second.

3.11.3 Transformation Propagation

When fraction of austenite reaches the value of 1 in any particular cell no further transformation update is produced in it and all its neighbors containing only ferrite are initialized for transformation using the initialization step described above.

3.11.4 Transformation Termination.

Different halting scenarios are possible.

1. Maximum temperature is above T_0 . When temperature rises above T_0 it is possible that all ferrite cells have been already transformed into austenite. If it is not so, then all remaining ferrite cells are transformed into austenite with concentration of carbon equal to that in ferrite. All two-phase cells are transformed into austenite with concentration equal to the average concentration in the cell. Further evolution involves only homogenization by solute diffusion in austenite. There are no closed boundaries for the diffusion inside the system, i.e., zero Neumann boundary conditions are applied. Diffusion homogenization is continued until temperature reaches $T_{c_0}^\gamma$ value during the cooling part of the cycle. The results from this solver are sent to a Kirkaldy-Watt type microstructure analysis to solve for the decomposition of austenite to pearlite, bainite and/or martensite with the obtained concentration field and austenite grain size computed by the austenitization solver.

2. Maximum temperature is below T_0 . Transformation continues as temperature rises to maximum and then cools down to $T_{c_0}^\gamma$ ($T_{c_0}^\gamma$ is the equilibrium austenitization temperature corresponding to the average alloy composition c_0). If all ferrite is transformed to austenite then diffusion homogenization is continued until T_γ is reached. The results from this solver is sent to a Kirkaldy-Watt type microstructure analysis to solve for the decomposition of austenite to pearlite, bainite and/or martensite with the obtained concentration field computed by the austenitization solver computed at

$$T = T_{c_0}^\gamma .$$

3. Maximum temperature is below $T_{c_0}^\gamma$. There are some ferrite cells in the system. The results from this solver are sent to a Kirkaldy-Watt type microstructure analysis to solve for the decomposition of austenite to pearlite, bainite and/or martensite with the obtained concentration field and phase field obtained at $T = T_{max}$ computed by the austenitization solver.

4. If the state is "all cells are austenite" and temperature and composition are in the equilibrium austenite field and one cools into the austenite-ferrite field, then ferrite nuclei would be located on the grain boundaries of the austenite grains. This assumes that austenite grains are present. Ferrite nuclei start the growth of ferrite grains and the dissolution of austenite grains.

3.12 Numerical Tests to Verify the Algorithm - 1D Benchmark Tests

Different scenarios were considered in order to verify the transformation behaviour. They are discussed in the next sections.

3.12.1 Peak Temperature Above T_e and Below $T_{c_0}^\gamma$ in the Two-Phase Region

A 1D $60 \times 1 \times 1$ element domain with one initial pearlite grain is considered as an initial synthetic microstructure. Pearlite is initialized with 0.77 wt% and the remaining ferrite with 0.025 wt% carbon and the average goes to 0.134918 wt% which is the alloy carbon (See Fig. 3.6). Cell size is chosen to be 5 μm and time step size is 0.5 s.

Fig. 3.8 summarizes the case where the peak temperature in the thermal cycle, T_{max} , is below $T_{c_0}^\gamma$. The nominal carbon composition of the alloy is c_0 . The simplified

Figure 3.6: Carbon concentration for in the initial microstructure. Red is the pearlite grain which transforms into austenite in heating .

thermal cycle is also shown in Fig. 3.7. In this test the temperature is raised from $T_e = 723^\circ C$ to $T_{max} = 823^\circ C$ with the isothermal heating rate of $1\ K/s$ in the domain. The domain remains at this temperature for a sufficiently long time. According to the Fe-C phase diagram, ferrite to austenite phase transformation will stop at equilibrium and we will end up with some ferrite cells in the system. During the growth, carbon composition in ferrite and austenite phases at the the interface cell are always at the the equilibrium values $c_e^\alpha(T)$ and $c_e^\gamma(T)$. For a sufficiently long holding time, carbon is homogenized in the final ferrite and austenite phases. Simple calculations give the carbon concentrations of $0.01047\ wt\%$ and $0.322463\ wt\%$ for c_e^α and c_e^γ respectively which is identical to the simulation results.

Fig. 3.9 illustrates the carbon distribution along the 1D bar for different solution times. Calculations using the phase diagram confirm the equilibrium carbon levels in both austenite and ferrite phases at the last time step.

Fig. 3.10 shows the evolution of the average austenite phase fraction in the domain which ends with 0.398 fraction austenite in the domain.

3.12.2 Maximum Temperature Above $T_{c_0}^\gamma$ and Below T_0

Assume that the maximum temperature, T_{max} is above $T_{c_0}^\gamma$ and below T_0 in the thermal cycle shown in Fig. 3.7. All ferrite grains transform to austenite for a sufficiently long time. Note that homogenization continues after all ferrite transforms to austenite and uniform carbon concentration is reached. Note that the phase transformation would

Figure 3.7: The simplified thermal cycle used for the bench mark tests. It includes one heating stage to the maximum temperature, T_{max} , and long holding time at that temperature. Choices of maximum temperature results in different transformation scenarios.

Figure 3.8: Test problem 1 where the maximum temperature is below $T_{c_0}^\gamma$.

Figure 3.9: Test 1; carbon distribution along the 1D bar as of function of time.

Figure 3.10: Time evolution of average fraction of austenite for test 1.

depend on how fast the heating stage is. Fig. 3.12 illustrate the carbon distribution in the bar as a function of time. As can be seen, homogenization is observed at the last time step where the carbon concentration is 0.134918 *wt%* in the domain.

Fig. 3.13 shows the evolution of the average austenite phase fraction in the domain which ends with fraction austenite in the domain equal to 1.0.

For whatever temperature above $T_{c_0}^\gamma$, the only thing which matters is the speed of homogenization due to the higher diffusion coefficient at higher temperatures.

Figure 3.11: Test problem 2 where the peak temperature is above $T_{c_0}^\gamma$ and below T_0 .

3.12.3 Maximum Temperature Above T_0

In this case austenization continues as the temperature goes up. As soon as temperature crosses T_0 , all remaining ferrite transforms to austenite instantaneously and carbon homogenization continues in the austenite. The heating rate of 1 *K/s* is used to raise the temperature from 723 °C to 917 °C for the results shown in Fig. 3.14.

Figure 3.12: Test 2; carbon distribution along the 1D bar as a function of time. Note the homogenization at $t=1000$ s with no interface (No discontinuity in the carbon concentration).

Figure 3.13: Time evolution of average fraction of austenite for test 2.

Figure 3.14: Time evolution of average fraction austenite for test 3. Note that at time $t=186$ s temperature reaches T_0 and all ferrite transforms to austenite

3.13 Austenization Validation Test

Palmer et al [12] ran an experimental study on the austenization process of 1005 C-Mn steel during the continuous heating. In their experiments, 3 samples are heated isothermally from room temperature to the peak temperature 1248°K and kept for 60 s at that temperature. The progression of austenization transformation is studied for heating rates of 1 K/s , 3 K/s and 10 K/s . The samples are AISI 1005 C-Mn steel (0.05 C 0.31 Mn 0.11 Ni 0.10 Cr 0.18 Si 0.008 Mo) and the equilibrium transformations temperature are reported as A_1 (720°C), A_3 (882°C), A_4 (1432°C), solidus (1506°C) and liquidus (1529°C) have been calculated based on a pseudo-binary phase diagram.

Fig. 3.15 shows the comparison between the experimental results and our austenite-ferrite solver results. We used two different cell sizes, $1\text{ }\mu\text{m}$ and $5\text{ }\mu\text{m}$ for our simulations. Choosing finer cell size results in a smaller pearlite grain size. We could not find a reason for a high fraction austenite immediately after austenization starts. The

Figure 3.15: Progression of austenitisation transformation in 1005 C-Mn steel as function of a time for heating rates of 1, 3 and 10 C/s [12]. Comparison between numerical and experimental results given in [12].

Figure 3.16: Austenization progression (right) and carbon field (left), simulated using austenite-ferrite solver, for the heating rate of 1 C/s. Initial pearlite grain is shown at $t=0$ s in red.

deviation could be the results of other alloying components present in the alloy that are not considered in our model. The overall trend suggests a reasonable agreement between experiments and numerical results. Fig. 3.16 shows the simulation results of austenite phase progression and carbon concentration in different stages of the thermal cycle for the heating rate of 1 K/s .

3.14 Microstructure Evolution in the Heat-affected zone of a Weld-HAZ Microstructure Framework

3.14.1 Introduction

A framework for a workflow is described in this section which links the macro weld model to the micro-model for the evolution of microstructure in a low-alloy steel weld. The goal is to compute the correlation between the weld process parameters in the macro model of a welded structure such as weld process type, weld current, voltage, weld heat input, weld speed, base metal and filler metal composition and the solid state phase transformations and the mechanical properties in a neighbourhood of a point in the weld HAZ.

The work flow in the framework for the micro-model shown in Fig. 3.17 illustrates the flow of data through the different solvers in the HAZ model. The rectangular boxes with red numbers from 1 to 6 indicate the six solvers used in the software framework. The oval boxes indicate the data fields computed by each solver and the small circular disks indicate the data field that flows from one solver to the next solver along the arrow joining the solvers. Note this work flow is embedded in the holistic model of a welded structure that could have multiple weld joints.

The macro-weld model, Solver 1 in Fig. 3.17, has typical length scales ranging from about 1 mm to several meters and time scales ranging from about 1 second to times as long as days. In contrast, the austenite-ferrite micro heat-affected zone microstructure model, solver 2 in Fig. 3.17 has typical length scales ranging from less than 1 micron to less than 1 mm and time scales ranging from about 1 microsecond to 0.1 s. The time scales in the micro-model for solid state microstructure transformations, solvers 2, 4 and 5 in Fig. 3.17, solute diffusion and stress models can range from seconds to hours. Each solver shown in Fig. 3.17 is described briefly in the following sections.

Figure 3.17: Work flow in the HAZ microstructure framework is shown.

In a framework, unlike in libraries or normal user applications, the overall program's flow of control is not dictated by the user, but by the framework [49].

In addition to executing the workflow described in this figure for a particular point in the HAZ, each solver can write a complete report on the transient evolution of the fields that it solves, including the images, figures, tables relevant to each particular analyses from a template for a HAZ microstructure analyses. The user can also edit the template to add user defined text, tables and figures to the template to create a new template.

3.14.2 No. 1: Macro-Weld Solver

Welds are simulated for given weld process parameters such as weld speed, heat input, and cooling condition. This macro-model computes the weld pool geometry. The macro-weld pool model could include dilution and mixing in dissimilar metal welds, i.e., the average composition of the micro-model (SPH weld pool model). An FEM weld model such as a double ellipsoidal heat source model [41] can be also used for macro weld simulations. Another alternative is to use a fourth generative heat source model that is a function of the welding process type and weld process parameters [1].

A typical thermal cycle obtained for an spatial point in the HAZ of a weld is schematically shown in Fig. 3.18.

Figure 3.18: Schematic of a typical thermal cycle of a point in HAZ.

3.14.3 No. 2: Austenite-Ferrite Solver

This solver, described in section 3.9, simulates the dissolution of ferrite in to austenite on heating and ferrite into austenite on cooling in a low-alloy steel weld. Austenite cooling below the eutectoid temperature transforms to to pearlite, bainite and/or martensite using the Watt-Kirkaldy algorithm. In this solver, a synthetic microstructure model is introduced that contains a representation of individual grains in the microstructure.

3.14.4 No. 3: Carbon Diffusion Analysis in the Solid State

As the micro domain is cooled down from A_1 (point c in Fig. 3.18) to room temperature, the transient carbon distribution is computed by solving the diffusion equation for the diffusion of carbon in the solid micro-model. It is solved with zero flux, i.e., zero Neumann BCs, with an implicit conjugate gradient FEM solver. This conserves the mass of carbon. The solute diffusivity in each cell in each time step is for the solid phase in that cell, e.g., the solute diffusivity for carbon in ferrite is used in a cell that is ferrite. The solute diffusion of substitutional elements such as manganese is not solved because the diffusivity is so low that within the time and temperature to cool to room temperature, the diffusion of substitutional elements would be negligible.

3.14.5 No. 4: Microstructure Solver

The solid state phase transformations of austenite to ferrite, pearlite, bainite and/or martensite in a weld are modelled using an algorithm first proposed by Watt et al [40] and Henwood et al [11]. Their model extends the model developed by Kirkaldy and Venugoplan [39]. It is a density model that computes the phase fraction of each phase at each spatial point at each instant of time. It does not contain individual grains but it does have austenite grain size as a scalar field in space-time. This model does not

change the composition of phases, i.e., only the alloy composition is used. However, it does have a pseudo-binary Fe-C phase diagram that is used to compute equilibrium compositions of phases as functions of time and temperature. After cool-down to room temperature for a given point in the macro-model, an image of the hardness map and distribution of all phases is created.

3.14.6 No. 5 and 6: Stress Solvers

As the solid is cooled from solidification to room temperature, a quasi-static thermo-visco-plastic-elastic stress analysis is done (Quasi-static means that inertial forces and acoustic stress waves are neglected) with traction boundary conditions from the stress in the macro model at this point. See [45] for details on the continuum mechanics theory of this thermo-stress analysis. In the micro model the thermal stress and strain due to temperature changes, phase change and composition changes are computed as the micro-model cools toward room temperature. Note that each phase has its own material properties, i.e., each phase is an independent material with a complete set of properties. Additionally, a stress-strain analysis of a uni-axial tensile test is run at room temperature that is initialized with the microstructure, residual stress and residual strain after cool down to room temperature. A similar uni-axial tensile test could be run and results reported at any other specified temperature.

3.15 Demonstration Example

Results generated by the framework after running the HAZ microstructure workflow (Fig. 3.17) are presented. The framework solves and reports the final microstructures such as ferrite, pearlite, martensite, and bainite phase fractions, hardness and stress-strain curves ($\sigma_{xx} - \varepsilon_{xx}$, $\sigma_{yy} - \varepsilon_{yy}$, and $\sigma_{zz} - \varepsilon_{zz}$) in a uniaxial tensile test. It also allows a user to introduce a thermal cycle from an experiment, e.g. thermocouple

data of a weld, and run the framework.

Note that the whole HAZ frame work for the micro-model provides results only for the one macro spatial point selected in the HAZ of a specific macro model of a weld in welded structure. Any number of macro spatial points can be selected but each must be processed separately and a separate report is prepared for each macro spatial point. The framework would be repeatable for any given weld process, weld procedure, and material. The results for one point in a HAZ of a weld are provided here as an example.

3.15.1 Macro Weld Analysis Results

A bead on plate weld is made using an FEM weld model using a low alloy steel (0.13 C 1.57 Mn 0.2 Si 0.024 Nb) as a material. A thermal cycle of a point in the HAZ of the weld is shown in Fig. 3.19.

Figure 3.19: Sample point in a weld HAZ and its thermal cycle.

3.15.2 Austenite-Ferrite and Carbon Diffusion Solver Results

Austenite-ferrite solver results for the phase transformations and the carbon concentration on the path abc (Fig. 3.18) are presented. Initial microstructure which represents the structure of the base metal before welding is required to be specified. A $50 \times 50 \times 50$ element domain with a cell size of $1 \mu m$ was used. Pearlite grains are initialized with $0.77 \text{ wt}\%$ and ferrite grain with $0.025 \text{ wt}\%$ carbon. The thermal cycle shown in Fig. 3.19 was applied to the domain (note that the tail cools down to 400 K which is not shown). Note that the solver terminates when $T = T_e = 723^\circ \text{C}$ on cooling.

The carbon field from the austenite-ferrite solver is initialized into the solute diffusion solver. It solves for the carbon diffusion in the domain (from c to d).

The initial microstructure and the final carbon distribution are shown in Fig. 3.20.

Figure 3.20: Austenite-ferrite solver; Left: Initial synthetic microstructure. Pearlite grains are shown in red and blue represents ferrite, Middle: carbon concentration at T_e , Right: carbon concentration at room temperature.

3.15.3 Microstructure Solver Results

The carbon field from the solute-diffusion solver is mapped into the microstructure solver as a data flow. It solves for the microstructure evolution in the heat effected zone (from c to d) and a hardness map at the room temperature at d . Thermal cycle shown in Fig. 3.19 was applied to the domain. The Watt-Kirkaldy microstructure model results are shown in Fig. 3.21 for transformation of austenite below T_e .

3.15.4 Transient Thermal Stress Analysis Results

This stress solver used the phase IDs from the microstructure and temperature from the thermal cycle as a data flow to do the transient thermo-visco-plastic-elastic stress analyses. We leave the application of BCs from the macro stress analysis to future work. Here we simply constraint the rigid body modes (zero Neumann BC). The effective stress and effective plastic strain fields at 300 °K are shown in Fig. 3.22.

3.15.5 Room Temperature Uni-axial Tensile Test Results

The residual stress field computed in the previous step is initialized into a new project before doing a uni-axial tensile test. Then we pull the sample in 20 displacement increments such that 4 % strain is applied to the sample ultimately. The effective stress field is shown in Fig. 3.23 at the last loading increment in the uni-axial tensile test. The average σ_{xx} is plotted vs strain shown in Fig. 3.24. We are expecting different stress-strain curves in different direction.

In order to see the variation of stress-strain state of different spatial points in the sample and also the effect of residual stress-strain on the tensile test results, 20 Gauss points were chosen randomly on the mid-cross section of the sample (cross-section normal is along x axis).

Two cases are considered and they both use the evolved microstructure to room

Figure 3.21: Microstructure solver results; Final ferrite, pearlite, martensite, bainite, austenite phase fields and hardness map.

Figure 3.22: Stress solver; effective stress and effective plastic strain.

Figure 3.23: Stress solver; effective stress in a room temperature uni-axial tensile test at at 4 % strain.

Figure 3.24: Room temperature uni-axial tensile test results; average stress xx-strain curve.

temperature. In case A, the residual stress-strain is not initialized from the transient analysis. In case B, the sample is initialized with the residual stress evolved on cooling from the melting point in addition to the room temperature microstructure. Both cases stretched in the x direction. σ_{xx} in the tensile test is plotted vs macro strain for a set of Gauss points is shown in Fig. 3.25.

Figure 3.25: Room temperature uni-axial tensile test results; stress-strain curve. Left: Case A. Zero initial residual stress, Right: Case B. with residual stress initialized on cooling from the melting point to room temperature.

3.16 Summary

A framework for a work flow was developed which runs a family of 6 different solvers linked together by data flows to obtain the microstructure evolution of a point in the weld HAZ. They are *the thermal solver* which gives the spatial transient temperature, *austenite-ferrite solver* solves for the phase transformations and the carbon concentration in the HAZ, *microstructure solver* which gives the microstructure evolution as well as the hardness map, *transient stress solver* solves for the transient displacement and residual stress-strain and *stress solver* which solves for room temperature uniaxial stress-strain curve. An example was demonstrated in the end. The steps that are done in this framework are summarized in Box. 3.16.

Summary - HAZ Microstructure Framework.

1. Run a weld FEM (or SPH) analysis to get the temperature field (and possibly composition fields) in the neighborhood of the weld pool. This is done on a high resolution mesh for a given weld procedure and a given material in MatLib.
2. Pick macro points in the HAZ and find temperature vs time curves for the full thermal cycles.
3. Build a pqr mesh for each of these macro points. This is a Cartesian grid (in this test, 50 x50 x 50) and the element size is about 1 μm .
4. Make a synthetic microstructure as initialization structure with composition field for each phase.
5. Prepare an asutenite-ferrite project.
6. Setup the microstructure project using the same mesh. Take temperature from the FEM weld and run FEM microstructure solver with the carbon

concentration and phase evolution taken from asutemite-ferrite project (solver 2).

7. Compute a hardness map when the FEM microstructure solver has cooled to ambient temperature.
8. Set up a stress project and compute the residual stress-strain at cool down using the cooling curve and computed evolved microstructure.
9. Create a uni-axial tensile test using the same mesh used for the microstructure. Initialized with the computed residual stress-strain. Run it with prescribed displacement to give macro strain of 1 to 4 % in several time steps. Compute stress and strain and plots the stress-strain curve.

Chapter 4

Fusion Zone Microstructure

4.1 Dendrite Growth During the Weld Pool Solidification of a Low-Alloy Steel Welds

4.1.1 Introduction

This chapter presents a numerical model of dendrite growth during the weld pool solidification of a Fe-Mn-C ternary alloy system. A 3D cellular approach is used for the dendrite growth simulation in the micro-scale where the solid phase grows due to the constitutional and capillary under-cooling at the interface. Solute diffusion PDEs are solved in the micro model for the transient composition distribution. The present solidification model is tested using a prescribed temperature gradient and cooling rate in the domain to verify the theory described by S. David [50], J. DuPont [51]. To be tested for the weld pool, it was run in the FZM framework which is discussed in the second part of this chapter.

4.1.2 Weld Pool Solidification Overview

Welding parameters such as input power, weld speed and cooling conditions can influence the microstructure in a weld fusion zone. This is because the local solidification parameters at the liquid-solid interface are affected by the welding parameters. Moreover, microstructure can determine the mechanical properties of the fusion zone, particularly at the center line. As an example, growth of columnar grains to the center line can increase the susceptibility to hot cracking and reduced bending ductility of the weld [52]. Understanding the effect of welding parameters on the evolution of grain structure could help to minimize such drawbacks.

4.1.3 Solidification Parameters in a Weld Fusion Zone

The grain structure of a weld depends on solidification parameters, composition, and weld pool geometry [53]. Growth rate, R , temperature gradient, G , and the cooling rate are the three important solidification parameters governing the solidification in a weld pool [51]. The cooling rate, dT/dt , can be viewed as a dependent parameter and linked to the first two by $dT/dt = RG$. The growth rate is referred to as the rate at which the solid-liquid interface advances [50]. Note that the growth rate and solidification rate can be viewed differently. Growth rate is a local velocity of the liquid-solid interface in the micro-scale. Solidification rate can be seen as a macro quantity. For example the liquid pool boundary moves with the weld speed in the steady state condition. In this case the solidification rate of the weld pool would be at the weld speed. Fig. 4.1 depicts the isotherms in a weld pool taken from the analytical solution of a moving heat source in a plate [54]. Fusion line and center line are shown. Heat is extracted by the cold base metal at the fusion line which results in a higher temperature gradient at that region. As one moves along an iso-therms of the melting point towards the trailing edge, cooling rate and temperature gradient decrease and

Figure 4.1: Temperature field around the moving weld pool.

this slows the heat transfer from the weld pool.

The non-uniform temperature gradient and cooling condition around the weld pool result in different growth rates at different points on the liquid-solid interface at any instant of time. For a point at the interface, the growth rate R can be related geometrically to the weld speed V which is given mathematically by

$$R = \frac{V \cos(\alpha)}{\cos(\alpha - \beta)}. \quad (4.1)$$

Fig. 4.2 shows two snapshots of a steady state weld pool at time t (solid line) and $t + dt$ (dash line) and α and β angles. Vector $\mathbf{n}$ specifies the direction perpendicular to the interface which is along the maximum heat flow direction and the vector $\mathbf{R}$ is along the easy growth direction of the crystal. Sometimes it is assumed that $\alpha - \beta \approx 0$ which simplifies the equation to $R = V \cos(\alpha)$. From Eq. 4.1 it is concluded that the growth rate has its maximum values at the center line and minimum at the fusion line.

4.1.4 Grain Structure at the Weld Fusion Zone

There can be a transition from cellular or columnar to dendritic grains near the fusion line to equiaxed grains near the center line [51]. Fig. 4.3 shows such a transition in the fusion zone. Growth direction is governed by two main competitive conditions

Figure 4.2: Weld speed and solidification rate relationship (modified from [13].)

as the weld pool solidifies. The first is that, grains tends to grow in the direction of maximum temperature gradient and the second is that the solid crystal tends to grow in the easy growth crystallographic direction which is $\langle 100 \rangle$ for a material with BCC or FCC structure. Near the fusion line, the solidification starts directly from

Figure 4.3: Different solidification modes at fusion zone [13].

the solid substrate at the liquidus temperature of the alloy [51]. Since the weld pool is in direct contact with the partially melted base metal in the fusion line [13] and wets the base metal completely [55], the melt changes to solid without difficulty in $\langle 100 \rangle$ direction as the temperature drops. This growth is called *epitaxial growth*. The solidification of a single grain continues in a competitive manner and epitaxial

grain growth might be stopped by the other condition which is the grain growth in the maximum heat flow direction. Note that non-epitaxial growth, i.e., heterogeneous nucleation, may occur at the fusion boundary if the filler metal composition is very different from base metal. A proposal by Nelson [55] is that nucleation of solid weld metal takes place on heterogeneous sites on the partially melted base metal which results in random misorientations between base metal grains and weld metal grains.

The lower temperature gradient near the center line promotes more constitutional supercooling and *equiaxed* dendrite structure could start growing in the center line region [56]. Lancaster argues that the equiaxed grains are nucleated by heterogeneous nuclei and are not essentially related to the interface solidification parameters [53].

4.1.5 Effect of Welding Parameters on Weld Pool Solidification

Different thermal conditions around the weld pool result in different growth morphologies as one moves along the interface from the fusion line to the center line. This morphology variation is also altered by the welding parameters and material properties. The welding parameters such as input power and welding velocity together affect heat and mass transfer that changes the weld pool geometry and therefore the isotherms. This implies that different welding parameters change the growth morphology [51]. For a low to moderate speed the weld pool shape tends to be elliptic. For high speed welding, the weld pool can have a tear drop shape which is characterized by the higher growth rate, lower temperature gradient and possibly composition changes due to segregation to the center line.

As argued by David [50], the maximum solidification rate is not always at the center line. It happens for certain weld speeds. In fact, there is a critical welding speed such that the growth rate and weld speed are equal [50]. Above the critical

welding speed the growth rate is smaller than the weld speed. From the quality of weld point of view, this is not a desired condition since the low strength region falls at the transient tensile stress envelope behind the weld pool and may increase the risk of center line cracking [57] .

For conventional welding processes such as shielded metal arc (SMAW) and gas tungsten arc (GTAW), the cooling rate may vary in the range of 10 to 10^3 K°/s [50]. For processes such as laser or electron beam welding which use a high power density beam, the cooling rate typically varies from 10^3 to 10^6 K/s [50, 58].

As another example, a temperature gradient of $720K/cm$ in the liquid was measured for a GTAW of plain carbon steel by Matsuda. The heat input can be used as a general guideline to evaluate the temperature gradient variation due to the heat input. For example lower heat input results in a lower thermal gradient near the fusion line [50]. Cooling rate decreases as the power per unit length is increased [59, 60]. It is equivalent to say that with a constant speed, an increase in power would results in a lower cooling rate. Reader should pay attention to fact that these experimental measurements of cooling rate and temperature gradient are rough approximations and typically limited to the solid region around the weld pool. The real thermal condition in the liquid side is strongly affected by the welding parameters and convection in the weld pool. A good numerical model of a weld pool can give more realistic insight about the thermal conditions in the weld pool.

4.1.6 Undercooling

According to nucleation theory, some undercooling is needed for nucleation but the amount of that undercooling is thought to be small for welding since epitaxial growth is common in welding [50]. The undercooling discussed below is restricted to the growth process. Several terms may contribute to the total undercooling of the liquid

as

$$\Delta T = \Delta T_c + \Delta T_{capillary} + \Delta T_k + \Delta T_t \quad (4.2)$$

where ΔT_c is constitutional undercooling, $\Delta T_{capillary}$ capillary undercooling, ΔT_k kinetic undercooling and ΔT_t the thermal undercooling. Constitutional and capillary terms make the largest contribution to the total undercooling in a welding process. Constitutional undercooling occurs when the solute composition deviates from the bulk composition and has the largest influence on ΔT at the interface. The solute rich boundary layer established in front of the interface lowers the melting temperature of the alloy and provides the driving force for nucleation and growth. Contrary to most casting processes, capillary effects or supercooling due to interface curvature can be significant in a welding process since much finer grains are developed during weld solidification. The capillary effect is confided through $\Delta T_{capillary} = \Gamma \cdot \kappa_{int}$ where κ_{int} is the local curvature and Γ is the Gibbs-Thompson coefficient. Thermal and kinetic undercoolings appears to make a small contribution to the total undercooling which can be ignored [50].

4.2 Mathematical Description and Numerical Modeling

4.2.1 Solidification Model

The cellular approach is used to simulate dendrite growth during the solidification process. The mathematical and numerical formulations have been described in detailed by Artemev and Goldak [43] and its application to the solidification modeling was analyzed by Martinez [61] and Alsoruji [62].

In this approach, the control volume is divided into n equal size cells. Each cell is assigned a phase field f which represents the state of material in that cell. A fully solid cell has $f = 1$. For a fully liquid cell $f = 0$ and $0 < f < 1$ represents a partially solidified cell. The liquid-solid interface is specified by either a cell with phase of 1 or between 0 and 1.

4.2.2 Heat and Mass Transfer

The evolution of temperature and concentration fields controls the solidification conditions in the cells with $0 < f < 1$. In the first stage and for test purposes, the spatial temperature evolution is prescribed in the control volume by using a constant temperature gradient and a cooling rate (Fig. 4.4). In the next stage of development, the temperature is taken from a macro FEM heat transfer model (see section 3.5.1) of a weld which can provide more realistic thermal conditions.

Figure 4.4: Left: Initial phase field, Right: Initial temperature field

$$\frac{Dh}{Dt} = \nabla \cdot (\kappa(T)\nabla T) + Q_v \quad (4.3)$$

where h is the enthalpy per unit volume, T is temperature, κ thermal conductivity. Mass transfer of solute is governed by Fick's second law of diffusion.

$$\frac{DC}{Dt} = \nabla \cdot (D\nabla C) + C(1 - k)\frac{\partial f}{\partial t} \quad (4.4)$$

where D is the diffusivity of the solute which is assumed to be constant in the present model and k is the distribution coefficient. The second term in the right hand side represents the source term due to the solute rejection from the solid to the liquid at the interface. This term is updated in each time step as the interface moves. Periodic boundary conditions are considered at the external side boundaries of the control volume. Solute diffusion in the solid is not considered in the model since the diffusion coefficient in the solid is around 1000 times smaller than that of the liquid phase and can be neglected for the solidification time scale. During the solution procedure, homogenous cells ($f=1$ or $f=0$) take a single value of concentration and the cell with $0 < f < 1$ takes different concentration values for solid phase and liquid phase. An implicit 3D solver is incorporated to solve Eq. 4.4 for the transient solute distribution for each solute, i.e., Mn and C in this case. This allows larger time steps than an explicit solver whenever they are justified.

4.2.3 Dendrite Evolution

The liquid-solid interface growth rate is proportional to the total amount of undercooling, ΔT , at the interface (See Eq. 4.2). Taking the two most important terms, the interface velocity would depend on the melting temperature of the pure metal,

solute concentrations in the liquid and curvature. It is expressed by:

$$V_{int} = \mu_k \cdot \Delta T = \mu_k \cdot (T^* + m_l^X c_l^X + m_l^Y c_l^Y - \Gamma \cdot \kappa_{int} - T_a) \quad (4.5)$$

The proportionality coefficient μ_k (m/Ks) is a material property of an alloy called the kinetic coefficient. T^* is the melting temperature of the pure alloy and T_a is the local actual temperature imposed by the thermal process. c_l^X and c_l^Y are the concentrations of the alloying components X and Y in the liquid phase at the interface, m_l^X and m_l^Y are the liquidus line slopes in $Fe - C$ and $F - Mn$ systems respectively, κ_{int} is the curvature of the interface which by convention is positive for a convex surface towards the liquid and Γ is the Gibbs-Thomson coefficient. The value of the kinetic coefficient is found experimentally and usually is difficult to obtain for metallic alloys. The most suggested value of 0.01 m/s K was adopted for the simulations [63]. Suppose that a pre-existing solid phase is at the bottom of the control volume. If the solid layer is flat the interface will grow in a flat configuration where the solute rich boundary layer exists in front of the growing interface.

Adding any perturbation to the surface curvature can break down the growth to a different growth morphology because non-uniform curvature of the interface and the subsequent solute distribution ahead of the perturbed interface will change the equilibrium melting temperature due to the capillary and compositional effects. The combination of these effects along with the thermal conditions at the interface can result in local positive (solidification) or negative (re-melting) velocity of the interface. The evolution of the phase field in cell i, j, k is numerically expressed as

$$f_{ijk}^{t+1} = f_{ijk}^t + \left(\frac{\Delta t \cdot V_{ijk} \cdot S}{\Delta x \Delta y \Delta z} \right) \quad (4.6)$$

where S is the surface area of the interface inside the cell which moves with the velocity

V_{ijk} .

4.2.4 Curvature

The curvature of the interface is computed on the average phase field, g as

$$\kappa_{int} = \nabla \cdot \frac{\nabla g}{|\nabla g|}. \quad (4.7)$$

Computing the curvature on the phase field, f , does not provide a smooth variation of the surface normal and therefore the average phase field, g , is used instead to avoid abrupt changes in the computed curvature of the interface. Special care should be taken in choosing the element size since the element size affects the tip radius computations. When the cell size is too large, the tip radius is dictated by the mesh, not by the physics of the problem [61].

4.2.5 Define Control volume, Initial and Boundary Conditions

In order to reach a steady state solution in the solidification model, the domain should be long enough such that it covers the mushy region. The minimum required length can be approximated using $L = (T_e - T_m)/G$ where the temperature gradient G can be taken from the heat transfer simulation or can be chosen. T_e is the cut off temperature which is chosen to be 1770 K for a steel alloy, and T_m is the equilibrium melting temperature. This will ensure that when the bottom of the domain becomes fully solid, the dendrite tip is a safe distance from the other end of the domain. The nominal concentration of the alloy specifies the initial equilibrium melting temperature as

$$T_m = T^* + m_l^C c_0^C + m_l^{Mn} c_0^{Mn}. \quad (4.8)$$

Table 4.1: Properties of alloying components.

Properties	Symbol	Units	Value
Initial concentration (Carbon)	c_0^C	wt%	0.205
Initial concentration (Manganese)	c_0^{Mn}	wt%	0.8
Distribution coefficient (Carbon)	k^C	—	0.17
Distribution coefficient (Manganese)	k^{Mn}	—	0.73
Liquidus line slope (Carbon)	m_l^C	$K/\text{wt}\%$	-81
Liquidus line slope (Manganese)	m_l^{Mn}	$K/\text{wt}\%$	-5.1
Diffusion coefficient (Carbon)	D_l^C	m^2/s	2.32×10^{-8}
Diffusion coefficient (Manganese)	D_l^{Mn}	m^2/s	3.83×10^{-9}
Gibbs-Thompson coefficient	Γ	mK	2.0×10^{-7}

where T^* is the melting temperature of the pure iron.

4.2.6 Material Parameters

The model for the tests in this thesis use the input parameters listed in Table. 4.1.

4.3 Simulation Results

4.3.1 Effect of Initial Nuclei and Noise on Dendrite Growth

In this study, a random noise is applied to the system which is an artificial representation of thermal fluctuations. Depending on the noise amplitude, positive or negative undercooling can occur on the interface. The first observation from the simulation is that applying noise to the system is enough for nucleation and growth and there is no need to make pre-existing nuclei. However using nuclei and noise results in a more uniform distribution of dendrites. Fig. 4.5 shows the effect of noise on the dendrite shapes. The corresponding average solid phase fractions are plotted as a function of

height in Fig. 4.6 for four cases.

Figure 4.5: Effect of noise: a) Initial nuclei, b) Initial nuclei plus noise, c) Only noise, d) Noise amplified noise by factor 2

4.3.2 Effect of Initial Temperature on Dendrite Growth

A solute rich boundary layer and curvature lower the initial equilibrium melting temperature to some degree. For the growth to start, the real temperature of the melt should be equal or less than the equilibrium melting temperature. A set of simulations was investigated which provides an estimate on the amount of under cooling required for growth. The melting temperature at the initial concentration of the alloy was computed as 1792 K . Keeping temperature gradient and cooling rate identical for all cases, different initial temperatures were considered. The initial temperatures were applied in such away that the bottom temperature of the control volume is 1, 2, 7, 12, 17, and 22 K below the melting temperature of the system at the initial concentration.

Figure 4.6: Average solid fraction in every layer for four cases.

Fig. 4.7 shows the maximum dendrite tip position along the growth direction as a function of time. Each curve represents the tip position for a certain amount of initial supercooling. Lower initial melt temperatures resulted in a fast growth at the beginning coming into the steady state regime. As is seen in all cases, the steady state growth rates are identical. The results also suggest that for a certain amount of supercooling the steady state solution for the dendrite tip should start in a few time steps.

4.3.3 Cell Size Effects

In the solidification model, the cell size is another factor which controls the geometry of the growth in addition to the physics of the problem. Very big cells can not accurately resolve the curvature at the dendrite tip and will raise the equilibrium melting temperature and the growth is no longer controlled by the tip geometry. Martinez [61] showed that below a certain value the predicted geometry is unaffected by the element size.

In order to find the optimum cell size for our simulations and understand the

Figure 4.7: Tip position vs time for different initial temperature of the liquid.

effects of the cell size on geometry and growth rate, a series of tests were conducted. A control volume of size $50 \times 50 \times 100 \mu m$ was discretized by the cell sizes of $5 \mu m$, $2.5 \mu m$, $1.25 \mu m$, $0.525 \mu m$, and $0.3125 \mu m$.

Consider the case where the temperature gradient in the control volume is fixed in space and time (No cool down). The melting temperature for the initial composition is calculated using Eq. 4.8 as $1792 K$ by ignoring the curvature effects. The temperature is imposed in such a way that the mid-plane is equal to $1792 K$. This suggests that the dendrite growth should stop near the mid-plane.

Fig. 4.8 shows the maximum tip position as a function of time. Theoretically, in all cases, if the interface composition is constant, the dendrite growth rate must come to zero at a certain height where the equilibrium melting temperature for that composition and curvature is equal to the actual temperature. The results suggests that by decreasing the cell size, the growth rate curves, i.e., the slopes curves, approaching each other.

Figure 4.8: Plot of dendrite tip positions as a function of time for different cell sizes. Slopes gives the grow rate. Temperature varies linearly in the domain from the cold bottom to the top. No cool down is considered.

4.3.4 Effect of Solidification Parameters on the Dendrite Growth

As reviewed in the beginning, different morphologies of growth could generate from point to point in a fusion zone which is controlled by solidification parameters. To explore the growth morphology space, two control variables, temperature gradient, G and cooling rate, dT/dt are considered. A range of variables were selected according to the experimental approximation for the weld pool and the cell size of $0.625 \mu m$ was chosen in all tests. Fig. 4.9 shows the input parameters and the results taken from the simulations in the steady state regime (Figs. 4.10 to 4.12).

Project	Domain size	Cell size (μm)	Cooling rate (K/s)	Temperature gradient (K/mm)	R= (dT/dt)/G (m/s)	Tip velocity (m/s) -model	Maximum Tip Temperature (K)	Mushy zone length (mm)	CPU time (hours)
P1	100x100x200	0.625	100	160	0.001	-	-	-	-
P2			500		0.003	-	-	-	-
P3			1000		0.006	0.0058	1786.45	0.104	30.7
P4			2500		0.015625	0.0146	1785.5	0.0988	6.25
P5			5000		0.031	0.0288	1774.11	0.0844	6.6
P6	100x100x400		100	80	0.001	-	-	-	-
P7			500		0.006	0.0057	1786.45	0.2075	82.6
P8			1000		0.013	0.0115	1785.63	0.1975	38.8
P9			2500		0.03125	0.0278	1783.15	0.167	14.4
P10			5000		0.063	0.0544	1779	0.114	7.66
P11	100x100x800		100	40	0.003	-	-	-	-
P12			500		0.013	0.0113	1786.34	0.383	156.8
P13			1000		0.025	0.023	1785.63	0.3481	75
P14			2500		0.0625	0.055	1779	0.2275	29.8
P15			5000		0.125	0.0984	1772.52	0.068	13.3

Figure 4.9: Projects list.

Figure 4.12: Dendrite geometry for Tests, P12(bottom), P13, P14 and P15 (top).

Figure 4.10: Dendrite geometry for Tests, P3 (bottom), P4 and P5 (top). Red represents fully solid and blue represents fully liquid.

Figure 4.11: Dendrite geometry for Tests, P7(bottom), P8, P9 and P10 (top).

4.4 Summary

A cellular model of the dendrite growth was presented. The details for the numerical modeling and some of its aspects and applications were demonstrated by [43], [61] and [62].

The main purpose of the first part is to verify the correctness of the solidification model mathematically and tuning physical and solver parameters, and machinery for software development. We tested the dendrite growth model using constant cooling rates and temperature gradients applied to the entire control volume. The steady growth rates are in a good agreement with the growth rate given by $R = (dT/dt)/G$. However, in a real welding process, the temperature gradient and cooling rate won't be constant and may vary in time for a point in the fusion zone during the solidification time. In addition, the available experiments on cooling cycles of weld usually give only a rough approximate of the thermal cycle.

To get more realistic thermal condition the temperature is mapped from a macro weld pool model to the micro domain for the solidification process. This will be explained in the next part along with introducing the fusion zone microstructure framework.

4.5 Microstructure Evolution in the Fusion Zone of Low Alloy Steel Welds-FZM framework.

4.6 Introduction

The mechanical properties of steels are controlled by its microstructure. The microstructure of steel generally refers to the specific shape, size, distribution, and phase types of the grains in the steel. The microstructure itself is greatly affected by heat

treatment. During a fusion welding process, melting and re-solidification of base and filler metals occurs in the fusion zone with a complex texture of columnar to exquiated dendrite structure in the grains. (See points A and B in Fig. 4.13)

The base metal in the HAZ (see point C in Fig. 4.13) does not go above the melting temperature. However the temperature is high enough such that the original microstructure is altered which is controlled by the thermal cycle imposed by the weld heat input. Understanding the microstructure in the fusion zone and HAZ may help to control the mechanical properties of the weld zone.

Figure 4.13: Fusion and HAZ in a weld.

The goal is to develop a micro-model for the evolution of microstructure in a low-alloy steel weld that is coupled to a macro-model of the weld in a welded structure. It is desirable to compute the correlation between the weld process parameters in the macro-model such as weld process type, weld current, voltage, weld heat input, weld speed, base metal and filler metal composition and the solidification microstructure as well as the solid state phase transformations after solidification in the micro-model. This would predict the evolution of microstructure in the neighbourhood of a point in the weld fusion zone of the macro-model. This is important because the transient microstructure determines the temperature dependent material properties of the fusion zone such as yield stress, creep rate, strength, hardness and toughness as a function of time and temperature. Solid state phase transformations can dramatically change the residual stress and distortion.

The micro-model represents the microstructure in the neighbourhood of a point

Figure 4.14: Work flow in the Fusion zone microstructure framework is shown.

in the macro-model. The work flow in the software framework for the micro-model shown in Fig. 4.14 illustrates the flow of data through the solvers. It is similar to the framework discussed in previous chapter for the HAZ including 6 solvers but the ausenite-ferrite solver has been replaced by the *Dendrite solver* which gives the dendrite morphology and composition distribution in the micro-model.

4.7 Implementation

The first stage of the micro-model solves the solidification, i.e., the formation of dendrite, columnar, cellular or planar solid crystals including the segregation of solutes. In the example described, the solutes are C and Mn . The boundary conditions are the

transient temperatures imported from the macro-model. The size of the micro-model domain is roughly $0.1 \times 0.5 \times 0.05 \text{ mm}$ with a typical grid of $100 \times 100 \times 160$. The second stage of the micro-model uses the same grid. The transient temperature is prescribed from the macro-model as it cools from the solidification temperature to room temperature. It solves for diffusion of carbon. Below T_e the solid state phase transformation of austenite to pearlite, bainite and/or martensite are modelled using an algorithm first proposed by Watt et al [40]. The residual stress created by the phase transformations during cooling is computed. The hardness maps are created in the micro-mesh at room temperature.

Finally, in a third stage longitudinal and transverse uni-axial tensile tests are pulled to about 4% macro strain at room temperature in an attempt to predict the stress-strain curve for the fusion zone microstructure.

4.7.1 No. 1: Macro-Weld Solver

The macro-model computes the weld pool geometry for given weld process parameters such as weld speed, heat input, and cooling condition. Also the macro-weld pool model could include dilution and mixing in dissimilar metal welds, i.e., the average composition of the micro-model if an SPH weld pool model is used. An FEM weld model such as a double ellipsoidal heat source model [41] can be also used for macro weld simulations. Another alternative is to use a fourth generation heat source model such as the SPH weld pool model that is a function of the welding process type and weld process parameters [1].

A typical thermal cycle of a point in the weld fusion zone at the neighborhood of the solid-liquid interface in a weld pool is shown in Fig. 4.15.

Figure 4.15: A typical thermal cycle of a point in the weld fusion zone at the neighborhood of the solid-liquid interface in a weld pool.

4.7.2 No. 2: Dendrite Solver

A cellular automata approach is used to simulate the dendrite growth during the solidification process. The mathematical and numerical formulations have been described by Artemev and Goldak [43] and its application to the solidification modeling was analyzed by Martinez [61] and Ghazi [62]. The liquid-solid transformation uses a thick interface cellular automata algorithm. A high order phase diagram controls phase composition in interface cells that contain both liquid and solid phases. An implicit solute diffusion solver is applied to all solutes in the liquid. Solute diffusion in the solid is neglected because the diffusivity in the solid is so much lower than the solute diffusivity in liquid and the solidification time is so short. The cooling rate is assigned to be the cooling rate for the point in the macro-model.

Solidification analysis in the micro-model is done for a sample point on the cooling side of the liquid-solid interface for the geometry of the weld pool computed in a macro-model. This solidification analysis will provide dendrite morphology and composition distribution in the micro model. This solidification analysis terminated when the

mushy zone and a solid region below the mushy zone has reached steady state. This steady state solid region of the solidification model is taken to be the micro-model for the solid state analysis described below. T_{per} (peritectic) is defined as the cut off temperature. When the temperature of a cell drops below T_{per} all remaining rich solute liquid turn to solid.

Fig. 4.16 shows a representation of a steady state weld pool at time t and $t + \Delta t$ and the orientation of the micro control volume (typically $n \times n \times m$) for the solidification analysis. It is along the direction of maximum heat flow.

Figure 4.16: Two snapshots of solidification process in the bounded by the control volume at times t and $t + \Delta t$ for a weld pool with the traveling speed V towards the left.

4.7.3 No. 3: Carbon Diffusion Solver

As the domain is cooled down to the room temperature, the transient carbon distribution is computed by solving the diffusion equation for the diffusion of carbon in the solid micro-model solved with, initial carbon composition from solidification solver,

zero flux, i.e., zero Neumann BCs, with an implicit conjugate gradient FEM solver. This conserves the mass of carbon.

4.7.4 No. 4: Microstructure Analysis

The solid state phase transformation of austenite to pearlite, bainite and/or martensite in a weld uses Watt-Kirkaldy algorithm.

4.7.5 No. 5 and 6: Stress Solvers

As the solid is cooled from solidification to room temperature, in a similar way to the HAZ microstructure (section 3.14.6), a quasi-static thermo-visco-plastic-elastic stress analysis is done with traction boundary conditions from the stress in the macro-model at this point. Then, a stress-strain analysis of a uni-axial tensile test is run at room temperature that is initialized with the microstructure, residual stress and residual strain after cool down to room temperature.

4.8 Demonstration Example, Fusion Zone

Note that the whole fusion zone microstructure framework for the micro-model provides results only for the one macro spatial point selected in the fusion zone of a specific macro-model of a weld in welded structure. Any number of macro spatial points can be selected but each must be processed separately and a separate report is prepared for each macro spatial point. The framework would be repeatable for any given weld process, weld procedure, and material. The results for one point in a macro-model fusion zone of a weld are provided here as an example.

Table 4.2: Welding parameters used in welding simulations (Fig. 4.17).

Project	Weld speed, m/s	Input power ($V \times I$), W	Arc efficiency	Double ellipsoid f, r, d, w
W1	0.0226	26×394	0.9	0.003, 0.017, 0.003, 0.003

4.8.1 Thermal Analysis

A weld is made on a steel plate (0.11 C 1.4 Mn 0.225 Si 0.5 Ni- 0.2 Mo- 0.5 Cr) using an FEM weld model. The parameters taken from the weld procedure of a submerged arc weld (SAW) weld ([64]) listed in Table 4.2. On the liquid-solid interface of the quasi-steady state weld pool, sample points *A* and *B* were chosen. Fig. 4.17 shows the temperature distribution around the weld pool as well as the thermal cycle for the two sample points on the liquid-solid interface. Point *B* is selected in order to demonstrate how the framework operates.

Figure 4.17: Thermal cycle of the sample points on the iso-surface at the liquidus temperature.

Table 4.3: Properties of alloying components used for the solidification analysis.

Properties	Symbol	Units	Value
Initial concentration (Carbon)	c_0^C	$wt\%$	0.11
Initial concentration (Manganese)	c_0^{Mn}	$wt\%$	1.2
Distribution coefficient (Carbon)	k^C	—	0.17
Distribution coefficient (Manganese)	k^{Mn}	—	0.73
Liquidus line slope (Carbon)	m_l^C	$K/wt\%$	-81
Liquidus line slope (Manganese)	m_l^{Mn}	$K/wt\%$	-5.1
Diffusion coefficient (Carbon)	D_l^C	m^2/s	2.32×10^{-8}
Diffusion coefficient (Manganese)	D_l^{Mn}	m^2/s	3.83×10^{-9}
Gibbs-Thompson coefficient	Γ	mK	2×10^{-7}

4.8.2 Solidification Test

A grid size of $80 \times 80 \times 500$ for point B was created and cell size of $0.75 \mu m$ was chosen. The temperature for the thermal cycle is mapped from the macro-FEM weld model. Table 4.3 shows the parameters used for the solidification analysis. Fig. 4.18 illustrates phase field, and solute distributions in the domain for the steady state condition. A sample can be taken from the fully solid region in order to do solid state solute diffusion, microstructure evolution and stress-strain evolution.

4.8.2.1 Partial mesh from the Dendrite Mesh

The idea is to take a smaller sample out of the micro-domain in the steady state regime in the solidification project. This saves computational time for the subsequent solvers in the framework, carbon diffusion, micro-structure, cool down stress and room temperature tensile analysis. A partial mesh can be $m \times n \times l$ in size and should be taken from the steady state fully solid region of the solidification project. The average fraction solid vs height can be used to construct such a mesh. The idea of making

Figure 4.18: Solidification solver results; Top: average phase field, Middle: carbon distribution Bottom: Manganese distribution.

a sub-domain mesh is illustrated in Fig. 4.19. The xyz mapping is used to map composition fields from a dendrite project into the microstructure project.

Figure 4.19: Making partial mesh based on average fraction solid.

4.8.3 Carbon Diffusion Analysis

The FEM solute diffusion solver is initialized with the carbon and manganese composition map from the dendrite solver. Diffusion of other substitutional alloying components such as manganese are ignored since their diffusion coefficient is about $1e3$ times smaller than that of carbon. However they do change the diffusivity of C in Fe. The temperature as a function of time is taken from the FEM thermal analysis (Fig. 4.17). Fig. 4.20 shows the carbon field initialized from the solidification solver

Figure 4.20: Carbon distribution from the carbon diffusion solver; Left: immediately after solidification is completed Right: at the room temperature.

(point *b* in Fig. 4.15) and the the final distribution (point *c* in Fig. 4.15).

4.8.4 Microstructure Analysis

To do the Watt-Kirkaldy microstructure analysis, the FEM micro mesh is initialized with the composition map of carbon and manganese from the dendrite solver. For each time step, the carbon field is imported as data from the FEM solute diffusion solver for carbon. The temperature evolution is taken from the thermal cycle of a sample point in a macro model. The analysis gives the microstructure evolution. Also the hardness map is reported for the microstructure at the room temperature.

For the decomposition of austenite below T_e to pearlite, bainite and/or martensite, the Watt-Kirkaldy microstructure model results are shown in Fig. 4.21.

4.8.5 Transient Thermal Stress Analysis Results

Before doing the uni-axial tensile test on a micro mesh, the transient residual stress-strain from solidification to room temperature are computed. Each phase evolving

Figure 4.21: Microstructure solver results; Final ferrite, pearlite, martensite, bainite, austenite phase fields and hardness map.

during the cool down has its own thermo-mechanical properties. This stress solver used the phase IDs at each Gauss point from the microstructure and temperature from the thermal cycle as a data flow to do the transient thermo-visco-plastic-elastic stress analysis. We leave the application of BCs from the macro stress analysis to future work. Here we simply constraint the rigid body modes (zero Neumann BC). Examples of the transient effective stress and effective plastic strain fields are shown in Fig. 4.22.

Figure 4.22: Stress solver results at room temperature for the cool down transient stress-strain; Left: effective plastic strain and Right: effective stress.

4.8.6 Room Temperature Uni-axial tensile Test Results

Before doing a uni-axial tensile test, the domain is initialized with the phaseIds, residual stress and residual strain after cool down to room temperature.

The sample is then pulled in 20 displacement increments in the direction of the dendrite axis such that 4 % macro strain is applied to the sample ultimately. The effective stress field is shown in Fig. 4.23 at the last loading increment in the uni-axial

tensile test. The average stress is plotted vs strain shown in Fig. 4.23. Different stress-strain curves in different uni-axial test directions. are expected.

Figure 4.23: Room temperature uni-axial tensile test results; stress-strain curve.

Similar to the way described in section 3.15.5, 30 Gauss points were chosen randomly on the mid-cross section of the sample in order to estimate the variation of stress-strain state at spatial points in the sample and also the effect of residual stress-strain on the tensile test results.

Two cases are considered. They both use the evolved microstructure to room temperature. In case A, the residual stress-strain is not initialized from the transient analysis. In case B, the sample is initialized with the residual stress evolved on cooling from the melting point in addition to the room temperature microstructure. Both cases stretched in the x direction. σ_{xx} in the tensile test is plotted vs macro strain for a set of Gauss points in Fig. 4.25.

Figure 4.24: Room temperature tensile test results; Average stress macro strain.

Figure 4.25: Room temperature uni-axial tensile test results; stress-strain curve. Left: Case A. Zero initial residual stress, Right: Case B. with residual stress initialized on cooling from the melting point to room temperature.

4.9 Summary - Weld Fusion Zone Microstructure Framework.

1. Run a macro weld FEM or SPH analysis to get the temperature field in the neighborhood of the weld pool. This is done on a high resolution mesh for a given weld procedure and a given material in MatLib.
2. Pick points on or near the liquid-solid interface and find temperature vs time curves for the full thermal cycles.
3. Build a dendrite mesh for each of these points. This is a Cartesian grid (in this test, $80 \times 80 \times 500$) and the element size is about $1 \mu m$.
4. Setup a dendrite project for each point selected. Select alloying element and set the data flow to the FEM weld project in step 1. It uses temperature and temperature gradients from the FEM weld.
5. Run the dendrite project for each point until the domain is fully solidified.
6. Setup the carbon diffusion project using the same mesh or partial mesh. Take the carbon field from the dendrite project and thermal cycle from the macro-FEM weld. This would compute a new transient carbon field.
7. Setup the microstructure projects using the same mesh or partial mesh. Take the temperature from the FEM weld, manganese field computed by the dendrite solver and carbon field computed by the solute diffusion solver. Run FEM microstructure solver.
8. Compute hardness map in Watt microstructure solver when the FEM microstructure solver has cooled down.
9. Set up a stress project and compute the transient residual stress-strain from solidification temperature to cool down using the cooling curve and computed microstructure.

10. Create a uni-axial tensile test using the same mesh used for the microstructure, initialized with the residual stress-strain. Run tensile test with prescribed displacement to say a macro strain of 4 % in several time steps. Compute stress and strain and plot stress-strain curve.

Chapter 5

Conclusion and Suggested Future Works

5.1 A Holistic Macro-Micro Model for Welds and Welded Structures

To the authors knowledge, this is first examples of computational micro-models of the weld pool, FZ and HAZ that are integrated into a holistic computational model for welding a welded structure that could have multiple weld joints, with multiple electrodes in each any weld pass and with multiple wed passes with dissimilar metal weld joints. These are operational models, to change the welded structure, weld joint or weld procedure designs, simply requires changing the input data.

5.2 SPH Weld Pool Model

A Smoothed Particle Hydrodynamic (SPH) method was implemented to model the weld pool. The model solves the transient 3D non-linear energy equation for temperature and fraction solid and the Navier-Stokes equations for velocity and pressure. In the initial testing stage of the model, we concluded that

- This method is robust and has a capability to capture the transient behavior of

the weld pool. Large deformations and free surface are treated easily without requiring an unduly complex computational model.

- As long as computational resources allow, a high resolution weld pool can be modeled. With the current machinery a weld pool with 500 K to 1M particle can be modeled without difficulty within a reasonable physical time and particle spacing of 0.1 mm.
- Since each particle carries its own material type, mixing and dilution can be captured very well. This is important for the welds in which filler metal composition and material properties are very different from that of base metal. This means that composition at any spatial point in the weld pool is different from both filler and base metal. This affects the microstructure and stress of that point as it evolves in time. SPH can provide an average composition for each spatial point in the fusion zone which can be used as input data for the fusion zone microstructure framework.
- The effect of droplet size, frequency and impact speed has a great influence on the weld pool disturbance and mixing behavior of the weld pool. Simulation using the known data for the droplet frequency, size, and velocity confirms this effect. Experiments are needed to validate this.

5.2.1 Suggested Works for the Model Improvement

- The SPH method, including the current model, suffers from the poor approximation of the density near the boundary. This is due to the fact that there are no particles beyond the boundary to contribute in the summation for the density. The change in density results in change in pressure which generates the force due to the pressure gradient. One possibility is to initialize the system

after equilibration. As an example, 2D and 3D droplets can be equilibrated and cached in a library. They can be inserted to the model at any time at an equilibrium state.

- To avoid allocating computing resources to the regions where high resolution particles are not necessary, a two scale SPH can be used as proposed by Solenthaler [65]. The idea is almost identical to that in FEM where a coarse and fine mesh descretization is used. A fine particle spacing can be used for the weld pool and coarse particle spacing can be used for the mushy and solid regions.
- One of drawbacks of SPH is using an explicit time integration scheme in which a large number of time steps is required. This is because time step size is determined by stability requirements. Implementing an implicit SPH solver for quasi-static or dynamic problems would be useful. A system of equations are generated which can be solved implicitly for the unknown degree of freedoms. This allows choosing longer time steps based on required accuracy.
- Add surface tension effects to the model.
- Add a magneto-hydrodynamic to model the plasma in the arc.

5.3 Fusion Zone Microstructure

A computer model was presented which describes the columnar dendritic growth mechanisms during the weld pool solidification considering capillary and constitutional under-coolings as the two main driving forces for the solid-liquid interface progression. This procedure results in computing a dendrite structure and solute segregation in the domain. The process was tested using the temperature mapped from a macro weld analysis (SPH or FEM) into the micro dendrite domain. The composition map from

the dendrite analysis were used for the microstructure analysis to compute different phases formed during the cool down. A transient micro stress-strain from melting point to room temperature was performed and a room temperature tensile test analysis was done. The process generates a Latex-pdf report including compositions map at different stages of the cooling cycle, room temperature microstructure, hardness map and stress-strain curve.

- Two main challenges in the dendrite simulation were using a large enough domain and choosing a sufficiently fine element size to resolve the curvature of the tips. This results in a large domain size that may lead to a long CPU times.
- To increase the performance and accuracy, adaptive mesh refinement can be used for the dendrite tip region where a coarse mesh is used for the regions that are fully solid or mushy regions.
- Different curvature computation algorithm can be used in order to manage fluctuations and very high local curvature values which causes very high local interface velocities.
- Fully automate the procedure such that a general user is only required to select a sample point in the weld fusion zone and setting all computing procedure will done in the background by a software wizard. This would make it easy to define a DOE matrix and run multi-projects to explore a design space.
- It is planed to to add high order phase diagrams to deal with variations in substitutional alloying elements and to deal with alloys other than low-alloy steels, e.g., stainless steels, Inconels, aluminium alloys and cast irons. This is important for modelling fusion zone microstructures because of segregation during solidification and because of mixing and dilution of filler metal and base metal, particularly in dissimilar metal welds.

- Solidification in the Micro Domain With Latent Heat Release at the Interface

In the current code temperature is prescribed in the dendrite domain as a linear function or mapped from a macro weld analysis in which no latent heat release during the solidification is considered. It would be better to input the latent heat release at the interface into the micro problem. Then add the source term, $L_m df/dt$ where L_m is latent heat of fusion, in the energy equation by using the information from the dendrite solver.

5.4 Heat-Affected Zone Microstructure

An implementation of a synthetic microstructure was implemented that has the capability to match a given known microstructure data for the initial microstructure. Each grain in a generated synthetic microstructure has its phase type and its own composition. Contrary to the work of Kirkaldy [39] that assumes homogenous composition, the synthetic microstructure can give a more realistic initial phase and alloying component distributions. The microstructural changes are then driven by the thermal cycle, the phase diagram and solute diffusivity for each individual grain.

In the next step, a ferrite-austenite transformation solver for the temperatures above T_e was implemented. A synthetic microstructure is initialized for this solver. The phase change is then driven by temperature and the diffusion of carbon. This means that the final shape of a grain would be different from that in the initial microstructure. In addition, the carbon distribution across each grain will not be constant and could decrease or increase from the middle to the interface. The model significantly improves the Watt-Kirkaldy model.

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Appendix A

SPH-Solution Steps

A.1 Introduction

Three SPH Energy solvers have been developed. The SPH Energy Solver that solves the energy equation with temperature as the independent variable, the energy equation with enthalpy and phase fraction as the independent variables, the energy equation with enthalpy and pressure as the independent variables. The SPH NS solver solves the momentum equation for velocity for compressible or for incompressible flow. For all SPH solvers, there are some common steps as well as specific steps for an individual solver that are described in the following sections.

A.2 Conservation of momentum: Incompressible Flow

Incompressible fluid flow motion can be described by the Navier-Stokes equations for an incompressible viscous fluid. Conservation of momentum in a material coordinate system is given by

$$\rho \frac{D\mathbf{v}}{Dt} = -\nabla p + \mu \nabla^2 \mathbf{v} + \mathbf{f} \quad (\text{A.1})$$

where $\mathbf{v}$ is the flow velocity, ρ is the fluid density, p is the pressure, μ is the dynamic viscosity (kg / ms), and $\mathbf{f}$ represents the body force vector per unit volume. For an incompressible flow, the velocity is divergence free and this viscosity acts on the deviatoric strain rate $\nabla \mathbf{v}$. In a compressible flow, one might have a volumetric viscosity that acts on the volumetric strain rate. The pressure for an incompressible flow is a Lagrange multiplier that enforces the incompressibility constraint that keeps the velocity field divergence free. In a compressible flow, pressure is a thermodynamic variable.

A.2.0.1 Conservation of Mass or Continuity Equation

Conservation of mass is given by the continuity equation. In a Lagrangian formulation it is given by

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} = 0 \quad (\text{A.2})$$

For incompressible flow, it is usual to enforce the constraint $\nabla \cdot \mathbf{v} = 0$. This is usually done by solving the Pressure Poisson equation. See Yabe's methodology.

A.2.1 Conservation of Energy with temperature as the independent variable

The conservation of energy equation in a Lagrangian formulation has the following forms

$$\begin{aligned}\rho c_p \frac{DT}{Dt} &= \nabla \cdot (\kappa(T) \nabla T) + Q \\ \rho \frac{DH}{Dt} &= \nabla \cdot (\kappa(T) \nabla T) + Q\end{aligned}\tag{A.3}$$

where ρ is the local density of the medium, c_p is the specific heat, T is the temperature (K), and $\kappa(T)$ is the temperature-dependent thermal conductivity. In the second form, DH/Dt is the rate of change of specific enthalpy, i.e., $H(T) = \int_{T_{Ref}}^T c_p dT$. The formulation assumes that there are no phase changes.

A.2.2 Conservation of Energy with Enthalpy and Phase Fraction

In this formulation, we deal with the energy equation that allows phase changes with zero velocity.

In this second form, DH/Dt is the rate of change of specific enthalpy and the latent heat due to a phase change with latent heat $f_i(T)L_{f_i \rightarrow f_j} df_i$ due to change in mass or volume phase fraction df_i , i.e.,

$$h(T) = \int_{T_{Ref}}^T c_p dT + \int_{f_{ref}}^{f_i} f_i(T) L_{f_i \rightarrow f_j} df_i.\tag{A.4}$$

In this formulation we assume that there are phase changes. This effectively uses the

Bousinesq approximation for changes in density.

A.2.2.1 FEM Thermal Solver

All of our FEM thermal solvers solved the correction to the temperature with the right-hand side the current residual. From the temperature correction in a Newton-Raphson iteration, a correction to the nodal enthalpy is computed. This is or should be true for all of SPH Thermal solvers. The SPH Thermal solver should not compute pressure. Only the SPH NS for compressible flow computes pressure and velocity. The SPH NS solver should never update enthalpy or temperature.

Combining $G c_p DT + G DH_{Latent} = G DH$ where G is the Gram matrix and DT and DH are temperature and enthalpy increments, we write

$$\begin{aligned}
 c_p G (dT) + \delta \theta K (dT) + G (dH_{Latent}) = \\
 -G DH \\
 -K (\delta(\theta DT + T_1)) \\
 -\delta \theta S_3 - \delta (1 - \theta) S_1
 \end{aligned} \tag{A.5}$$

For some solving strategies such as domain decomposition it is an advantage to compute the residual from the global stiffness matrix for a given linearization. This can be achieved by writing $DH = c_p DT + LDFs$, setting $G (dH_{Latent}) = 0$ and then rewriting the above equation in the following form in which $(c_p G + \delta \theta K)$ is the global stiffness matrix. In Eq. A.6, RHS, the two terms in square brackets can be viewed as the internal nodal thermal load and the external nodal thermal load. If Dirichlet values on a sub-domain in a domain decomposition solver change, i.e., DT changes, then only the first term in square brackets needs to be recomputed to evaluate the RHS vector for a new linear solve.

$$\begin{aligned}
& (c_p G + \delta \theta K) dT = \\
& - [(c_p G + \delta \theta K) DT] \\
& - [GLDfs - \delta \theta K T_1 - \delta \theta S_3 - \delta (1 - \theta) S_1]
\end{aligned} \tag{A.6}$$

A.2.3 Conservation of Momentum: Compressible Flow

The flow motion can be described by the Navier-Stokes equations for an compressible viscous fluid coupled with the conservation of mass and energy. (Unlike incompressible flow, compressible flow cannot be solved without coupling to the energy equation.)

Conservation of momentum in a material coordinate system is given by

$$\rho \frac{D\mathbf{v}}{Dt} = -\nabla p + \mu \nabla^2 \mathbf{v} + \left(\zeta + \frac{1}{3}\mu\right) \nabla(\nabla \cdot \mathbf{v}) + \mathbf{F} \tag{A.7}$$

where $\mathbf{v}$ is the flow velocity, ρ is the fluid density, p is the pressure, μ is the dynamic viscosity(kg/ms), $\zeta = \lambda + \frac{2}{3}\mu$ is often called the coefficient of bulk viscosity, and $\mathbf{f}$ represents the body force vector per unit volume. This viscosity acts on the deviatoric strain rate $\nabla \mathbf{v}$. In a compressible flow, one might have a volumetric viscosity that acts on the volumetric strain rate. The pressure field for a compressible flow, is a thermodynamic variable.

A.2.4 Conservation of Mass

Conservation of mass is given by the continuity equation. In a Lagrangian formulation, it is given by

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} = 0. \quad (\text{A.8})$$

Note that now the density ρ is usually time dependent.

A.2.5 Solve the Energy Equation in Terms of Temperature

- Create an FEM mesh and position one particle at the centroid of each FEM element. This positions the particles in a grid (Sec. 2.7.1).
- Assign particle type (Sec. 2.7.2)
- Assign the particle attribute and material properties to each particle (Sec. 2.7.3).
- For each particle, for each sub step, the code computes the list of nearby particles (Sec. 2.7.4).
- Compute mass of each particle in each part based on the volume of the element and the reference density for that element (Sec. 2.7.5).

To solve the energy equation for the transient temperature with zero velocity, for any particle s ,

1. Compute the density (using Eq. 2.4).
2. Define the initial temperature or enthalpy.
3. Apply boundary condition, Dirichlet, flux or convection BCs.
4. Compute the rate of change of the internal energy per unit mass (using Eq. 2.43).
5. Update the temperature, enthalpy or internal energy using an integration scheme.
6. Compute temperature at any position in the domain using SPH interpolating function.

Note that SPH energy equation is solved in terms of temperature. If the latent heat is considered, the initial phase fraction is defined and then temperature is corrected

using enthalpy-temperature relation at a constant pressure in each time step. If latent heat and pressure needed to be considered, initial phase fraction is defined and then temperature is corrected using enthalpy-pressure-temperature relationship in each time step.

A.2.5.1 Verification Test problems for the Energy Equation in Terms of Temperature

The following tests were set up:

A.2.5.1.1 Heat conduction in a semi-infinite bar. See reference [66] for the analytical solution.

TestSuite project name: SPHVerification-SPHEnergy-SemiInfiniteSlab

A.2.5.1.2 Heat conduction in a composite bar. See page 236 of reference [22] for the description.

TestSuite project name: SPHVerification-SPHEnergy-Cleary1999-Section5.1-P236

A.2.5.1.3 Heat conduction in a bar with discontinuous thermal conductivity. See page 243 of discontinuous [22] for the description.

TestSuite project name: SPHVerification-SPHEnergy-Cleary1999-Section6.2-P243

A.2.5.1.4 Heat conduction in a bar with sinusoidal initial temperature. See page 249 of reference [22] for the description.

TestSuite project name: SPHVerification-SPHEnergy-Cleary1999-p249

A.2.6 Solve the Energy Equation in Terms of Enthalpy and Phase Fraction

In order to solve the energy equation in terms of enthalpy and phase fraction, do the following setting:

Set up $\longrightarrow$ Process Parameters $\longrightarrow$ SPHParticleEnergy

Set the Solidification flag to 1

With this setting, the solver does the correction to the temperature based on the Enthalpy-Temperature relationship defined in material library.

A.2.6.1 Verification Test problems for the Energy Equation in Terms of Enthalpy and Phase Fraction

The Stefan problem was simulated using SPH. See page 691 of reference [67].

TestSuite project name: SPHVerification-SPHEnergywithEnthalpyPhaseFraction-StefanProblem-Monaghan2005-P691

A.2.7 Solve the Momentum Equation in terms of Velocity and Pressure for Weakly Compressible Flow

Force balance equation is solved for each particle for the acceleration vector $\mathbf{a}$. From $\mathbf{a}$, velocity vector $\mathbf{v}$ and displacement or position are computed by the integration. Verlet time integration scheme is discussed in Sec. .

1. Create an FEM mesh and position one particle at the centroid of each FEM element. This positions the particles in a grid (Sec. 2.7.1).
2. Assign particle type (Sec. 2.7.2)
3. Assign the particle attribute and material properties to each particle (Sec. 2.7.3).
4. For each particle, for each sub step, the code computes the list of nearby particles (Sec. 2.7.4).

5. Compute mass of each particle in each part based on the volume of the element and the reference density for that element (Sec. 2.7.5).
6. Define the initial states, initial velocity, acceleration.
7. Compute the density (Using 2.4).
8. Update boundary condition.
9. Compute the rate of change of the velocity.
10. Update the velocity, position. Verlet scheme is used for the time integration.

A.2.7.1 Verification Test Problems

The following test was set up in order to qualitatively check the correctness of the SPH NS solver. A column of fluid collapses under the gravitational force. One may check the effect of speed of sound on the fluid behavior. Lower speed of sound will result in more compression and higher density for the compressed fluid at the bottom.

TestSuite project name: SPHNS-SummationDensityTest

A.2.8 Solve the Coupled Energy and Momentum Equations

A.2.8.1 Verification Test problems for the Coupled Incompressible Flow and Energy Equation in Terms of Temperature Changes

Heat transfer by conduction and convection. See page 315 of reference [68] for the description.

TestSuite project name:

SPHVerification-AdvectionDiffusion-Chung-P315-SPHEnergy

SPHVerification-AdvectionDiffusion-Chung-P315-SPHNS

A.2.9 Time Step Size

For a transient dynamic problem, time step size, δ is limited by stability in an explicit time integration scheme. In this case, the stability requirement is normally controlled by the Courant, Friedrichs, Lewy (CFL) condition expressed as

$$\delta = CFL \frac{h}{c_s} \quad (\text{A.9})$$

where the value of CFL is between 0 and 1 and c_s is the speed of the sound. Using the real bulk modulus of a material can result in a very small time step size. In order to reduce CPU time for problems in which we are not interested in stress waves, an artificial smaller bulk modulus is used which gives an artificial slower speed of sound. Note that according to [69] the time step size is controlled by viscosity for highly viscous flows. Eq. A.9 is used in the present model to determine the time step size for explicit solver. The time step size requirement given in other references are discussed next. Cleary [70,71] suggests the time step size as

$$\Delta t = \min_a \left(\frac{0.5h}{c_s + \frac{2\xi\mu_a}{h\rho_a}} \right) \quad (\text{A.10})$$

where the minima is over all particles ‘a’ and μ_a is the dynamic viscosity of particle ‘a’. ξ is undefined in Cleary 2002 but it is defined in Cleary 1998 p 873, just below Eq. 4 to have the value $\xi = 4.96333$. Cleary 1998 claims this value is independent of the value of the viscosity. ξ is a constant calibration factor for the viscosity. The local sound speed in each time step is assigned a value $c_s = 100 V^2$ where V is the maximum particle speed in the domain. Bonet and Lok [21] use the following statement for the time steps size in their work.

$$\Delta t = CFL \left(\frac{h_{min}}{\max(c_s + \|\mathbf{v}_a\|^2)} \right) \quad (\text{A.11})$$

where the maxima is over all particles ‘a’, $0 < CFL \leq 1$ is the Courant Number for the assigned sound speed, $c_{max} = m\|v_{max}\|$ and $k = c_{max}^2 \rho / \gamma$, m is a scaling parameter that was chosen in the range $[10, 1000]$ and $c_s = \sqrt{\gamma k / \rho}$ is the speed of sound.

(k is the same as the constant B used in the equation of state (Eq. 2.33))

A.2.10 SPH Thermal Time Step Length

Cleary [22] suggests the following equation to compute the time step size for the explicit time integration.

$$\Delta t = \beta \rho c_V h^2 / k;$$

where ρ is density, c_V is specific heat at constant volume, h is particle spacing and k is thermal conductivity. β is a scaling factor chosen to achieve stability. Doing a wide range of test problems [22] suggests assigning a value of $\beta \leq 0.15$ for stable integration. For example, for $h = 1.2\Delta x$ and $\beta = 0.1$ the above equation becomes

$$\delta = 0.144 \frac{\rho c_v \Delta^2 x}{\kappa} \quad (\text{A.12})$$

which suggests a Fourier number of 0.144.

A.3 Time Integration

Having the acceleration vector computed, the Verlet algorithm [72] is used to compute velocity and position vectors at time $n + 1$ as

$$\begin{aligned}
 \mathbf{a}_a(n+1) &= \frac{d\mathbf{v}_a(n)}{dt} \\
 \mathbf{v}_a(n+1) &= \mathbf{v}_a(n) + 0.5\delta [\mathbf{a}_a(n+1) + \mathbf{a}_a(n)] \\
 \mathbf{r}_a(n+1) &= \mathbf{r}_a(n) + \delta\mathbf{v}_a(n) + 0.5\delta^2\mathbf{a}_a(n) +
 \end{aligned} \tag{A.13}$$

Appendix B

SPH Model-Verification Tests

B.1 Introduction

In order to ensure that the SPH code gives the expected accuracy for a certain problem, a series of test problems were set up to compare the SPH modeling results with known exact solutions or trusted numerical solutions. The following tests were considered for SPH Solver's verification:

B.2 SPH Energy

- 2D Transient heat diffusion in a semi-infinite bar. See B.2.1 of this document.
- 2D Transient heat diffusion in a finite composite bar.
(Cleary, Sec 5.2., and 5.3. [22])
- 2D Steady state heat diffusion in a finite composite bar with fixed end temperatures.
(Cleary, Sec 6.1., 6.2., and 6.4. [22]).
- 2D Transient heat diffusion in a finite bar with disordered particles. See B.2.2
(Cleary, Sec 8. [22])
- Uniform temperature raise in a bar due to constant volumetric source.

- 2D Solidification test, Stefan problem, See B.2.4 of this document.

(Monaghan 2005, Sec 3.1. p 690 Figure 1 [67]).

B.2.1 Heat Conduction in a Semi-infinite Bar

This test verifies that the SPH-Energy code models the 1D heat diffusion in a semi-infinite slab correctly. Note that, for all SPH Energy tests given in this document, the simple Forward Euler scheme is used for time integration.

For a semi-infinite bar with initial temperature T_0 and Dirichlet temperature T_1 at $x = 0$, the exact solution is given by

$$T(x, t) = (T_1 - T_0) \operatorname{erf}\left(\frac{x}{2\sqrt{\alpha t}}\right) + T_1 \quad (\text{B.1})$$

where α is the thermal diffusivity. To set up a SPH test problem, a 50×5 particle grid with the spacing $\Delta x = 0.02$ is built. All considered parameters are $h = 1.2\Delta x$, $\rho = c = \kappa = 1$ and $T_1 = 1$ and $T_0 = 0$. Figure B.1 shows the grid configuration. Figure

Figure B.1: 2D error function test set up.

B.2 displays the comparison between exact and SPH solution at 3 different times.

Figure B.2: Comparison between SPH and exact solutions at $t = 3s$, $t = 18s$, and $t = 36s$. Empty circles represent SPH results.

B.2.2 The Infinite Composite Solid

Suppose that we have two regions with the plane of separation located at x_0 . For region $x > x_0$, κ_1 , ρ_1 , c_1 , the initial temperature is T_0 . For region $x < x_0$, κ_2 , ρ_2 , c_2 , the initial temperature is 0. The transient temperature distribution in each region has the following form [66].

(Note! the equation given by [22] has an important typo error.)

$$T_1(x, t) = \frac{\kappa_1 \sqrt{\alpha_1} T_0}{\kappa_1 \sqrt{\alpha_1} + \kappa_2 \sqrt{\alpha_2}} \left\{ 1 + \frac{\kappa_2 \sqrt{\alpha_2}}{\kappa_1 \sqrt{\alpha_1}} \operatorname{erf} \left(\frac{x - x_0}{2\sqrt{\kappa_1 t}} \right) \right\} \quad x > x_0 \quad (\text{B.2})$$

$$T_2(x, t) = \frac{\kappa_1 \sqrt{\alpha_1} T_0}{\kappa_1 \sqrt{\alpha_1} + \kappa_2 \sqrt{\alpha_2}} \left\{ \operatorname{erfc} \left(\frac{|x - x_0|}{2\sqrt{\kappa_2 t}} \right) \right\} \quad x < x_0 \quad (\text{B.3})$$

Note that when $\alpha_1 = \alpha_2$ both equations in Eq. B.2 and B.3 become identical. The SPH simulation is done on a mesh of 40×20 particles with, $\Delta x = 0.0125 \text{ m}$ and $h = 1.2\Delta x$ using $\rho_1 = \rho_2 = c_1 = c_2 = \kappa_1 = \kappa_2 = 1$ and $T_1 = 1$ and $T_2 = 0$. Fig. B.4 shows the comparison between the analytical solution and SPH solution for $t = 0.07 \text{ s}$,

Figure B.3: Heat Diffusion in a composite solid. Initial temperature in each region (top), and temperature distribution at $t=11$ s (bottom).

4 s and 11 s.

B.2.3 Transient Heat Diffusion in a Bar with Sinusoidal Initial Temperature Varying in x .

This is a test problem given in [22]. A square grid with 51×10 particles with spacing $\Delta x = 0.02m$ is constructed. Material properties used are $\rho = 10$, $c = 1$ and $\kappa = 1$ and $h = 1.15\Delta x$. Two sides have fixed temperatures with $T_l = T_r = 0$ and top and bottom are adiabatic. The initial temperature of particles is defined as

$$T_0(x, y) = A_n \sin\left(\frac{n\pi x}{l}\right) \quad (\text{B.4})$$

where $l = 1 - \Delta x$ is the length of the square. The initial condition satisfies the boundary condition at $x = 0$ and $x = l$. The exact solution for this problem is given

Figure B.4: Comparison between the transient analytical solution and SPH solution at $t = 0.07 \text{ s}$, 4 s and 11 s .

as (Sec 3.3. in [66])

$$T(x, y, t) = A_n \sin\left(\frac{n\pi x}{l}\right) e^{-(n\pi/l)^2 \alpha t} \quad (\text{B.5})$$

Figure (addref) shows the comparison between the analytical solution and SPH solution.

B.2.4 Solidification Test

The solidification test is set according to the SPH example given by [67]. In this test which is basically the known Stefan problem, the jump in the heat flux at the melting interface is given by

$$\kappa_l \frac{\partial T_l}{\partial x} - \kappa_s \frac{\partial T_s}{\partial x} = \rho L_m V_{in} \quad (\text{B.6})$$

Figure B.5: 2D Heat Diffusion in a Bar with Sinusoidal Initial Temperature, Comparison between SPH and the exact solution at $t = 0.02$ s, 0.5 s and 1.5 s.

where κ_l and κ_s are thermal conductivity in liquid and solid phase respectively, L_m is the latent heat of melting and V_{in} is the interface velocity. Consider a semi-infinite bar with an initial uniform temperature of T_l which is above the melting temperature T_m . A fixed temperature T_s which is below the melting point is imposed at $x = 0$. There is an exact solution for the position of liquid-solid interface as well as the temperature distributions in both solid and liquid phases [67].

$$T(x, t) = T_s + \frac{T_m - T_s}{\text{erf}(\lambda)} \text{erf} \left(x \sqrt{\frac{\rho c}{4 \kappa t}} \right) \quad \text{in solid} \quad (\text{B.7})$$

$$T(x, t) = T_0 + \frac{T_m - T_0}{\text{erfc}(\lambda)} \text{erfc} \left(x \sqrt{\frac{\rho c}{4 \kappa t}} \right) \quad \text{in liquid} \quad (\text{B.8})$$

The interface position as a function of time is given by

$$x_{\text{interface}} = 2\lambda \text{erf} \left(\sqrt{\frac{4 \kappa t}{\rho c}} \right) \quad (\text{B.9})$$

A SPH problem is set up using 52 particle along x with spacing $\Delta x = 0.02m$ and $h = 1.2\Delta x$ and parameters $T_0 = 1.2$, $T_m = 1$, $T_s = 0.1906$ at $x = 0$, $\lambda = 0.5$. Material properties are set to $\kappa = 1$, $\rho = 1$, $c = 1$ for both liquid and solid phases. The bar should be long enough such that it satisfies semi-infinite assumption for the bar. The SPH solution of the temperature distribution in solid and liquid phases at $t = 0.0568s$ is shown in Figure B.6 which suggests a good agreement between SPH and the exact solution. The exact solution gives the interface position at $x = 0.238$.

Figure B.6: 2D Stefan Problem, Comparison between SPH and the exact solution.

B.3 SPH NS

- Hydrostatic pressure test.
- 2D Dam break test.
- 1D Rayleigh instability test-oscillating drop (Tartakovsky 2005, Sec 3. Figure 1 [73]) and (Nugent 2000 Sec 4. Figure 7 [74] and (Hu 2006, Sec 3.1. Figure 4 [75]) and (Morris 2000,Sec 8.3. Figure 6 [76])).

- 2D Couette flow test.
- 2D, 3D surface tension tests on a square (cube).
- Multi phase fluid interaction . (Hu 2006, Sec 3.2. Figure and 8 [75])

B.4 SPH Coupled

- 2D Steady state Convection-Diffusion test.
- 1D, 2D Sod shock tube tests. (Price 2012, Sec 6.3.4. Figure 8 and Fig. 10 [20])

B.4.1 2D Steady state Advection-Diffusion test

The purpose of this test is to demonstrate the effect of convective heat transfer verifying the coupled Navier-Stokes and Thermal SPH solvers. Consider a heat diffusion problem for a stationary fluid with two Dirichlet boundary conditions at the ends. The steady state solution is clearly linear. Now Consider another problem in which the fluid has constant velocity along x. In this case convective heat transfer is added to diffusive heat transfer. The exact solution [68] for such a problem is given by

Figure B.7: SPH set up for advection diffusion test.

$$T(x) = \frac{e^{Pe(x)} - 1}{e^{Pe} - 1} \quad (\text{B.10})$$

where $Pe = v/\alpha$ is the Peclet number in which, v is the fluid velocity and α is the thermal diffusivity.

The Peclet number can be looked at as the ratio of convective and diffusive heat transfer which is typically used to assess which phenomena is stronger. A high Peclet number suggests that the heat transfer by advection is dominant whereas, a small Peclet number suggests that heat transfer by diffusion is dominant in a thermal flow problem.

To set up a SPH test problem, a 52×10 particle grid with the spacing $\Delta x = 0.02$ is built (Figure B.7). All considered parameters are $h = 1.15$ and $T_{inlet} = 0$. Density, specific heat and thermal conductivity are set such that it gives the thermal diffusivity $\alpha = 0.2$

Three different speed $v = 0.01$, $v = 1$ and $v = 5 \text{ m/s}$ are tested. Note that we are seeking the steady solutions, so the problem should be solved for long enough times to reach the steady state solution. Note that, the problem should be setup such that all particles have uniform velocity along the x direction.

Figure B.8 shows the comparison between the exact solution and the SPH solution for three different speeds.

Figure B.8: Advection-Diffusion Problem, Comparison between SPH and the exact solution.