



Analysis on grain growth of SS316L induced by plasma cutting process using probabilistic FEM with experimental verification

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Abstract

This fundamental research was conducted to predict the grain size of austenitic stainless-steel after plasma cutting process using experiment and non-linear probabilistic numerical computation with self-developed algorithm which was written and compiled using Fortran-based subroutines and utility routines available in commercial FEM software. For grain modelling, the non-linear numerical programming codes consisted of fourth-order Runge–Kutta method for solving ordinary differential equation of grain growth formula with major parameters such as initial grain size, activation energy, and kinetic constant which were measured by using dilatometer on specimen samples at various temperatures and holding times. In order to replicate the actual thermal cutting process, customized conical heat source model was developed and employed. The probabilistic approach in numerical computation was executed using Monte Carlo method by setting major process parameter of input power based on normal distribution with defined mean and standard deviation which were randomized following linear congruential generator and Box-Muller algorithm. This comprehensive numerical computation based on deterministic and probabilistic FEM was established using nonlinear thermomechanical method with hexahedral element type including finer mesh on cutting section and coarser at base plate. For verification purpose, a series of experiments using fully automated system was carried out on SS316L plate with 4-mm thickness. From the analysis of results, acceptable discrepancy was achieved in grain size prediction obtained between numerical methods and experiment with the error percentage of up to 9.2% and 14.5% for probabilistic and deterministic analyses respectively.

Keywords Deterministic · Probabilistic · Grain size · Numerical Computation · SS316L

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1 Introduction

As one of the separating processes, thermal cutting is a very important method in fabrication industry. This process uses concentrated heat to be imposed on a metallic or non-metallic plate, causing the applied part to melt away. Typically, thermal cutting is an exothermal process where less heat is needed for maintaining the burning process. Main thermal cutting processes are flame, plasma arc, and laser cutting [1]. The most extensively utilized thermal cutting process is known as flame cutting due to its low-cost equipment and easy to handle. The flame cutting can be manually applied and also can be easily automated [2]. The flame cutting is also called as oxyfuel gas cutting and oxyacetylene cutting. This process is a thermochemical process that works by initially preheating the material to its ignition temperature which is lower than its melting point, and subsequently, the preheated area is subjected to pure oxygen jet to produce iron oxides which are then blown away by the oxygen jet to generate cut kerf that penetrating through the material. The flame cutting has the capability to produce good quality cutting which can be employed to cut material with the thickness ranging from 5 up to 120 mm [3].

In plasma arc cutting (PAC), the applied part of workpiece material is melted and partially vaporized away by extremely hot plasma gas that is produced through the combination of an arc with inert gas flow or pressurized air. Plasma arc is produced by means of heating the gas with an arc that results into partly ionized which is capable to conduct electricity. More accurate and hotter arc is generated by concentrating the plasma arc through a nozzle that can reach extremely high operating temperature of around 10,000 to 14,000 °C. Fast action of heating the gas when moving along the arc leads to expansion which then accelerates via the nozzle and focuses towards the workpiece. High speed of plasma gas jet is utilized to get rid of the molten materials. Types of gases that are typically used for plasma cutting process consist of air, argon, oxygen, nitrogen, and mixture of argon and hydrogen as well as mixture of nitrogen and hydrogen [4, 5].

Laser cutting is an advanced non-contact thermal cutting process which can avoid effects like tool wear, vibration of machine, and mechanically induced thermal damage [6]. Laser cutting can be used for nearly all types of materials such as metals, non-metals, composites, and ceramics. It has the capability to produce complex shapes and various geometries with the narrow kerf. As stated in [7], instead of mechanical properties, the potential of laser cutting primarily depends on thermal and optical properties. A cut kerf is formed by the action of removing the molten material as the assist gas blows it away where the molten material is produced as a result of locally focused laser beam onto the material.

Numerous thermal analyses have been performed by means of numerical methods. A thermomechanical numerical analysis was conducted on carbon steel material to observe the effects of flame cutting parameters on HAZ (heat affected zone) size [8]. The simulated HAZ size was found to be closer to the actual HAZ size obtained through experiment. The results showed that the increase in cutting speed led to decreasing in HAZ width at the center area. Meanwhile, the increase in ethylene (C_2H_4) flow rate caused the upper HAZ width to increase whereas the increasing flow rate of oxygen caused the widening of the lower HAZ width. Another research on numerical simulation of flame cutting on steel material had been performed in [9]. Referring to this research, a quasi-stationary state model can be used when the flame size is far much smaller than the plate size with straight cutting line. In addition, the quasi-stationary state model was coupled with transport equations to describe the transition of phase based on transient Leblond-Devaux model. A portion of molten material was removed during cutting process resulting in the formation of heat-affected zone (HAZ) in the region around the cut kerf. The HAZ is the area where transitions of phases take place as a result of austenitization. It can be found that the HAZ and kerf widths were reduced when the cutting speed was increased.

In [10], a study on forecasting distribution of temperature induced by thermal cutting on Inconel 718 was carried out. The numerical computation was made based on thermomechanical analysis using temperature-dependent properties of material. From the results, it was found that the estimated temperature distribution was in good agreement with the actual temperature measurement. The trend of temperature provided by 2-mm thickness specimen was slightly higher than that of 1-mm thickness specimen. According to [11], arc cutting and arc welding processes were based on the similar basic principles in which some parts of materials were removed in cutting process, whereas some filler materials in welding process were normally added up to the base material to form the joint. Research on numerical simulation of multipassed welding distortion induced in combined joint by gas metal arc welding (GMAW) was conducted in [12]. Commercial software SYSWELD was used for predicting the distortion which was implemented through thermomechanical plus metallurgical analysis. Plasticity criterion calculated using isotropic strain hardening caused by non-cyclic loading was defined for mechanical analysis whereas constitutive equation formulated by Leblond was defined for metallurgical history consideration. The results revealed that the angular distortion predicted through 2D analysis showed reasonable agreement with the prediction using 3D analysis. The 2D analysis has an advantage over 3D analysis in terms of computational time in which the 2D analysis was completed in much faster time compared to 3D analysis. A study on residual stresses produced in pipe girth weld of

316 stainless steel was carried out [13]. The residual stress prediction was computed through thermo-elastic-plastic mechanical analysis. The numerical analysis was implemented by means of three different hardening models comprising of isotropic, kinematic, and mixed hardening models which were computed depending on flow curves, bilinear-Ziegler rule, and Lemaitre-Chaboche model respectively. Comparing to experimental measurements, good predictions of axial stresses and hoop stresses were obtained through isotropic hardening model while the mixed hardening model provided the best prediction for hoop stresses. On the other hand, the numerical analysis via kinematic hardening model underestimated both predictions of axial and hoop stresses.

It is well known that finite element analysis is implemented typically based on deterministic method. However, in the deterministic analysis, even though all the criteria have been taken into account, it still leads to limited description of the characteristics of a system [14]. The research on complex phenomena like dynamic loading, inherent randomness of material, lack of data, and human error has always come up with various sources of uncertainty. In order to enhance the classical FEM, other new numerical approaches have been added up in the analysis which considered the uncertainty of parameters. This new type of analysis is identified as a stochastic finite element method [15], a random finite element method [16], and a probabilistic finite element method [17]. In addition, to enable the variation of stochastic scenarios, random fields are applied in the analysis for characterizing the nature of stochastic in the system. To determine the effects of random variations, the statistical information of the response variables is assessed by including the calculation on the probability of system output. In [18], research was conducted on optimization of laser cutting parameters via probabilistic FEM. The process parameters involved in the CO₂ laser cutting of stainless steel 304 comprised of travel speed, assist gas pressure and focus position, laser power, and kerf taper angle which were connected in the analysis through the implementation of artificial neural network-based mathematical model using Monte Carlo (MC) method. MC method is considered as a common mathematical tool used in numerical simulation for solving numerous problems which are operated by manipulating random numbers in the programming algorithm. The statistical result of kerf taper angle demonstrated good accuracy when compared to experimental measurement. The MC method was found to have the capability to minimize the kerf taper angle by optimizing the laser cutting parameters. Furthermore, an acceptable kerf taper angle was achieved by focusing the laser beam on about two-third of the thickness of material with the application of low assist gas pressure of 9 bar and also combining high cutting speed of 3 m/min with low laser power of 1.6 kW. The optimization through MC simulation could be resolved by generating random numbers that were

uniformly distributed in the range between 0 and 1. To fulfill the limitations of parameter values, manipulation of the random numbers was implemented with the purpose to generate uniformly distributed random numbers for each of the laser cutting parameter which was laid within the range of interest that could be accomplished.

A huge number of input parameters are involved in predicting oil and gas reserves and resources particularly in complex projects [19]. The prediction via deterministic method was normally faced with limited capability in order to take the effects of uncertainties such as seismic, petrophysics, and porosity into consideration. Therefore, probabilistic method was preferred because its projection was made by considering a lot of uncertainties which could provide higher confidence levels in evaluation. The advancement in computing technologies would provide better assessments through intensive probabilistic method with artificial intelligence. Due to unbiased results produced by probabilistic method, it was used in predicting the mainstream of reserves and resources which could assist the practitioners to describe the downside and upside of the projects. Based on research in [20], probabilistic and deterministic methods were implemented to evaluate marine pipeline corruptions which could adversely affect the structural integrity. Among the weaknesses produced via deterministic analysis were lack of understanding in importance of various input parameters, lack of understanding in influence of every single failure mechanism, uncertainties in the physical models, as well as variables were not taken into consideration. However, these limitations could be overcome through the implementation of probabilistic analysis. The load and strength variables were fixed in deterministic analysis, whereas these variables were normally distributed in probabilistic analysis. The defect assessment triggered by the corrosion can be estimated through the comparison of calculated failure pressure with the load imposed on the pipeline. As for deterministic method, the assessment can be made where the capability of the pipeline to withstand against the load increased with the increasing value of calculated failure pressure. In probabilistic method, the assessment can be defined by comparing the calculated failure probability with respect to the service time where the pipeline was increasingly susceptible to fail when the failure probability approached the value of 1.0. Through deterministic analysis, the increasing defect length led to decreasing failure pressure and thus lowered the capability of the pipeline to resist against the exerted load. However, in probabilistic analysis, all the approaches showed that the failure probability of pipeline reached the value of 1.0 which indicated towards the pipe failure when its service time closes to 20 years. The evaluation made based on probabilistic method could provide higher reliability on

the aging corroded marine pipeline performance towards its remaining service lifecycle. Through the probabilistic analysis, the current performance of the aging pipeline in service could be better assessed as compared to the result obtained from the deterministic analysis.

Numerous researches on the calculation of grain growth were performed previously especially due to heat-induced processes such as welding process [21–23]. Study on behavior of grain growth using stainless steel material in consequence of cooling rates was conducted in [24]. Calculations of cooling rates were made through numerical analysis using phenomenological model, whereas the microstructural measurements of secondary dendrite arm spacing (SDAS) were conducted on the welded samples using scanning electron microscopy (SEM) for verifying the predicted results. The computed results were in good agreement with the actual measurements, and the grain growth was found to be influenced by the cooling rate in which slower cooling rate would increase the grain size. As stated by research in [25], grain growth in the heat-affected zone (HAZ) of stainless-steel material was hugely depended on the main factors such as maximum temperature, rate of cooling, and a period of staying at high temperature. The grain was greater in size in the area that was undergoing higher maximum temperature when compared to the grain size in the area that was undergoing lower maximum temperature. The changes in temperature throughout heating and cooling cycles would influence the grain size in which the grain growth typically occurs between the temperature of 900 °C and its peak temperature. In addition, particle precipitation and grain boundary migration were also the major factors that could provide great impact on the grain growth in stainless steel material.

Based on reviewed literatures, there were only few attempts in comparative prediction of grain size using probabilistic and deterministic FEM especially for thermal cutting process due to limited numerical software capability to solve the problem by default which leads to the need of comprehensively advanced approaches using subroutines and utility routines. Therefore, in this study, non-linear thermo-mechanical probabilistic computation method based on Monte Carlo using FEM software Marc/Mentat 2016 was employed to model and simulate plasma arc cutting process for predicting the grain growth in 4-mm plate thickness of austenitic stainless steel 316L. A series of experiments were carried out using fully automated system for validating the simulated results. To measure the initial and final grain sizes of the specimen, an advanced system of metallurgical microscope was utilized. Finally, the simulation results were analyzed and concluded.

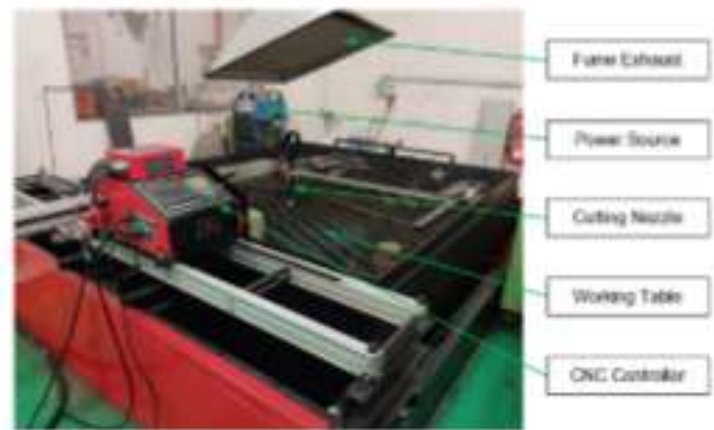


Fig. 1 CNC plasma cutting machine

2 Experimental set-up and procedures

At the initial stage of this research, a series of experiments were conducted using automatic CNC plasma cutting machine model HNC-1500 W with IGBT Inverter power source as displayed in Fig. 1. At the present time, plasma arc cutting process is normally integrated with Computer Numerical Control (CNC) system [26–28]. The implementation of CNC system in plasma cutting process could enhance the cutting flexibility especially to setup and control the torch movement. The type of material used in the experiment was stainless steel 316L with the specimen size of 100 mm in length and width as well as 4 mm in thickness. The cutting parameters applied during the experiment are tabulated in Table 1.

After the experimental cutting process was finished, the specimens were then used for metallographic preparations consisting of several steps prior to final grain size measurement. In preparing the metallographic samples, the specimens underwent sectioning process using abrasive cutter which then proceeded with mounting process by means of automatic mounting press. After finishing mounting process, the samples were subsequently used in crucial course and fine grindings using metallographic sand papers started with lower grade (coarser) and increased gradually to higher grade (finer) by means of grinding machine. Later, polishing process was implemented via polisher machine by utilizing three different grades of polishing agents which were diamond

Table 1 Thermal cutting parameters used for experimental investigation

Parameter	Value
Current, I [A]	30
Voltage, V [V]	80–100
Travel speed, v [mm/s]	5

suspensions of grades 6, 3, and 1 μm . Then, the preparation continued with etching process by using V2A etchant which was suitable for stainless steel material. For better metallographic examination, the inspection of material microstructure was performed just after the etching. The aim of the metallographic inspection was to conduct microscopic examination on the prepared sample in order to measure the grain size at the cut kerf area. The metallographic inspection was carried out using system metallurgical microscope model OLYMPUS BX60F-3. For microscopic measurement, the microscope was connected to a computer equipped with IMAPS 2.0 software. This software program allowed the grain image that was being observed through the microscope to be previewed on the computer which then could be captured and measured. The calculation of real average grain size was made by means of linear intercept method which was performed in accordance to ASTM E112 standard.

According to [29], one of the important parameters to calculate grain size is the modified kinetic constant. However, it is very difficult to find information and reference about the value of this particular parameter. As an alternative to obtain the parameter value, a heat treatment process was conducted using DIL 805A/D/T quenching and deformation dilatometer as shown in Fig. 2. The experiment was carried out on SS316L material in cylindrical shape of 5 mm $\times$ 10 mm in diameter and length respectively. A number of samples were heated and held isothermally at four different temperatures of 900 $^{\circ}\text{C}$, 1000 $^{\circ}\text{C}$, 1100 $^{\circ}\text{C}$, and 1200 $^{\circ}\text{C}$ with four different holding times of 30 s, 60 s, 120 s, and 240 s. Based on the results of grain sizes obtained from the heat treatment experiment, the values of modified kinetic constants at each temperature are stated in Table 2. The results of modified kinetic constants are to be implemented in the numerical simulation of grain growth.

Furthermore, a chemical analysis was conducted to identify the composition of chemical substances that were

Table 2 Modified kinetic constant parameters obtained from heat treatment experiment

Temperature [$^{\circ}\text{C}$]	Value [$\mu\text{m}^2\text{s}^{-1}$]
900	2.94×10^{13}
1000	6.79×10^{12}
1100	1.91×10^{12}
1200	3.22×10^{11}

present in the specimen. The chemical testing was performed using QMatrix Analysis by weight percent accomplished based on ASTM A240 specification. Table 3 shows the average results of chemical composition obtained from the experiment and compared with the chemical composition provided in material model from database.

Other factor that might contribute to the accuracy of numerical prediction is the heat transfer coefficient. For this reason, a thermal calibration was conducted in order to ensure the predicted temperature distribution resembling the actual behavior. As calibrating purpose, temperature distribution during the thermal cutting test was measured by means of thermocouples type-K connected to data logger ALMEMO 2890-9 for data recording at specific locations as demonstrated in Fig. 3. Table 4 presents the calibrated heat transfer coefficients obtained from the thermal calibration which were further implemented for the grain growth simulation. The thermal calibration was determined by comparing the temperature distributions obtained between simulation and experiment. Apart from that, the calibration was also made to validate that the chosen material property models used in the numerical analysis as shown in Fig. 6 could characterize the similar behavior as the actual material as displayed in Fig. 4.

3 Simulation method and procedures

3.1 Geometrical, material, and thermomechanical modelling

Figure 5 illustrates a schematic diagram of solid finite element model implemented in the numerical computation with the dimension of 20 mm (L) $\times$ 40 mm (W) $\times$ 4 mm (T). The arrow demonstrates the trajectory and direction of cutting. The geometrical model was built using three-dimensional hexahedral element type. In order to have better numerical prediction, the model was constructed using finer elements in the region close to the cutting trajectory.

For numerical simulation, the grain growth analysis was executed by means of material modelling of SS316L generated based on the chemical composition as disclosed in Table 3. The grain growth computation was made based on temperature distribution where non-linear thermomechanical



Fig. 2 Quenching and deformation dilatometer DIL 805A/D/T

Table 3 Chemical composition of SS316L

Material type	Chemical substance							
	C	Cr	Ni	Mo	Mn	Si	S	P
Specimen	0.017	16.760	10.190	2.148	1.475	0.340	0.0067	0.026
Database	0.018	16.630	11.180	2.050	1.570	0.480	0.0020	0.040

method was applied for the temperature analysis. Besides, in this study, the numerical computations were accomplished through temperature-dependent material properties as displayed in Fig. 6. In real situation, the specimen is subjected to high temperature throughout the cutting process which particularly could surpass its melting point at the main cutting area. Consequently, the heat will be transmitted via heat-affected zone (HAZ) region and passed on through base metal as well as ended up dissipating into the surrounding environment. Furthermore, this phenomenon leads to changes in magnitudes of certain material properties that are influenced by the temperature changes. Therefore, it is crucial in the numerical prediction to take the temperature-dependent material properties into consideration in order to replicate the actual condition.

The application of constant material properties could result in inaccurate prediction owing to the consideration that could merely be taken on material behavior at room temperature. On the other hand, due to insignificant changes in magnitudes of particular material properties towards the temperature variation, Poisson's ratio and mass density were possibly considered to be constant at 0.3 and 7850 kg/m³ respectively. This implementation could also permit reduction in computational time without compromising the accuracy of numerical prediction.

For thermal heat transfer, referring to research by [30], the governing equation for transient heat transfer analysis is represented by Eq. (1). In this equation, ρ is density of the material, c is temperature-dependent specific heat capacity, T is temperature vector, Q is thermal load vector (flux), t is time, and ∇ is the spatial gradient operator, whereas x , y , and z are coordinates in the reference system.

Table 4 Calibrated heat transfer coefficients

Type of heat transfer coefficient	Value
Convective, h [W/m ² K]	25
Contact, α [W/m ² K]	1000
Emissivity, ϵ	0.6

In addition, from the equation, $\vec{q}$ is the thermal conductivity vector in which non-linear isotropic Fourier heat flux constitutive equation is used with temperature-dependent properties.

$$\rho c \frac{\partial T}{\partial t}(x, y, z, t) = -\nabla \cdot \vec{q}(x, y, z, t) + Q(x, y, z, t) \quad (1)$$

In this numerical simulation, two types of system interaction between part and environment were considered, namely, mechanical and thermal boundary conditions. Fixed displacement on the nodal points was set up as the mechanical boundary condition. Meanwhile, as thermal boundary condition, the heat losses were taken into consideration in consequences of conduction (contact between two bodies), convection, and radiation. Equations (2), (3), and (4) are used to characterize the heat losses via conduction, convection, and radiation respectively. Referring to these equations, contact heat transfer coefficient, coefficient of convective heat transfer, Stefan Boltzmann's constant, and thermal emissivity are represented by α , h , σ , and ϵ respectively, while T_1 and T_2 are bodies' temperatures, whereas T_s and T_∞ define the surface and ambient temperatures respectively. Thus, for the thermal boundary condition, the total heat losses involved in the computational analysis could be expressed as Eq. (5).

$$q_{cond} = -\alpha(T_1 - T_2) \quad (2)$$

$$q_{conv} = -h(T_s - T_\infty) \quad (3)$$

$$q_{rad} = -\sigma\epsilon(T_s^4 - T_\infty^4) \quad (4)$$

$$q_{totallosses} = q_{cond} + q_{conv} + q_{rad} \quad (5)$$

Fig. 3 Data logger ALMEMO 2890-9 (left), type-K thermocouples (middle), and measuring point locations (right) used in thermal calibration



Fig. 4 Temperature measurements for thermal calibration

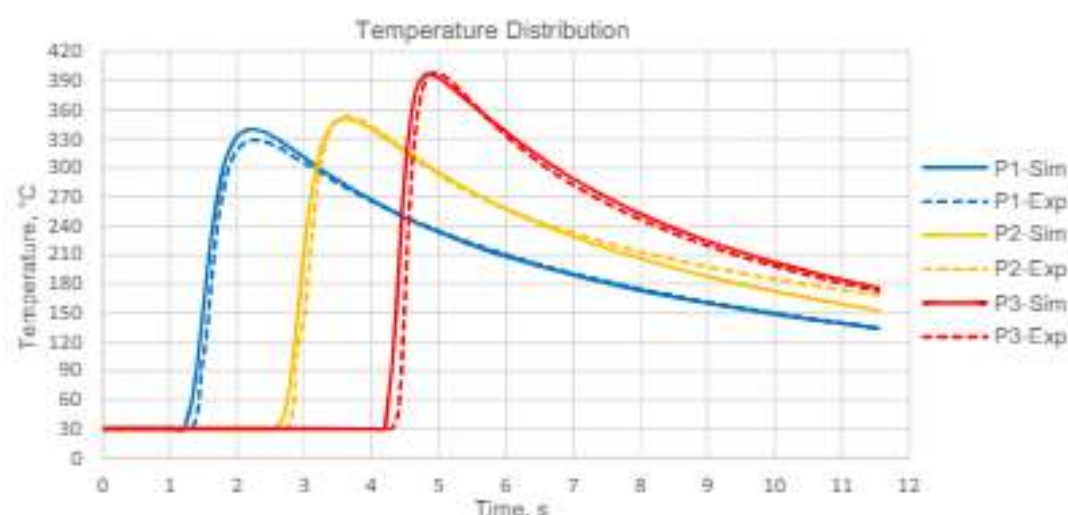


Figure 7 exhibits the basic overview of the coupled thermomechanical-metallurgical analysis. The heat input is defined by the volumetric conical heat source which will be modelled using Fortran-based subroutine and utility routine in FEM software MSC Marc/Mentat 2016.

3.2 Heat source modelling

The application of heat source model is one of the key steps in thermal cutting simulation. The implementation of correct model that is well suited to the simulation process being investigated can give a huge impact on the accuracy of prediction. The heat source model used for simulation

should be able to replicate the actual heat source profile. Therefore, in this study, the best preferred model is a volumetric conical heat source model. However, this type of heat source model is usually not provided by default and thus, customized model should be created. Since this simulation is executed using MSC Marc, the algorithm is formulated by means of Fortran-based subroutine. The volumetric conical heat source model implemented throughout this research was developed and formulated in [31] which was exceptionally arisen from derivation of heat intensity distribution from thermal energy conservation equation. The volumetric conical model equation is divided into two parts, where Eq. (6) is generated to characterize the heat intensity distribution of thermal arc while the following Eq. (7) is

Fig. 5 Geometrical model applied for numerical simulation

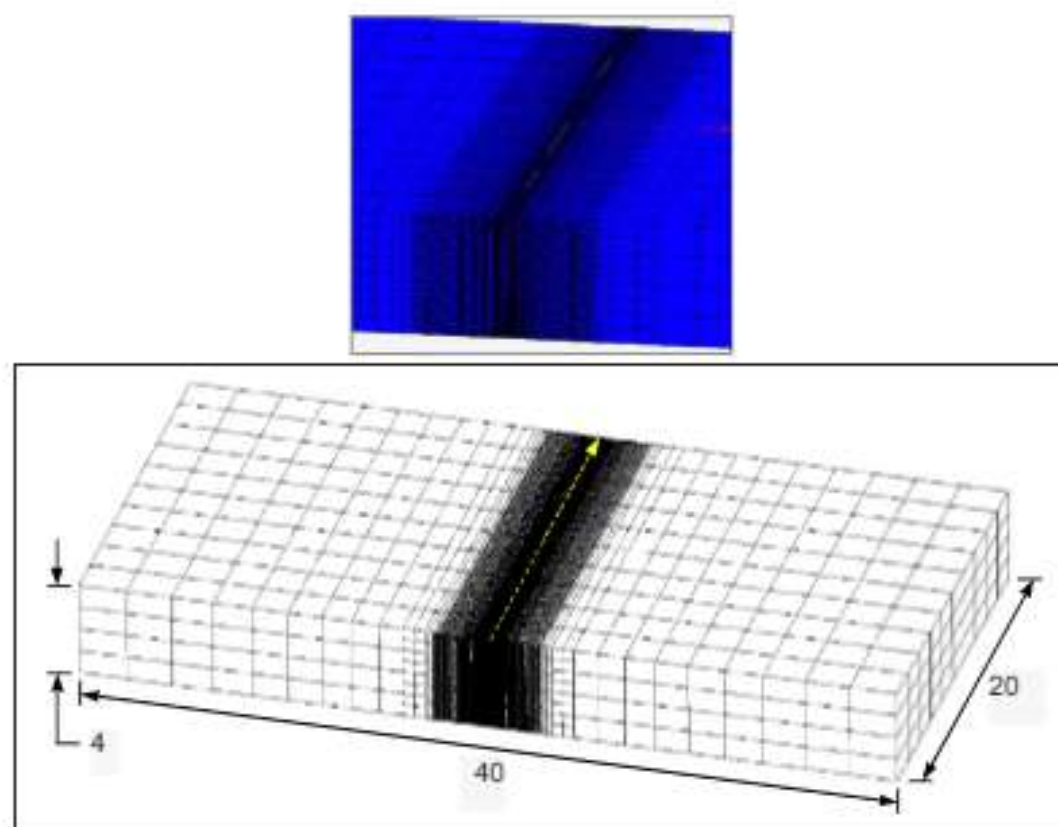
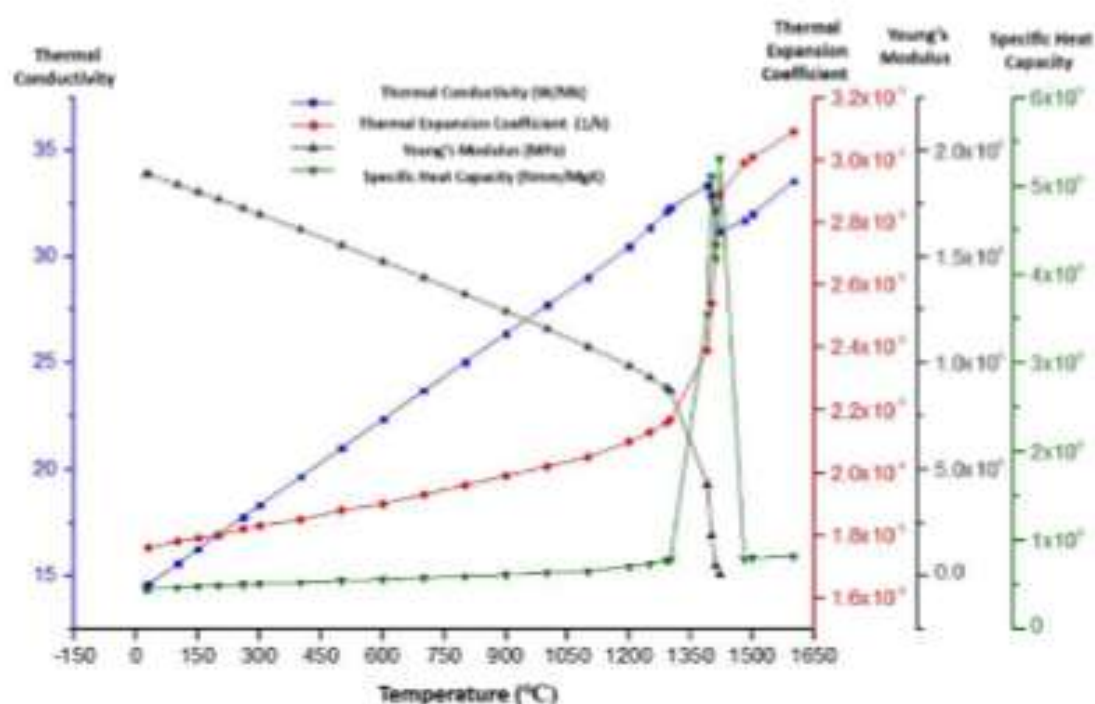


Fig. 6 Temperature-dependent mechanical and thermo-physical properties of SS316L



fraction of the abovementioned equation which manipulates the heat input intensity that deteriorates through the distance of material thickness. Referring to both formulae, the net heat flux, input power, radial coordinate, z -coordinate, and heat intensity distribution parameters are represented by q , Q_0 , r , z , and r_0 respectively. Meanwhile, r_e and z_e define the top surface radius and z -coordinate respectively, whereas the bottom surface radius and z -coordinate are defined by r_i and z_i respectively. Figure 8 demonstrates the volumetric conical heat source model configuration. The heat source variables applied in the numerical analysis were defined

through the thermal calibration that has been described as above, where the preferred heat source parameters obtained when the predicted temperature distribution could provide the similar behavior of temperature distribution as produced by experiment.

$$q(r, z) = \frac{9Q_0 \epsilon^3}{\pi(\epsilon^3 - 1)} \cdot \frac{1}{(z_e - z_i)(r_e^2 + r_e r_i + r_i^2)} \cdot \exp\left(-\frac{3r^2}{r_e^2}\right) \quad (6)$$

$$r_0(z) = r_i + (r_e - r_i) \cdot \frac{z - z_i}{z_e - z_i} \quad (7)$$

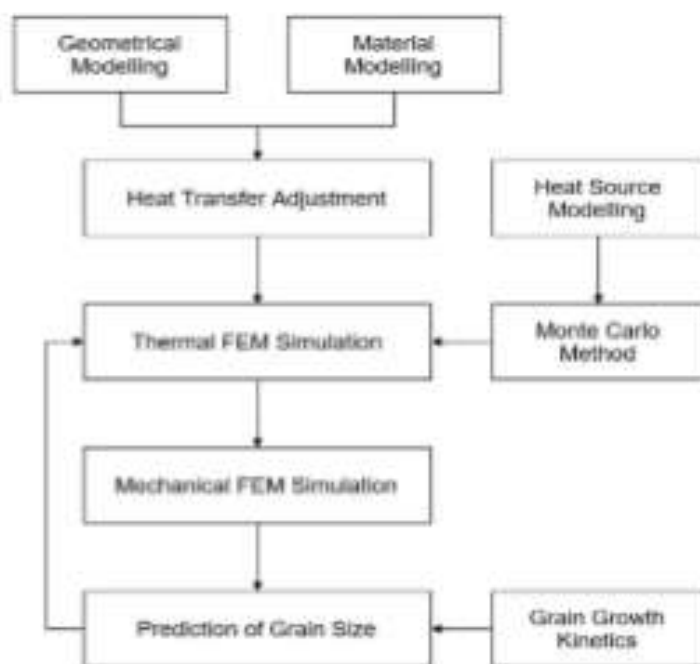


Fig. 7 The coupled thermomechanical-metallurgical analysis

3.3 Principle of Monte Carlo (MC) method

A numerical model that considers variability of inputs to predict the probable outputs is called MC method, which is also known as probabilistic analysis method. A lot of recalculations could be involved in the numerical analysis prior to finishing. Distributions of different outcome values are possible to be generated via this method. In order to execute the probabilistic analysis, the input powers of heat source energy are fluctuated in a particular range while maintaining the rest of important parameters.

To implement the MC analysis, the input power could be varied through the intervention of random variables. Hence, a source of random variables ought to be generated to implement this process. There are numerous existing random number generators; however, linear congruential generator (LCG) is the most broadly used which can be described as follows [32, 33]:

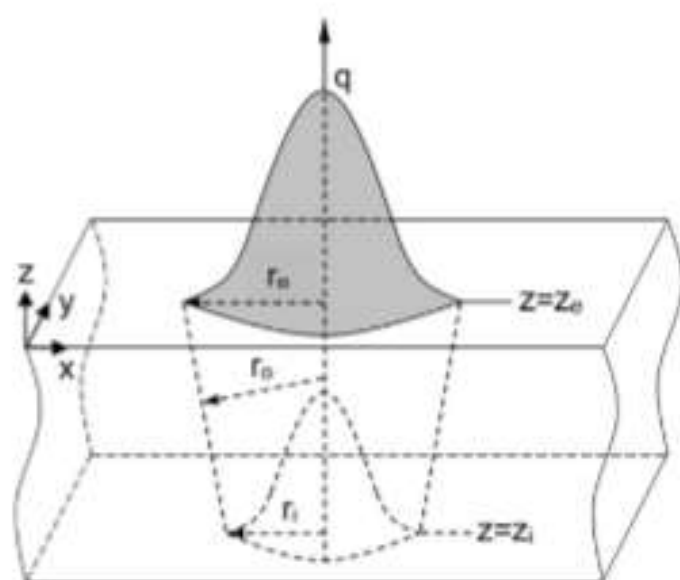


Fig. 8 Configuration of volumetric conical heat source model [31]

$$x_{i+1} = (a \cdot x_i + c) \bmod M, i \geq 0 \quad (8)$$

where a represents the multiplier, c denotes the increment, M is the modulus, and the seed (start value) is represented by x_0 . A sequence of integer pseudo-random numbers $\{x_i\}$ could be produced via this formulation. Afterwards, the random number x_i that was generated beforehand would be divided by M to transform it into random number X_i which laid in the range between 0 and 1 as presented below:

$$X_i = \frac{x_i}{M}, \quad i \geq 1 \quad (9)$$

The previously generated sequence of random numbers $\{X_i\}$ was distributed uniformly, $U(0,1)$. However, in probabilistic

analysis, it is more preferable to use Gaussian or normal random number, $N(0,1)$. Therefore, another model called Box-Muller method [34–36] would be engaged and used to convert the uniform random number into the normal random number. The execution of this technique could be made by manipulating a couple of uniform random numbers (X_1, X_2) to be transformed into a couple of normal random numbers (Y_1, Y_2) through the following formulae:

$$Y_1 = \sqrt{-2\ln(X_1)}\cos(2\pi X_2) \quad (10)$$

$$Y_2 = \sqrt{-2\ln(X_1)}\sin(2\pi X_2) \quad (11)$$

In order to ensure the accomplishment of MC method, the normal distribution of input powers predicted through the probabilistic algorithm was written and executed by means of Fortran 77 program. On account that the MSC Marc software was built based on the same platform, the Fortran programming language was chosen and executed for this purpose. In the investigated thermal cutting process, the value of power input is generated randomly following the increment size ($N=60$). Hence, the probabilistic algorithm was set to produce a sequence of 60 random values based on Gaussian distribution with defined mean and standard deviation as shown in Fig. 9. In the experiment, the magnitude of the voltage and current that have been set up before running the thermal cutting process were considered as the fixed input and mean power for the deterministic and probabilistic analyses respectively. Furthermore, based on the observed minimum and maximum power values during the experiment, the magnitude of standard deviation was approximated. Table 5 shows the thermal cutting parameters applied for both numerical methods.

Fig. 9 Normal distribution of random input powers

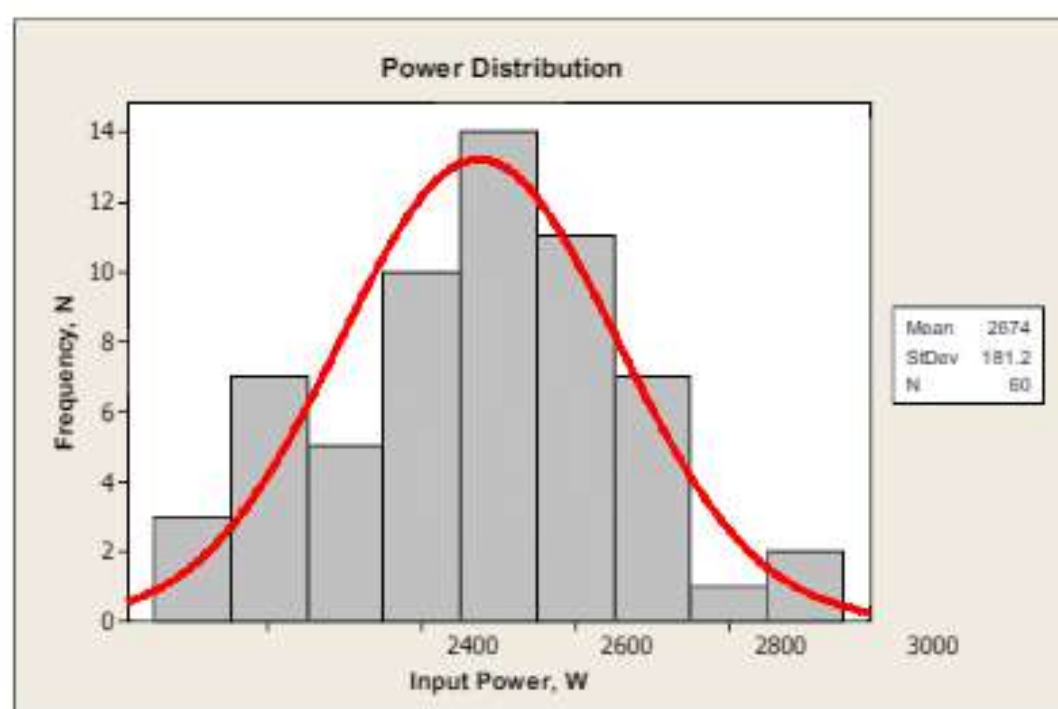


Table 5 Thermal cutting parameters used in numerical computations

Parameter	Simulation method	
	Normal (Deterministic)	Monte Carlo (Probabilistic)
Input power, P [W]	2700	Mean, $\mu = 2700$ Standard deviation, $\sigma = 190$ Size, $N = 60$
Cutting speed, v [mm/s]	5.0	5.0
Heat source model	3D conical	3D conical

4 Grain growth modelling

A metallurgical phenomenon identified as grain growth would occur as a consequence of kinetic energy produced by induced heat when metallic material is being subjected to particular thermal processes [29]. In addition, the existence of impurity and precipitation in certain conditions could also give an impact on the grain growth phenomenon. The precipitation is referred to a process of diffusion that depends on two major factors which are temperature and time. The calculation of grain growth can be made by using the mathematical formula as shown below:

$$\frac{d\bar{g}}{dt} = M_o^* \exp \left[-\frac{Q_{app}}{RT(t)} \right] \left[\frac{1}{\bar{g}} - \frac{1}{\bar{g}_{lim}} \right]^{(1-n)} \quad (12)$$

where Q_{app} is activation energy of grain growth (kJ mol^{-1}), M_o^* is modified kinetic constant ($\mu\text{m}^2\text{s}^{-1}$), $\bar{g}$ is initial grain size in average (μm), T is absolute temperature (K), t is time (s), n is time exponent, R is gas constant ($8.314 \text{ J K}^{-1} \text{ mol}^{-1}$), and $\bar{g}_{lim}$ is limiting grain size (μm).

According to [25], in stainless steel material, the grain can be grown in the temperature range between 900 °C and maximum temperature (peak) which happens throughout heating and cooling phases. In thermal processes such as arc welding and thermal cutting, the grain growth is mainly dependent on the rates of heating and cooling. In general, the period of heating phase is faster than cooling phase. Thus, more opportunity of grain growth can happen during the cooling phase. In this research, the grain growth was taken into account and calculated in both cycles of heating and cooling. Referring to [37], the presence of carbon in austenitic stainless steel can stabilize the austenite structure, but it provides disadvantage of attracting to chromium. Consequently, this strong attraction leads to the formation of chromium carbides (Cr_{23}C_6) that is also known as precipitation which can be further driven to occur when supersaturation levels in austenite are achieved by carbon. Moreover, carbon

level, temperature, and time are the main factors that influence the rate of precipitation where it typically takes place at the range of temperature between 500 and 800 °C, also called as sensitization.

Referring to the abovementioned chemical composition as stated in Table 3, with the confirmed carbon content, it is obviously found that a very long period of time (about 10 h or more) is required for the precipitation to take place. Hence, in this study, the calculation of grain growth was only considered based on the free grain growth phenomenon. By considering the absence of precipitates as described in Eq. (13), part of Eq. (12) could be eliminated, and thus the general grain growth formula could be reduced as presented in Eq. (14).

$$\bar{g}_{Lim} = k \left(\frac{r}{f} \right) \quad (13)$$

where k is zener coefficient, r is radius of precipitate (μm), and f is volume fraction of precipitate. When there is no precipitation, then $f = 0$ and thus $\bar{g}_{lim}$ becomes infinite. Therefore,

$$\frac{d\bar{g}}{dt} = M_o^* \exp \left[-\frac{Q_{app}}{RT(t)} \right] \left[\frac{1}{\bar{g}} \right]^{(1-n)} \quad (14)$$

By looking at the grain growth formula as expressed in Eq. (14), it is in the form of ordinary differential equation (ODE). As stated in [38], the ODE is an equation that contains a function of one or more ordinary derivatives with respect to only one independent variable. In general, the ODE can be solved by finding the anti-derivative that is reached through integration. However, the integration process is sometimes very difficult to be made especially involving complex differential equation which is also complicated to be solved through analytical method. The Fortran software used to write the program code may not solve the ODE directly. Therefore, in this case, an approximation will be used for solving the ODE. Referring to previous studies [39–42], a lot of researchers resolved the problems involving ODE through numerical approximation by using Runge–Kutta methods. Hence, through this study, a Runge–Kutta fourth-order method was selected to solve the ODE for calculating the average grain size. The Runge–Kutta fourth-order method was chosen as it may provide high accuracy of numerical approximation compared to the other numerical methods. The Runge–Kutta fourth-order method is obtained through derivation of equation from Taylor series which is taken from the first five terms. The implementation of Runge–Kutta method would eliminate the tricky integration process of exact solution and skip the difficult and lengthy higher order derivatives of functions as required

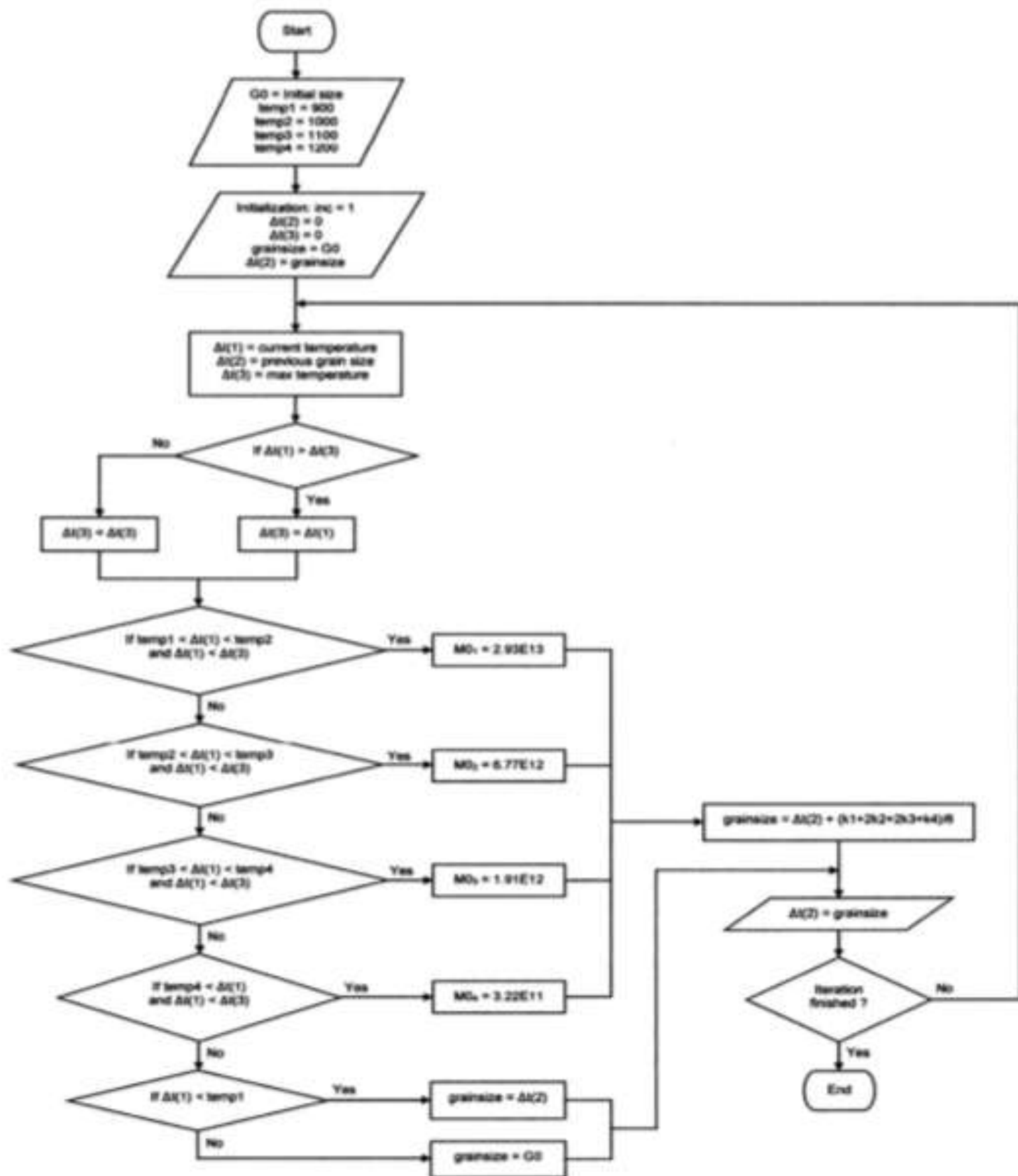


Fig. 10 Flowchart of grain size algorithm

in Taylor series. This numerical method is stable and easy to apply since it works by computing four different slopes within an interval and makes use of them as the weighted average slope to determine the next position at the end of

the interval. The size of interval used in the numerical computation was defined by the increment (time step) that had been set up for the simulation. The determination of step size was vital since it would have great influence on

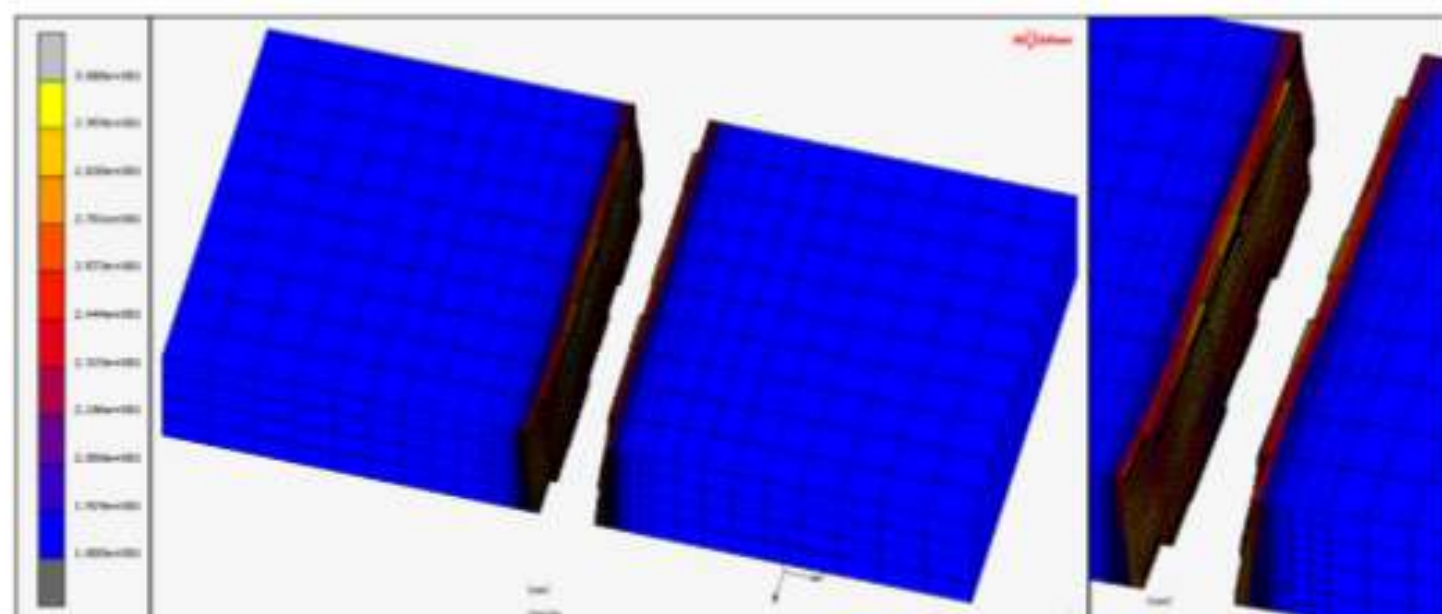


Fig. 11 Distribution of grain predicted via probabilistic analysis

the computational time and accuracy of prediction. The formulation of Runge–Kutta fourth-order method can be described as follows [43]:

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h \quad (15)$$

where $k_1 = f(x_i, y_i)$, $k_2 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1h)$, $k_3 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_2h)$, and $k_4 = f(x_i + h, y_i + k_3h)$.

In order to see how the algorithm works, the executed program for determining the grain size can be represented by the flowchart as exhibited in Fig. 10 below:

5 Results and discussion

Close analysis of postprocessing results could be performed upon the completion of thermal cutting simulations. The focal points of the result analysis were on the grain distributions predicted through probabilistic and deterministic methods. The temperature distributions would also be analyzed due to its strong impact on the grain growth. The grain distributions as forecasted by means of probabilistic and deterministic analyses are shown in Figs. 11 and 12 respectively. It could be seen that both numerical methods estimated the

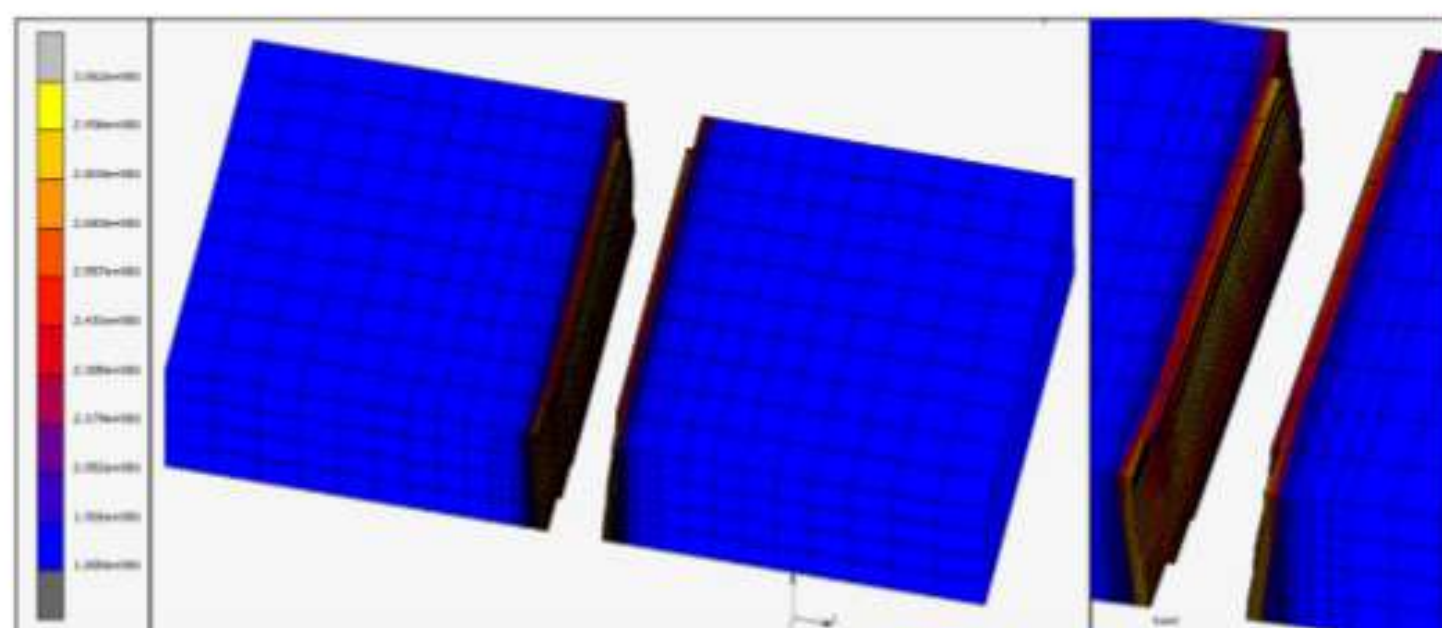
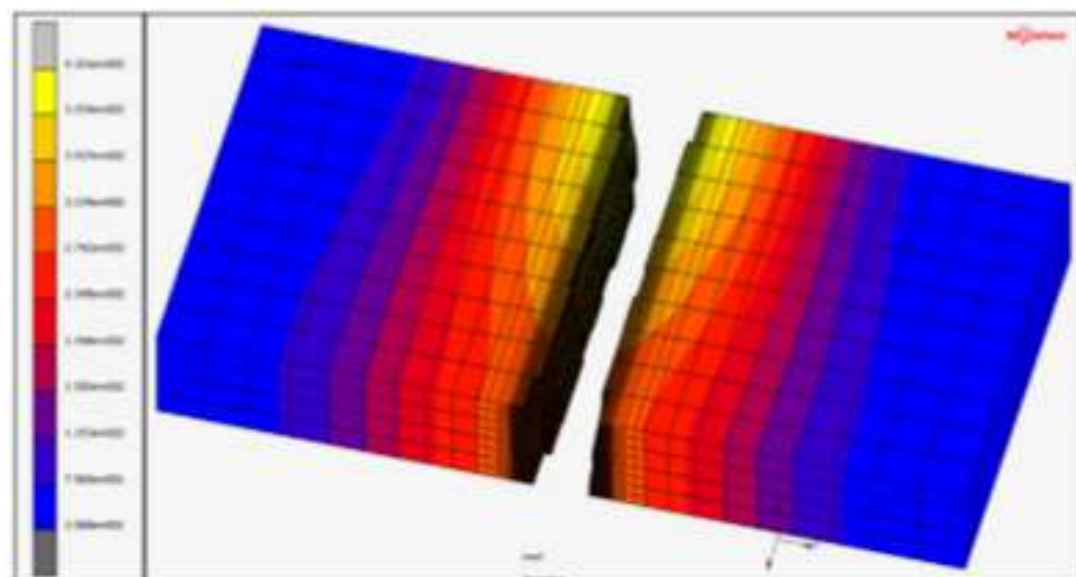


Fig. 12 Distribution of grain predicted via deterministic analysis

Fig. 13 Distribution of temperature estimated using probabilistic analysis



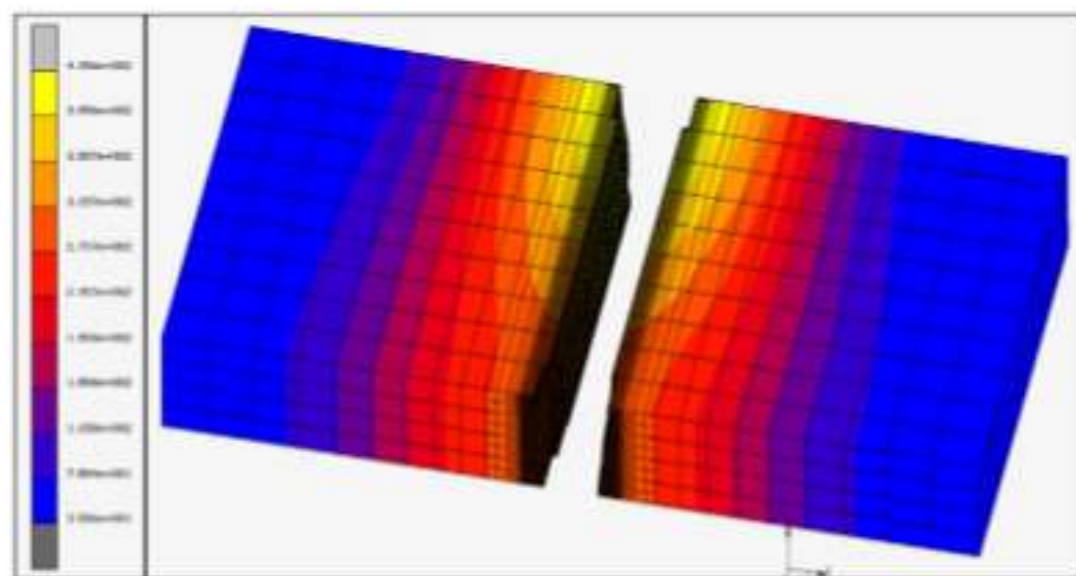
grain growth occurrence at the area around the cut kerf. The maximum size of grain was $30.88 \mu\text{m}$ as calculated in probabilistic analysis, whereas $30.62 \mu\text{m}$ was the maximum value of grain size as computed through deterministic analysis. Both grain growth analyses started from the initial value of $18 \mu\text{m}$. The results revealed slight differences in grain size distributions predicted between both numerical methods. Besides, based on the outcomes of grain distributions, it proved that the programming code for calculating grain growth was successfully implemented.

In addition, based on the estimated shapes of cut kerfs as displayed in figures above, the effects of analysis types could be observed where smooth cutting profile was generated through deterministic method, while the probabilistic method produced rough and uneven cutting profile. The

rough profile was generated as a result of input power fluctuation that was set up through the MC method. The cut kerf was created according to removal of materials (elements) that were implemented when the ongoing temperatures during simulation went beyond the melting point of SS316L material. Furthermore, based on the results obtained, it confirmed that the algorithm subroutine for thermal cutting simulation was effectively executed.

The grain growth occurred due to high temperature experienced by the material. Thus, the temperature distribution should also be examined. Figures 13 and 14 present the temperature distributions resulted from the thermal load of heat input which were predicted by means of probabilistic and deterministic analyses respectively. The temperature results in the figures were displayed at the final time of simulation

Fig. 14 Distribution of temperature estimated using deterministic analysis



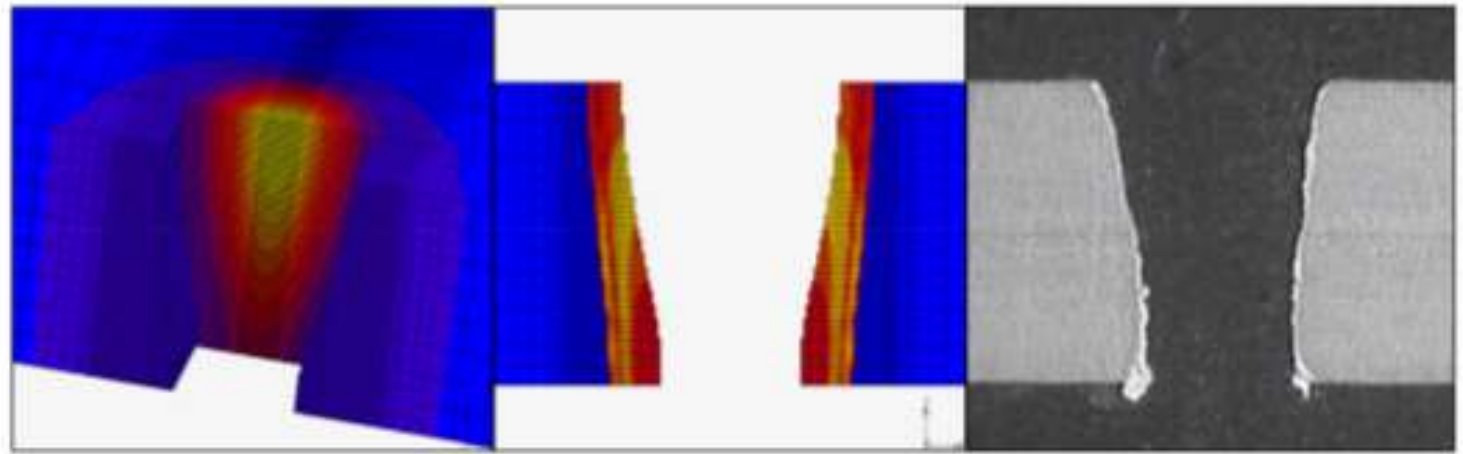


Fig. 15 Cross section images of forecasted (middle) and actual (right) cutting profiles

(6 s) that was 2 s after the completion of cutting. It could be observed that the maximum temperatures dropped under 500 °C, which was enough for grain growth analysis since the grain stopped growing when the temperature fell about under 900 °C. There were slight differences in temperature distributions estimated through both methods. The temperature difference confirmed that the predicted grain size distributions would differ between probabilistic and deterministic methods. The temperature values were dropping away from the cutting

points towards the adjacent base metal, and the induced heat was ended by dissipating into the surrounding environment.

Since the thermal cutting simulation was executed using customized conical heat source model, the effect could be seen via the shape of cross section area. Figure 15 exhibits the images of cutting profiles obtained from the predicted (middle) and actual (right) cross section areas. The shape of conical heat source model is demonstrated in Fig. 15 (left) as well. The conical contour of heat source caused the cut kerf

Fig. 16 Position of node 53,440

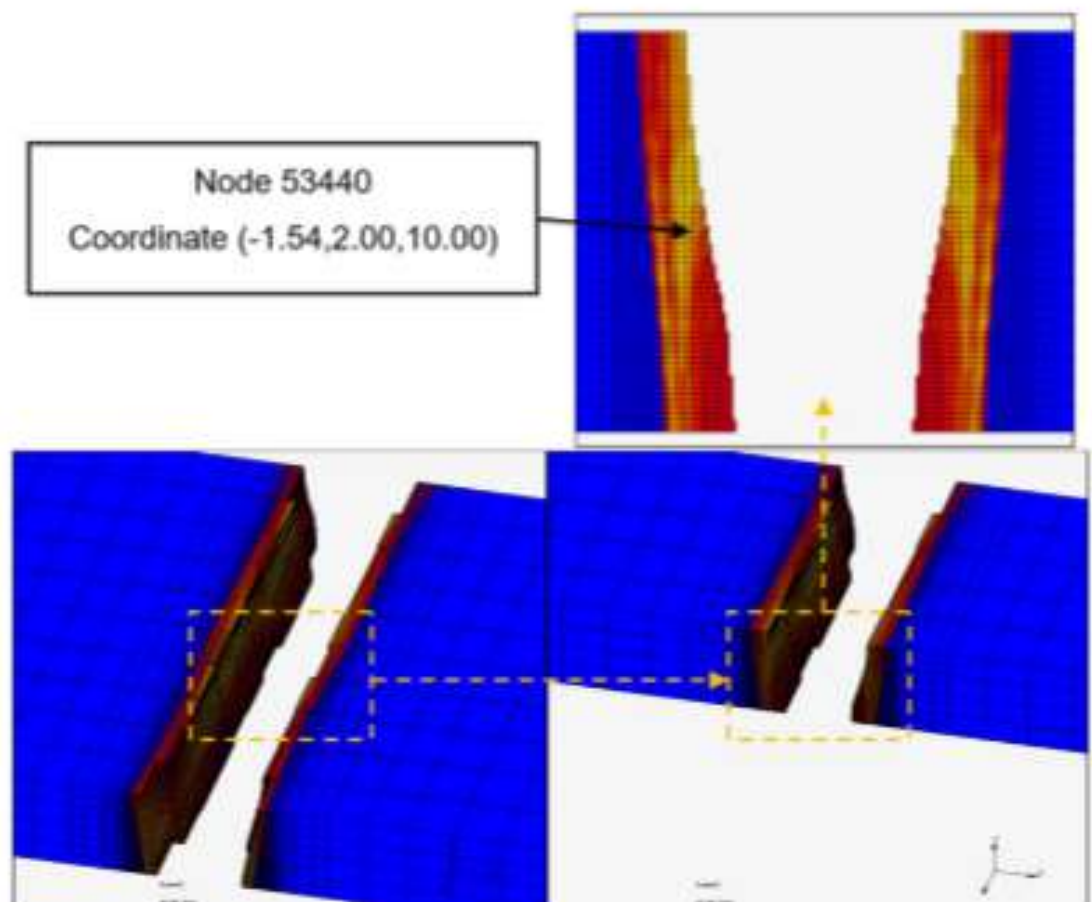
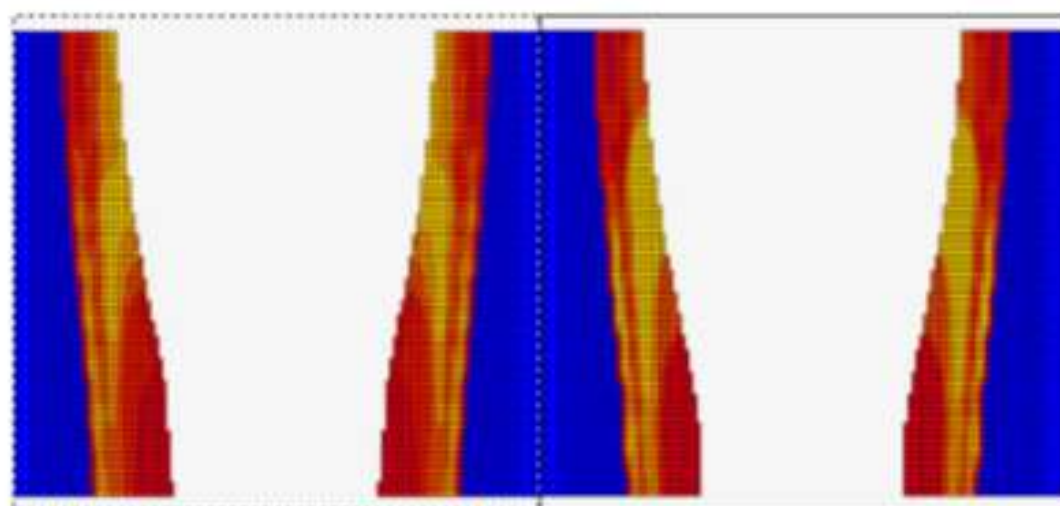


Fig. 17 Distributions of grain sizes predicted through probabilistic (left) and deterministic (right) methods



profile to be produced in V-shape. Both numerical methods produced similar cutting profiles. Moreover, the predicted cut kerf profile in V-shape was effectively produced as a result of implementing finer meshes in the surrounding area of cutting trajectory. The V-shape profile was difficult to be generated with the application of coarser meshes. However, the implementation of finer elements led to longer computational time which required good performance device to run the numerical simulation. When comparing the predicted cutting profile to the actual one, good agreement was achieved in which both cutting profiles looked similar. This result could be evidence that the programming subroutine of customized conical heat source model was successfully implemented for the thermal cutting simulation.

In order to observe the grain size, a specific node was selected for comparison of results. The selected one was node 53,440 which was located in the affected area of heat input as demonstrated in Fig. 16. More specifically, the node was taken from cross section area in the middle of the length. For verification, the actual grain size was measured from the similar position of the prediction as mentioned above.

Figure 17 displays the grain size distributions predicted using both numerical methods, where some differences were found between them. The different grain size distributions were produced as a result of different amount of induced heat input at the same location due to the variation of input power set up for probabilistic method. Both numerical methods estimated greater grain size in the middle

Fig. 18 Comparison of grain growth at node 53,440 calculated through probabilistic (broken line) and deterministic (solid line) methods

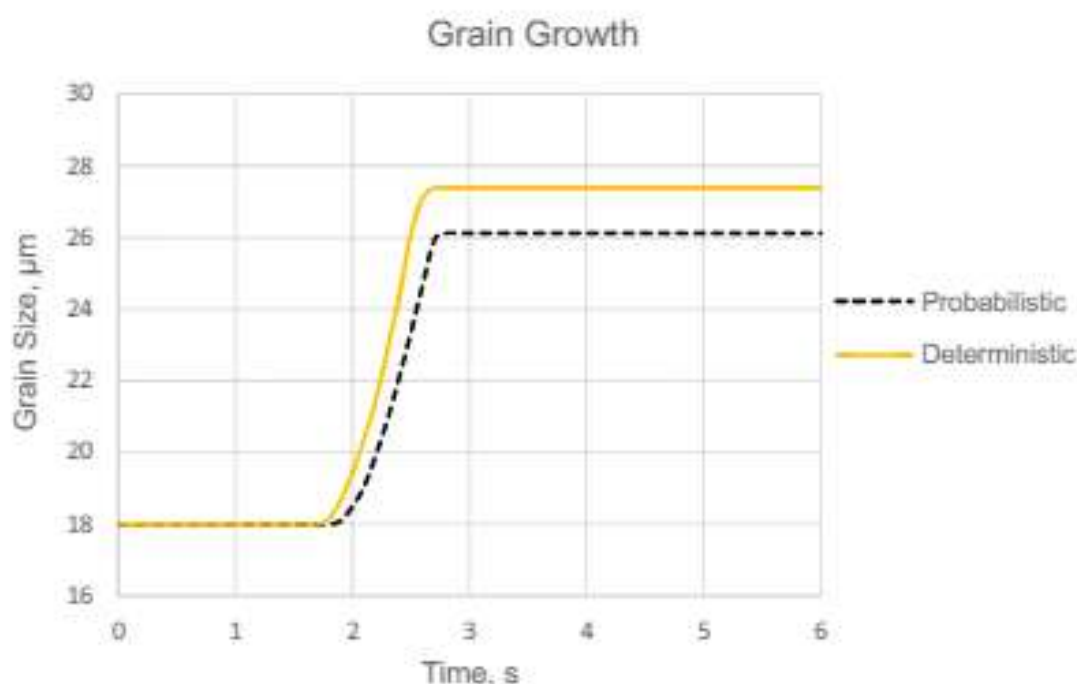
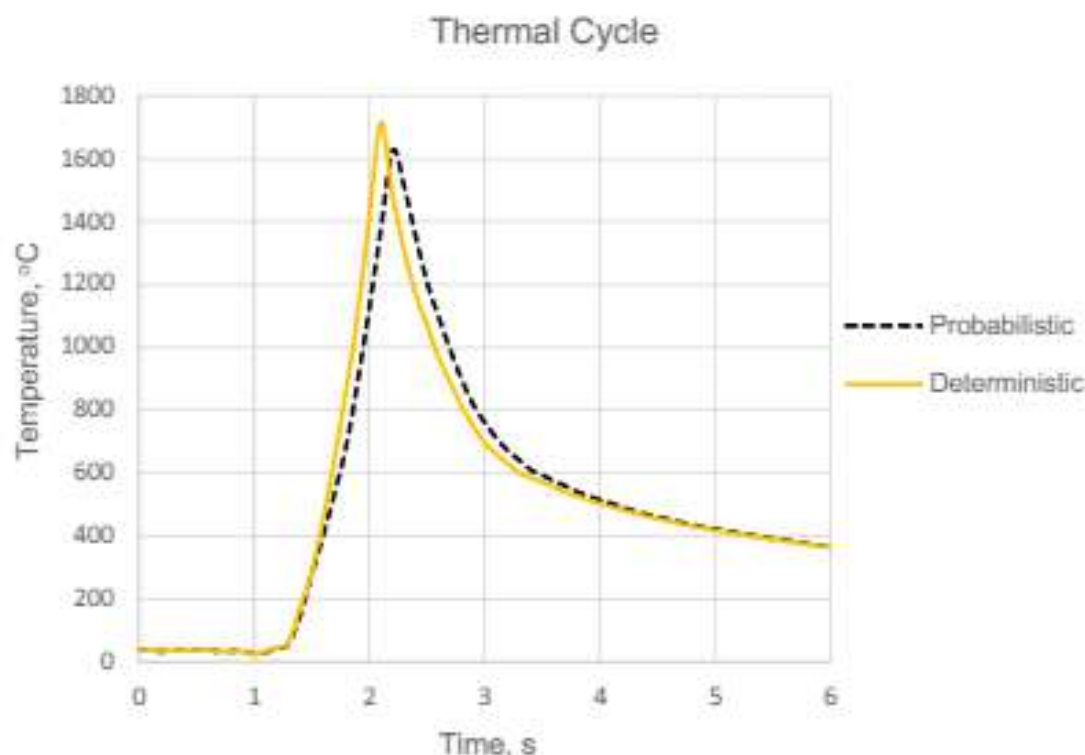


Fig. 19 Comparison of temperature history at node 53,440 calculated through probabilistic (broken line) and deterministic (solid line) methods



region area of material thickness caused by higher intensity of heat flux that led to higher degree of temperature. The detailed progresses of grain growths calculated at the specified node are presented in Fig. 18, while Fig. 19 reveals the temperature histories recorded at the same point. The maximum temperatures achieved by means of probabilistic and deterministic analyses were 1626.89 °C and 1715.00 °C respectively. Based on the graphs, it was found that the

probabilistic method estimated slightly lower maximum grain size compared to deterministic method, where this outcome was supported by the induced thermal cycles experienced at that same point in which higher maximum temperature was reached via deterministic method. It was clearly observed that the grain growth was greatly influenced by the thermal cycle induced through heat input during thermal cutting process, where the grain growth phenomena took place in very short period of time during heating and cooling cycles. For verification purpose, the average actual grain size was obtained and measured at the similar point as shown in Fig. 20. The numerical values of grain sizes predicted through both numerical methods and measured from experiment are presented in Table 6 for comparison of results. The actual grain size was measured on average using the method as explained in the experimental procedure. Based on the figures in the table, the final grain sizes predicted through both simulation methods reached a good agreement with the experimental measurement, where the deterministic method produced a bit higher final grain size prediction in comparison to the probabilistic method. Thus, the error percentage produced by deterministic analysis was a little higher compared to probabilistic analysis whereas the actual grain size

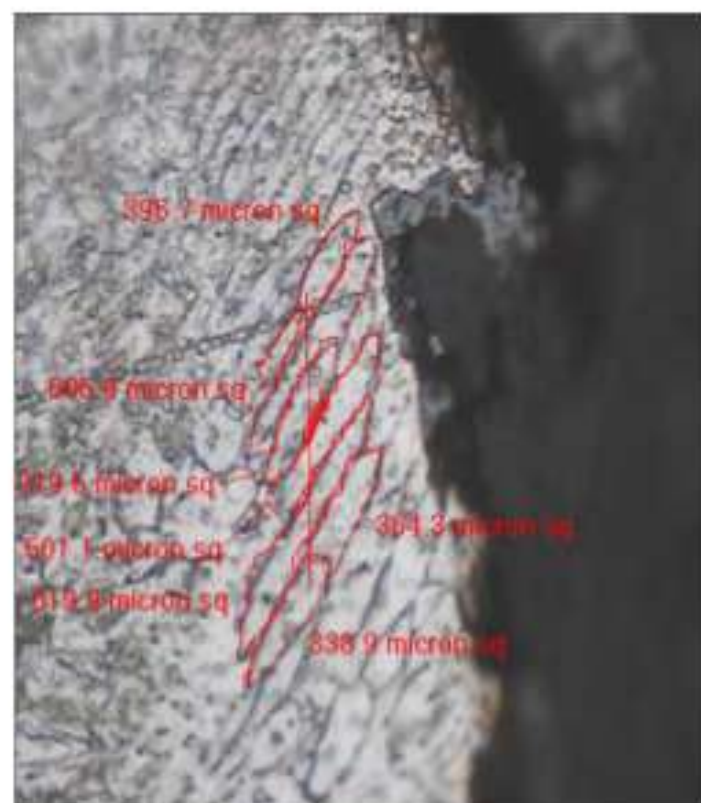


Fig. 20 Distribution of grain sizes obtained from actual sample

Table 6 Comparison of grain sizes obtained between numerical methods and experiment

Methods	Average grain sizes [μm]	Error percentages [%]
Probabilistic simulation	26.12	9.19
Deterministic simulation	27.38	14.46
Experiment	23.92	-

measurement was lower than both numerical predictions. However, both simulation methods generated good accuracy of prediction where the error percentages were computed below 15%.

6 Conclusions

In conclusion, the analysis of results from this research proved that the grain growth phenomenon occurred as a result of heat input induced in thermal cutting process could possibly be predicted by means of numerical computation. However, the grain growth calculation is not possible to be executed using default numerical analysis. Based on the research findings, the following outcomes derived from this study can be summarized as follows:

- Grain growth prediction is an advanced numerical simulation that could only be performed through customized simulation using particular subroutines. The subroutines involved in this study were the programming codes for conical heat source model which included MC method, contour plotting of desired output, thermal cutting implementation through activation and deactivation of elements, as well as grain size calculation based on Runge–Kutta fourth-order method.
- Based on the numerical analysis, thermal cycle was found to have an impact on the grain growth phenomenon. Furthermore, the reliable calculated grain size obtained from the numerical computation proved that the compiled customized subroutines were successfully implemented to predict the grain growth behavior.
- There were little differences in distributions of grain size estimated through both numerical analyses. However, the probabilistic method predicted closer to the actual grain size value at the specified node as compared to the deterministic method. Therefore, grain growth prediction could be better performed through probabilistic analysis.
- Grain size prediction achieved via probabilistic method provided with higher accuracy in which the percentage of error was less than 10%. Even though the deterministic method ended up with a slightly higher percentage of error, it still managed to provide good prediction with the accuracy of more than 85%.
- The different predictions produced by probabilistic analysis occurred as a result of implementing MC method which considered the variation of input power parameter along the simulation process, where the variation was provided based on normal distribution predicted from the sequence of random numbers that was generated using simple random number generator.
- Moreover, the factors that could lead to result deviations might be caused by chemical composition, material proper-

ties, geometrical size, theoretical model, and approximation method.

Appendix

In this numerical analysis, the subroutine algorithm executed for computing the grain growth can be expressed as follows:

Algorithm 1. Algorithm of metallurgical analysis for calculating grain size.

```

1: procedure grain size calculation
2:   Set the initial grain size,  $G_0$ .
3:   Specify the limit temperatures for selecting grain boundary mobility,  $M_0$  value.
4:   Assign the parameters of current temp as  $\Delta t(1)$  and maximum temp as  $\Delta t(3)$ .
5:   Assign the parameter of previous grain size as  $\Delta t(2)$ .
6:   Initialize the grain calculation by setting the starting values for the parameters.
7:   iteration  $\leftarrow 1$ 
8:   Repeat
9:     Define the maximum temperature,  $\Delta t(3)$ .
10:    if the current temperature,  $\Delta t(1)$  is between temp1 and temp2
11:      Select relevant  $M_0$ , by referring to Table 2.
12:      Calculate grain size using Equation (15) based on Equation (14).
13:    else if the current temperature,  $\Delta t(1)$  is between temp2 and temp3
14:      Select relevant  $M_0$ , by referring to Table 2.
15:      Calculate grain size using Equation (15) based on Equation (14).
16:    else if the current temperature,  $\Delta t(1)$  is between temp3 and temp4
17:      Select relevant  $M_0$ , by referring to Table 2.
18:      Calculate grain size using Equation (15) based on Equation (14).
19:    else if the current temperature,  $\Delta t(1)$  is greater than temp4
20:      Select relevant  $M_0$ , by referring to Table 2.
21:      Calculate grain size using Equation (15) based on Equation (14).
22:    else if the current temperature,  $\Delta t(1)$  is lower than temp1
23:      No grain growth.
24:    Else
25:      Grain size is same to the initial size.
26:    end if
27:    iteration  $\leftarrow$  iteration + 1
28:  until the maximum number of iterations is completed
29: end procedure

```

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Declarations

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