Numerical investigation of temperature distribution and melt pool geometry in laser beam welding of a Zr–1% Nb alloy nuclear fuel rod end cap

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Abstract. Zr–Nb alloys are used in the nuclear and chemical industries, in which the welding of an end cap to a fuel rod is a critical issue in manufacturing processes. To identify the optimal process parameters for achieving good-quality welds, it is necessary to investigate the thermal environment in the fusion and heat-affected zones. A three-dimensional computational fluid dynamics analysis is performed with a volumetric heat source by simulating the interaction of the heat source and the material and by accounting for the phase change during welding. The model incorporates the buoyancy force and Marangoni stress and generates the temperature distribution, weld bead geometry and fluid flow in the weld pool during the laser welding process.

Keywords. Computational fluid dynamics; fusion zone; heat-affected zone; laser beam welding; weld depth; zirconium alloy.

1. Introduction

Safe and economical operation of nuclear power plants depends primarily on the selection of materials and the processes of construction. End plug welding is a crucial welding process in boiling water reactors and pressurized water reactor technologies [1,2]. A hermetically sealed cladding tube with end caps is loaded with pellets. The fuel rod is designed as a pressure vessel to prevent failure of the cladding and the release of radioactive fission products. Defects in circumferential joints cause leaking of radioactive fission products during the irradiation process. The cladding tube and end caps are made of a zirconium alloy [3]. The assembly of the top and bottom end caps of a fuel rod with fuel pellets is shown in figure 1 [4].

The bottom end cap is welded circumferentially to an empty cladding tube at atmospheric pressure in a helium or argon environment in a welding chamber. Later, the fuel pellets are loaded and the fuel rod is evacuated. The top end cap is pressed against a plenum spring force. The rod and the welding chamber are pressurized with helium. The pressure is monitored and controlled to compensate for the change caused by the rise in the temperature during the welding process. Oxygen monitors are used in weld chambers to avoid air intrusion during welding. Upset shape welding, laser beam welding and electron beam welding processes are used in end cap joining. In upset shape welding processing, a high current is passed through the end cap, the cladding tube and the interface between them to generate a high temperature

[5]. The heated parts are forged together by pressing the end cap into the cladding tube. The laser beam welding process produces a deep penetration weld with a small heat-affected zone (HAZ). Welding is performed in an open atmosphere. CO₂ and Nd:YAG lasers do not require an evacuated welding chamber. To protect the weld pool from oxidation, the inert gas helium or argon or a mixture of both is used as the shielding gas. The weld properties depend on the weld geometry and microstructure changes during the process in the fusion zone (FZ) and HAZ [6,7]. Studies on laser welding simulations are categorized into four groups [8–25]: analytical solutions, thermal analysis using a conduction model with the effective thermal conductivity, thermal analysis including a convection component and a pure conduction model with a stress distribution described by finite element analysis.

This paper examines the effect of the laser process parameters on the weld bead geometry and thermal history during the laser welding of an E110 zirconium alloy end cap to the fuel rod assembly. A three-dimensional (3D) computational fluid dynamics (CFD) analysis is performed by incorporating the buoyancy force and Marangoni stress and using the temperature-dependent material properties.

2. Geometry and grid structure

The geometry of the top end cap and fuel rod is shown in figure 2. The tube has an outer diameter of 11.2 mm and a

Figure 1. Assembly of the top and bottom end caps of a fuel rod with fuel pellets [4].

Figure 2. End cap and tube assembly.

Figure 3. Computational domain.

thickness of 0.6 mm. A computational domain that is 20 mm in length and 11.2 mm in diameter is created, as shown in figure 3. It is divided into a ring with a width of 2 mm (called the source zone in which the laser heat source is applied at the centre) and the remainder (see figure 4). Figure 5 shows the selected grid structure, which is refined near the heat source and a coarse grid away from it. The source zone is divided into 75 components along the circumferential direction and 20 components with a width of 2 mm. The domain consists of 51,120 nodes and 58,432 elements. The laser source position is fixed, whereas the domain rotates with a specified angular velocity. The number of iterations was selected to achieve the maximum variations in the temperature and weld geometry properties within 2%. The composition of zirconium alloy E110 (wt%) is: 0.9–1.1 Nb; 0.015 Fe; 0.007 Ni; 0.004 Al; 0.003 Ti; 0.02 C; 0.004 Si; 0.05 O; 0.003 N; 0.001 H and

Figure 4. Portion of the source zone (green ring) and remainder.

balance Zr. Table 1 shows the physical properties of the zirconium alloy E110 [26,27].

3. Thermo-fluid analysis

The finite volume method code in ANSYS is integrated with user-defined functions (UDF) to examine the thermo-fluid phenomena in the laser welding process by solving the Navier–Stokes equations with the standard $k-\epsilon$ equations in the weld pool and mushy zone (MZ) regions [28]. The density, time and weld pool velocity are denoted as ρ , t and $\vec{V}$, respectively, and the continuity equation is:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0. \quad (1)$$

Using the liquid and solid mass fractions (f_L and f_S), the average density is evaluated as:

$$\rho = \rho_L f_L + \rho_S f_S = \rho_L f_L + \rho_S (1 - f_L). \quad (2)$$

The liquid mass fraction $f_L = 0$ for $T \leq T_S$ and $f_L = 1$ for $T \geq T_L$, whereas for $T_S \leq T \leq T_L$, $f_L = (T - T_S)(T_L - T_S)^{-1}$. Considering the static pressure (p), viscosity (μ) and gravitational body force ($\rho \vec{g}$), the momentum equation for the flow of liquid metal in the weld pool is [29]:

$$\frac{\partial (\rho \vec{V})}{\partial t} + \nabla \cdot (\rho \vec{V} \vec{V}) = -\nabla p + \mu \nabla^2 \vec{V} + \rho \vec{g} + \vec{S}_w. \quad (3)$$

Figure 5. Grid structure.

Table 1. Thermo-physical properties of E110.

Property	Empirical relation
Density, ρ (kg m^{-3})	$\rho = 6636 - 286\zeta$ for $T \leq T_m$ $= 6844.5 - 609.8\zeta + 205\zeta^2 - 44.783\zeta^3 + 3.265\zeta^4$ for $T > T_m$
Heat capacity, C_p ($\text{J kg}^{-1} \text{K}^{-1}$)	$C_p = 238 + 159\zeta$ for $T \leq 1100 \text{ K}$ $= 281 + 66.3\zeta$ for $1100 \text{ K} \leq T \leq T_m$ $= -1480 + 1745.88\zeta - 5.262\zeta^2 + 55.68\zeta^3$ for $T > T_m$
Thermal conductivity, κ ($\text{W m}^{-1} \text{K}^{-1}$)	$\kappa = 23.5 - 19.2\zeta + 16.8\zeta^2$ for $T \leq 1100 \text{ K}$ $= 1.5 + 20\zeta$ for $1100 \text{ K} \leq T \leq T_m$
Coefficient of volumetric expansion, β (K^{-1})	$\beta = 39 \times 10^{-6}$
Dynamic viscosity, μ (Pa s)	$\mu = 8 \times 10^{-3}$
Surface tension, σ (mN m^{-1})	$\sigma = 1459 - 0.244(T - T_m)$
Heat of fusion (J kg^{-1})	153,000
Melting point, T_m (K)	2130
Solidus temperature, T_S (K)	2098
Liquidus temperature, T_L (K)	2158
Boiling point, T_b (K)	4680
Surface tension gradient ($\text{N m}^{-1} \text{K}^{-1}$)	$\frac{\partial \sigma}{\partial T} = -0.000244$

$+\zeta = 10^{-3} T$ is for the empirical relations of ρ , C_p and κ .

The source term in terms of the MZ constant (A_{mush}) and pull velocity ($\vec{w}$) is:

$$\vec{S}_w = (1 - f_L)^2 (f_L^3 + 0.001)^{-1} (\vec{w}) A_{\text{mush}}. \quad (4)$$

Equation (4) represents the frictional dissipation of momentum in the MZ [30,31]. The enthalpy–porosity technique [32] is employed to trace the interface resulting from the phase change. Considering the thermal conductivity (κ) and volumetric heat source (S), the energy equation is written in terms of the enthalpy H ($\equiv h + \Delta H$) as:

$$\frac{\partial(\rho H)}{\partial t} + \nabla \cdot (\rho \vec{V} H) = \nabla \cdot (\kappa \nabla T) + S. \quad (5)$$

Here, $h = h_{\text{ref}} + \int_{T_{\text{ref}}}^T C_p dT$ is the sensible heat, C_p is the specific heat and h_{ref} is the reference enthalpy. The latent heat (ΔH) is zero for a solid, whereas $\Delta H = f_L L$ for a liquid, where L is the latent heat of the liquid metal. The normal velocity component to the flat weld pool top surface is zero. The shear stress in the momentum equation is:

$$\tau = \frac{\partial \sigma}{\partial T} \nabla T. \quad (6)$$

Convection and radiation boundary conditions are imposed on all surfaces using the lumped convection coefficient $h_c = 2.4 \times 10^{-3} \varepsilon T^{1.61}$ [33]. A transient heat flux due to the laser is considered on the top surface. Using the Stefan–Boltzmann

Table 2. Properties of SS304L.

Solidus temperature = 1697 K
Liquidus temperature = 1727 K
Specific heat of solid = 712 J kg ⁻¹ K ⁻¹
Specific heat of liquid = 800 J kg ⁻¹ K ⁻¹
Density of solid = 7800 kg m ⁻³
Density of liquid = 7000 kg m ⁻³
Thermal conductivity of solid = 27 W m ⁻¹ K ⁻¹
Viscosity = 0.007 Pa s
Temperature coefficient of surface tension = -0.00049 N m ⁻¹ K ⁻¹
Enthalpy of solid at melting point = 120 kJ kg ⁻¹

constant (σ_{SB}), emissivity (ϵ) and the ambient temperature (T_a), the energy balance is written as:

$$\kappa \frac{\partial T}{\partial z} = q - h_c(T - T_a) - \sigma_{SB}\epsilon(T^4 - T_a^4). \quad (7)$$

The Gaussian distribution of the volumetric heat flux in terms of the absorbed laser power (P), laser beam radius (r_0), current radius (r), current depth (y) and the total depth (Y) is:

$$q = \frac{2P}{\pi r_0^2 Y} \exp\left(1 - \frac{r^2}{r_0^2}\right) \left(1 - \frac{y}{Y}\right). \quad (8)$$

4. Validation of numerical simulations

The adequacy of the developed 3D heat transfer and fluid flow model is examined by performing numerical simulations for SS304L and comparing the results with the experimental data [34–36]. To have a comparison, the temperature-independent material properties shown in table 2 specified in the numerical computation [36] are mentioned in the present numerical simulations. With regard to experimentation, welding has been carried out on 152.4 × 25.4 × 9.5 mm plates using a Rofin Sinar DY-022 diode-pumped continuous wave Nd:YAG laser with a maximum power output of 2200 W. Figure 6 shows the weld depth and FZ width for input laser powers ranging from 1330 to 1980 W at a constant welding speed of 19.1 mm s⁻¹. Figure 7 shows the weld geometry for welding speeds ranging from 6.4 to 19.1 mm s⁻¹ at a constant input laser power of 1980 W. The simulated results in figures 6 and 7 agree well with the existing test results. Figure 8 shows the comparison of the experimental and simulated weld pool cross-section at a welding speed of 19 mm s⁻¹ and an input power of 1000 W. The black line separating melted weld pool from an un-melted base metal is the predicted profile from the finite element analysis for the isothermal solidus temperature of 1697 K [36], which resembles the present CFD-simulated weld profile. The present model can accommodate the temperature-dependent material properties. The generic nature of the model can be used for any material and fusion welding process with laser

Figure 6. Simulated and experimental weld dimensions of SS304L with different input laser powers at a constant welding speed of 19.1 mm s⁻¹.

beam specifying the material properties using UDF, which is being assessed by conducting case studies on different materials (viz., zircaloy-4, carbon steel and E110 (Zr-1% Nb)) [28,37].

5. Results and discussion

To examine the effects of the laser welding parameters on the temperature profile, fluid flow and weld bead profile on end plug joint, numerical simulations were performed for various laser-absorbed powers and welding speeds. The laser source is fixed and the cladding tube assembly is rotated at 1, 3 and 5 RPM to realize the cir seam weld joint. A full penetration joint occurs when the weld depth is 0.6 mm (the thickness of the cladding tube). Thermo-fluid analysis was performed on a 2 mm wide XY plane and a circular YZ plane passing through the centre of the laser heat source (see figure 3). When the laser beam strikes the metal, a portion of the absorbed energy is used to increase the enthalpy of the metal and the remaining portion is conducted into the solid base metal. In the initial stage, heat conduction is the major mode of energy transfer. As the laser-on time increases, the metal melts and fluid convection causes deformation of the free surface of the

Figure 7. Simulated and experimental weld dimensions of SS304L with different welding speeds and a constant input power of 1980 W.

Figure 8. Comparison of experimental and simulated weld pool cross-section of SS304L at a welding speed of 19 mm s^{-1} and an input power of 1000 W.

weld pool. The welding process influences the resulting phase components and their distribution in the FZ and HAZ, including the macro- and micro-segregation and microstructural morphology. The FZ is a homogeneous mixture of completely molten base metal (mass fraction, $f_L = 1$). The main driving forces for convective transport of heat and the resulting mixing of molten metal in the weld pool are the buoyancy force and surface tension gradient force. The microstructure in the weld FZ is expected

Figure 9. Weld pool shape for a power of 400 W and a welding speed of 3 RPM.

Figure 10. Weld depth with welding speed for the specified input power.

to change significantly owing to melting and solidification of metal at temperatures exceeding the effective liquidus temperature. Figure 9 shows the weld pool shape for a power of 400 W and a welding speed of 3 RPM. It also shows the MZ separating the FZ and HAZ.

The weld geometry depends on the power density, interaction time of the laser beam source and heat transfer in the weld pool. The power density (W cm^{-2}) is the ratio of laser power to the area of laser beam. The interaction time (s) is the ratio of the beam diameter to the welding speed. The heat transfer in the weld pool is mainly due to convection and the molten weld pool moves from inward to top or in the reverse direction, depending on the surface tension gradient that exists on the top surface of the pool. The convective movement within the weld pool influences the geometry of the weld.

Figures 10 and 11 show the variation of the weld bead geometry of the welding speed of 400 and 500 W for power inputs. The high weld depth and fusion width of the weld pool were observed at 500 W due to the high energy input. The weld depth increases with welding speed initially and decreases with further increase. The convective movement of the weld pool influences the welding speed to a certain level, causing an increase in the weld depth. With a further increase in the welding speed, the interaction time of the laser beam with the metal is found to decrease, which decreases the energy

Figure 11. FZ width with welding speed for the specified input power.

Figure 12. Weld pool maximum temperature with welding speed for the specified input power.

Figure 13. Velocity on the top surface of the weld pool.

input, resulting in a lower weld depth. The circumferential rotation of the component also influences the weld size due to the flow of the molten metal on the top surface. The weld depth is found to be high at 3 RPM and is the highest at these two welding powers, as shown in figure 10. The FZ width also follows the same trend as shown in figure 11. The maximum weld pool temperature depends only on the power density and not on welding speed, as shown in figure 12.

The velocity vectors and XY plane are shown in figures 13 and 14. A maximum fluid flow velocity of 25.11 mm s^{-1} is found for a laser absorbed power of 400 W. Figure 15 shows

Figure 14. Velocity in the XY plane of the weld pool.

Figure 15. Weld pool velocity with welding speed for the specified input power.

the increase of the weld pool velocity with welding speed and laser power. The velocity is strongly influenced by the surface tension gradient and surface temperature. For a power of 400 W, the temperature is 3480 K at the centre of the weld pool, whereas it is 2588 K at the end of the FZ. For the negative coefficient of the surface tension, the molten metal flows from the centre to the periphery of the weld pool.

The relative rate of heat transfer by conduction and convection is given by the Peclet number $P_e = L_R C_p \rho u / \kappa$, in which u is the velocity of the weld pool, ρ is the density of the liquid, C_p is the specific heat, L_R is the characteristic length taken as the pool radius and κ is the thermal conductivity of the liquid metal. In the present study, P_e is of the order 3 that indicates convective heat transfer, which plays an important role in the transport of heat in the weld pool. The rate of heat transfer due to convection is higher than that of heat transfer due to conduction.

The driving forces in the weld pool flow are the Marangoni force (Ma) and the buoyancy force. The ratio of Ma and Gr (where Gr is the Grashof number) shows the relative importance of these forces.

Figure 16. Temperature contour plot for the specified source zone power of 400 W and welding speed of 3 RPM.

Figure 17. Temperature contour plot on the YZ circular plane for the specified source zone power of 400 W and the welding speed of 3 RPM.

$$Ma = \frac{\rho L_R}{\mu^2} \frac{\partial \sigma}{\partial T} \Delta T, \quad (9)$$

$$Gr = g \rho^2 \beta L_B^3 \frac{\Delta T}{\mu^2}, \quad (10)$$

where g is the gravitational acceleration, ΔT is the difference between the peak temperature of the weld pool and the solidus temperature and L_B is the characteristic length for the buoyancy force in the liquid pool, which is approximated as one-eighth of the width of the weld pool [7]. In this study, the ratio Ma/Gr is of the order of 10^5 ; this value clearly establishes the weld pool flow, which is driven mainly by surface tension.

The effect of the laser power on the weld geometry is investigated for a welding speed of 3 RPM. Weld penetration of

Figure 18. Weld depth and FZ width with absorbed power for the specified welding speed of 3 RPM.

Figure 19. Weld pool maximum temperature with power.

Figure 20. Temperature on the XY-plane with the circumferential position.

74% of the full depth with a narrow FZ is achieved at an absorbed power of 400 W. Figures 16 and 17 show the temperature contours on the source zone ring and YZ circular plane, respectively. Figure 16 also shows the weld pool contour for $f_L = 1$ (outlined in black). These are helpful in predicting the weld pool microstructure. The power density or laser power with a constant beam diameter influences the weld size and weld pool temperature. Both the weld depth and FZ increase with an increase in power (see figure 18). The maximum weld pool temperature increases with an increase in power (see figure 19).

Figure 20 shows the variation of temperature on the YZ plane circular surface. It shows the temperature at various

Figure 21. Temperature variation in the axial (X) direction for 400 W at 3 RPM.

Figure 22. Width of MZ, HAZ and WZ with power.

points on the circumference of the weld centre line when the laser source is at 0° . The temperature drops steeply to 50% of the maximum weld pool temperature. The variation in temperature in the X direction (parallel to the fuel rod and end cap axis) from the weld line at circular positions of 90° , 180° and 270° , when the welding source is at 0° , is shown in figure 21. Figure 22 shows the influence of power on the weld zones (WZs). It shows negligible variation of the MZ width with laser power. The WZ and HAZ widths increase with an increase in power.

6. Concluding remarks

The welding of an end cap to an irradiation tube to form a fuel rod is a critical welding process in the nuclear industry. A 3D numerical heat transfer and fluid flow model was developed to simulate the evolution of the temperature and weld geometry, using a volumetric heat source during laser beam circumferential welding of the end cap to the cladding tube. Using this model, it is possible to select the optimal circumferential welding speed to achieve the required weld depth and FZ combination for the end cap and cladding tube. The weld pool dimensions are obtained in terms of the laser power and welding speed. The temperature profiles will be useful in

assessing the size of the HAZ and the microstructure in the WZ.

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