

Article

Computational Investigation of Friction Stir Processing of Ti-6Al-4V Alloy for Biomedical Applications Using FEM and Taguchi Design

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Abstract

Friction stir processing (FSP) is an advanced solid-state surface modification technique for biomedical titanium alloys. This study presents a computational investigation of FSP applied to Ti-6Al-4V alloy through three-dimensional finite element modeling and Taguchi-based statistical optimization. A Taguchi L9 orthogonal array evaluated rotational speed (400–1000 rpm), traverse speed (50–100 mm/min), shoulder diameter (6–18 mm), and pin diameter (2–6 mm), reducing the required simulations from 81 (full factorial) to nine (88.9% reduction). A calibrated friction model ($\mu = 0.35/0.25/0.20$ for 400/800/1000 rpm, $F = 6000$ N) yielded maximum temperatures of 870–1384 °C; all predicted temperatures remained below the melting point of Ti-6Al-4V (1660 °C). These values are consistent with experimentally reported ranges for FSW/FSP of Ti-6Al-4V. Traverse speed is the dominant parameter (ANOVA contribution: 63.1%, $F = 10.44$), followed by rotational speed (26.7%) and shoulder diameter (4.1%). Simulation 3 (400 rpm, 100 mm/min, $D_s = 18$ mm, $T_{\max} = 870$ °C) appears to be the most promising thermal condition for preserving the fine-grained $\alpha + \beta$ microstructure, as it remains below the β -transus temperature (980 °C) throughout the processed zone.

Keywords: friction stir processing; Ti-6Al-4V; finite element method; Taguchi design; ANOVA; biomedical; Abaqus; DFLUX subroutine; thermal calibration; model validation



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1. Introduction

Titanium and titanium alloys are among the most attractive metallic materials for biomedical applications due to their excellent corrosion resistance, favorable strength-to-weight ratio, and superior biocompatibility. Ti-6Al-4V alloy has become the most widely used titanium alloy in orthopedic and dental implants because of its ability to provide long-term mechanical stability while maintaining adequate biological performance [1]. The functional performance of biomedical titanium components is strongly influenced by surface characteristics including microstructure, hardness, wear resistance, and surface integrity.

Friction stir processing (FSP), derived from friction stir welding (FSW), utilizes a rotating non-consumable tool to generate frictional heat and severe plastic deformation,

promoting dynamic recrystallization and grain refinement without melting [2,3]. Unlike fusion-based methods, FSP avoids solidification-related defects and can selectively modify surface layers. The foundational work of Zhu and Chao [4] demonstrated that the heat flux distribution under the FSW tool shoulder can be effectively modeled using a linearly distributed annular source validated against neutron diffraction data—an approach adopted in the present study.

Experimental investigations of FSP applied to Ti-6Al-4V have demonstrated its effectiveness for biomedical surface engineering. Singh et al. [5] applied FSP to electron-beam-melted Ti-6Al-4V and reported that the process eliminated surface porosity, refined the as-built columnar microstructure into fine equiaxed grains, and significantly enhanced cytocompatibility, confirming the biomedical relevance of FSP-treated Ti-6Al-4V surfaces. Pilchak et al. [6] showed that FSP of investment-cast Ti-6Al-4V introduces measurable tool-derived tungsten contamination in the stir zone and demonstrated that a post-process α/β heat treatment can be used to dissolve the tungsten-rich particles and restore a homogeneous microstructure, highlighting the importance of tool material selection and post-processing for biomedical applications. Zykova et al. [7] investigated friction stir alloying of Ti-6Al-4V with copper powder using multiple processing passes and found that the resulting in situ Ti–Cu intermetallic-reinforced composite exhibited substantially increased microhardness relative to the unreinforced base alloy, illustrating that FSP-based alloying can be used to tailor surface mechanical properties beyond what is achievable with single-material processing.

Computational thermal and thermo-mechanical modeling has played an increasingly central role in understanding and optimizing FSP. Beyond the foundational FSW heat-flux model of Zhu and Chao [4] adopted in the present study, finite-element-based phase-change formulations have been developed for related multiphysics problems: Vasilyeva et al. [8] and Ammosov and Vasilyeva [9] presented finite element and online multiscale finite element implementations of coupled thermo-mechanical models with phase transition, providing numerical strategies for handling temperature-dependent material behavior that are conceptually relevant to the β -transus phase change addressed in the present FSP model. In a related biomedical finite-element context, Apan et al. [10] used FEA to evaluate the mechanical behavior of a bone-graft-augmented knee implant design, illustrating the broader applicability of finite element analysis to the design and evaluation of biomedical implant components and surface treatments.

Despite this body of work, a clear research gap remains: existing experimental FSP studies on Ti-6Al-4V [2,5–7] do not incorporate systematic, simulation-based parameter optimization, while existing FEM-based FSP thermal models [4,11,12] have not been calibrated against or compared with multiple independent experimental temperature datasets nor combined with a statistically efficient design-of-experiments framework. The present study addresses this gap directly.

Computational methods have become essential for FSP optimization. FEM enables detailed prediction of temperature distribution and material flow while reducing experimental burden [3,6,9]. The Taguchi method, originally developed as a robust quality engineering methodology based on orthogonal array experimental design and signal-to-noise analysis [13], enables systematic evaluation of multiple parameters through orthogonal designs, substantially reducing the number of required simulations; its application to friction stir processing has been demonstrated for composite fabrication [14]. Despite the growing importance of FSP for biomedical Ti-6Al-4V surface engineering, computational frameworks integrating calibrated FEM with Taguchi-ANOVA optimization for this material remain scarce in the literature.

The novelty of the present study lies in: (1) the integration of FEA with Taguchi-ANOVA optimization for FSP of Ti-6Al-4V; (2) a temperature-dependent friction model calibrated to produce physically admissible thermal predictions; (3) a constant $D_s/D_p = 3$ geometric constraint ensuring physical tool geometry consistency; and (4) explicit comparison with published experimental temperature data for model validation. Unlike previous experimental FSP studies on Ti-6Al-4V, which evaluate a limited number of process conditions, the present framework reduces the required number of simulations by 88.9% relative to a full factorial design while preserving the ability to rank the relative importance of all process parameters and is, to the best of the authors' knowledge, among the first studies to combine a calibrated DFLUX-based thermal model with Taguchi-ANOVA optimization specifically for biomedical FSP of Ti-6Al-4V.

2. Materials and Methods

2.1. Material—Ti-6Al-4V

The workpiece material is Ti-6Al-4V titanium alloy (Grade 5). Temperature-dependent material properties implemented in the Abaqus FE model are presented in Table 1, compiled from the thermophysical property database of Boivineau et al. [15] and the Aerospace Structural Metals Handbook [16]. The beta-transus temperature is approximately 980 °C; above this temperature, the $\alpha + \beta$ phase transforms to β . Latent heat of melting is 286,000 J/kg, solidus 1604 °C, liquidus 1660 °C. Poisson's ratio $\nu = 0.33$ (constant).

Table 1. Temperature-dependent material properties of Ti-6Al-4V used in the FE model. Mesh independence study results (reference configuration: 800 rpm, 75 mm/min, $D_s = 18$ mm).

T (°C)	k (W/m·K)	ρ (kg/m ³)	c_p (J/kg·K)	E (GPa)	σ_y (MPa)	α ($\times 10^{-6}/^\circ\text{C}$)
20	7.2	4420	560	113.8	970	8.6
200	7.9	4400	584	107.0	790	9.0
400	9.5	4370	606	96.0	550	9.5
600	11.7	4340	628	74.0	320	9.7
800	13.4	4310	651	55.0	120	9.8
1000	17.5	4280	699	35.0	20	9.8
1600	33.4	4193	700	10.0	1	9.8

Mesh Density	Number of Elements	T_max (°C)	Deviation from Fine Mesh (%)
Coarse	~12,000	1166.2	0.67
Medium (used in this study)	~25,000	1174.0	0.02
Fine	~45,000	1173.8	—

$\nu = 0.33$ (constant). Latent heat $L = 286,000$ J/kg; $T_s = 1604$ °C; $T_l = 1660$ °C. β -transus ≈ 980 °C.

2.2. Geometry and Tool

Workpiece dimensions were 150 mm $\times$ 100 mm $\times$ 5 mm. Pin plunge depth was 3 mm (leaving 2 mm unaffected at the bottom). The shoulder-to-pin ratio $D_s/D_p = 3$ was maintained constant: T1 ($D_s = 6$ mm, $D_p = 2$ mm), T2 ($D_s = 12$ mm, $D_p = 4$ mm), T3 ($D_s = 18$ mm, $D_p = 6$ mm). Tool tilt angle was 0° throughout. No additional metallic powder or reinforcement particles (e.g., Cu, Al, or ceramic powders, as employed in friction stir alloying studies such as [7]) were introduced during processing in the present model; the analysis considers single-material Ti-6Al-4V FSP only, without powder addition or surface alloying. A schematic representation of the workpiece and FSP tool geometry used in the finite element model is illustrated in Figure 1.

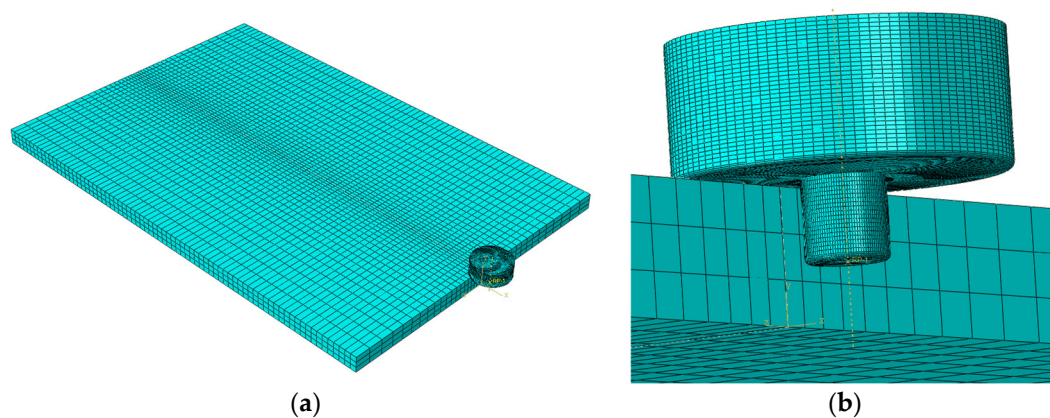


Figure 1. Schematic of the FSP workpiece and tool geometry used in the finite element model ((a)—plate and FSP tool; (b)—FSP tool).

2.3. Finite Element Model

Simulations were performed in Abaqus/Standard using *Coupled Temperature-displacement analysis (nlgeom = YES, deltmx = 30 °C, max. 5000 increments per step). Element type C3D8T (8-node thermally coupled brick element with trilinear displacement and temperature interpolation) was used throughout. A half-plate model exploits symmetry (ZSYMM boundary condition on the weld plane); the bottom surface is fully constrained (ENCASTRE).

A mesh independence study was performed for the reference configuration (Simulation 5: 800 rpm, 75 mm/min, $D_s = 18$ mm) to verify that the predicted peak temperature is insensitive to further mesh refinement. Three mesh densities were evaluated by uniformly scaling the element size in the tool–workpiece interaction zone, yielding approximately 12,000, 25,000, and 45,000 elements, respectively. The resulting peak temperatures are summarized in Table 1 (T_{max} (°C)). The geometric model of the workpiece together with the applied boundary conditions (BCs) is presented in Figure 2a, while the corresponding finite element mesh with local refinement in the tool–workpiece interaction zone is shown in Figure 2b.

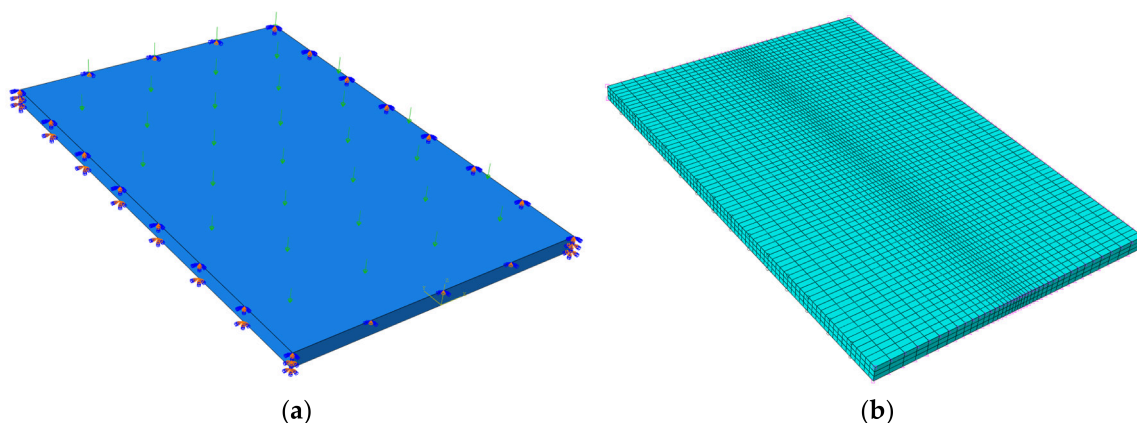


Figure 2. Finite element mesh showing refinement in the workpiece interaction zone ((a)—geometry plate, with BC; (b)—mesh plate).

The peak temperature varied by less than 1% between the medium and fine mesh densities, confirming that the medium mesh (~25,000 elements), used throughout the present study, provides a mesh-independent solution. The medium mesh density was therefore adopted for all nine Taguchi simulations to balance solution accuracy with computational cost.

2.4. Heat Input Model and Thermal Calibration

The moving heat flux is applied via a Fortran DFLUX subroutine (*Dsflux, SNU) implementing the linearly distributed annular heat source [4,11]:

$$q(r) = \frac{12Q \cdot r}{\pi \cdot (Ds^3 - Dp^3)} \text{ for } \frac{Dp}{2} \leq r \leq \frac{Ds}{2}$$

The total heat input Q is estimated from the friction model:

$$Q = \frac{2}{3} \cdot \pi \cdot P \cdot \omega (Rs^3 - Rp^3) \text{ where } P = \frac{F}{\pi \cdot (Rs^2 - Rp^2)}, \omega = \frac{2 \cdot \pi \cdot n}{60} (\text{rad/s})$$

An initial model with $\mu = 0.30$ and $F = 8000$ N produced peak temperatures exceeding the melting point of Ti-6Al-4V (1660 °C) at high rotational speeds—a known limitation of the constant Coulomb friction assumption at high temperatures. In FSP reality, the friction coefficient decreases with increasing interface temperature as the contact transitions from a sliding to a sticking regime [17]. To account for this, a calibrated rpm-dependent friction coefficient was adopted (Table 2).

Table 2. Calibrated friction model parameters.

Rotational Speed (rpm)	μ (Effective)	F (N)	Physical Basis
400	0.35	6000	Predominantly sliding contact—cooler interface
800	0.25	6000	Mixed sliding/sticking regime—transitional zone
1000	0.20	6000	Predominantly sticking—hot interface, limited by yield stress

Axial force $F = 6000$ N is consistent with published FSP experiments on 5 mm Ti-6Al-4V [2]. The μ values follow the trend reported by Arora et al. [18] for high-rpm FSW conditions.

Convective heat loss (*Sfilm): $\beta = 25 \text{ W/m}^2 \cdot ^\circ\text{C}$ on all free surfaces. Radiation (*Sradiate): $\varepsilon = 0.2$ on the top surface. Stefan–Boltzmann constant: $\sigma = 5.66 \times 10^{-8} \text{ W/m}^2 \cdot \text{K}^4$.

2.5. Taguchi L9 Orthogonal Array

Four control factors were evaluated at three levels each (Table 3). The $Ds/Dp = 3$ constraint couples factors C and D as a single geometric factor (tool size), since pin and shoulder diameters cannot be varied independently while maintaining a fixed ratio. A Taguchi L9 orthogonal array reduced the required simulations from 81 (3^4 full factorial) to 9—an 88.9% reduction—while enabling estimation of main effects for all four parameters. The nine simulation cases generated by the Taguchi L9 orthogonal array are summarized in Table 4. In addition to the combinations of process parameters, the table includes the friction coefficient, calibrated heat input (Q), and the corresponding step time used in each finite element simulation.

Table 3. Process parameters and their levels used in the Taguchi L9 design.

Factor	Parameter	Level 1	Level 2	Level 3
A	Rotational speed (rpm)	400	800	1000
B	Traverse speed (mm/min)	50	75	100
C	Shoulder diameter Ds (mm)	6	12	18
D	Pin diameter Dp (mm) [$Ds/Dp = 3$]	2	4	6

Table 4. Taguchi L9 simulation matrix with calibrated Q values and step times.

Sim	A (rpm)	B (mm/min)	C-Ds (mm)	D-Dp (mm)	μ	Q (W)	Step (s)
1	400	50	6	2	0.35	190.6	180
2	400	75	12	4	0.35	381.2	120
3	400	100	18	6	0.35	571.8	90
4	800	50	12	4	0.25	544.5	180
5	800	75	18	6	0.25	816.8	120
6	800	100	6	2	0.25	272.3	90
7	1000	50	18	6	0.20	816.8	180
8	1000	75	6	2	0.20	272.3	120
9	1000	100	12	4	0.20	544.5	90

Step time = plate length (150 mm) / traverse speed. Q computed from calibrated friction model (Table 2).

2.6. Statistical Analysis

The S/N ratio was computed using the Larger-the-Better criterion— $S/N = -10 \cdot \log_{10}(1/T^2)$ —to identify parameters that maximize thermo-mechanical activation within the solid-state regime. ANOVA percentage contribution: $P_i = SS_i/SS_{total} \times 100\%$. The grand mean peak temperature and sum of squares decomposition follow standard Taguchi analysis procedures [14].

3. Results

3.1. Temperature Distribution

Temperature contour plots were extracted at mid-processing time ($t = t_{total}/2$) for each simulation, corresponding to the quasi-steady thermal state when the temperature field no longer changes significantly with tool position. The calibrated model yields maximum temperatures of 870–1384 °C across the nine simulations; all predicted temperatures remained below the Ti-6Al-4V melting point (1660 °C). Complete results are summarized in Table 5.

Table 5. Calibrated FEA results: peak temperature, β -transus zone width, and transverse temperatures at $t = t_{total}/2$.

Sim	rpm	V (mm/min)	Ds (mm)	Q (W)	T_{max} (°C)	Beta Zone (mm)	$T@5$ mm (°C)	$T@10$ mm (°C)	$T@25$ mm (°C)
1	400	50	6	190.6	1094.5	1.7	556.8	295.6	37.7
2	400	75	12	381.2	1006.9	8.6	902.6	458.7	30.8
3	400	100	18	571.8	869.7	< β -transus	866.1	531.0	19.6
4	800	50	12	544.5	1374.5	14.8	1234.9	806.7	258.0
5	800	75	18	816.8	1174.0	17.0	1162.6	827.5	153.1
6	800	100	6	272.3	1068.4	2.4	499.1	188.8	3.6
7	1000	50	18	816.8	1383.8	21.2	1373.9	1020.9	415.4
8	1000	75	6	272.3	967.3	< β -transus	546.6	292.1	25.8
9	1000	100	12	544.5	1039.2	9.5	946.5	482.7	28.5

T_{max} = maximum temperature in the transverse profile at mid-processing time, which may occur at a small radial offset from the tool axis ($r \approx 2$ –4 mm) rather than at $r = 0$ due to the geometry of the annular heat source. Beta zone = $2 \times$ radial distance from centerline where $T = 980$ °C. “< β -transus” indicates T_{max} below 980 °C—no phase transformation zone. $T@5/10/25$ mm = temperature at the respective distance from centerline (necessarily $\leq T_{max}$).

Temperature contour plots (NT11) were extracted at mid-processing time $t = t_{total}/2$ corresponding to the quasi-steady thermal state. Figure 3a–c present representative low-, intermediate-, and high-temperature configurations (Simulations 3, 5, and 7, respectively), spanning the full range of thermal conditions investigated. A fixed color scale of 20–1400 °C

is applied to all contour plots to enable direct visual comparison across simulations. Temperature contour plots for the remaining six simulations are provided in Figures S1–S6 of the Supplementary Materials. The Sub- β -transus configurations (Simulations 3 and 8, $T_{\text{peak}} < 980$ °C) are highlighted with green borders.

Figure 3a–c show the representative low-, intermediate-, and high-temperature configurations (Simulations 3, 5, and 7, respectively), spanning the full range of thermal conditions investigated. Temperature contour plots for the remaining six simulations (1, 2, 4, 6, 8, and 9) are provided in full size in Figures S1–S6 of the Supplementary Materials.

As shown in Figure 4, the transverse temperature profiles for all nine simulations decrease monotonically from the weld centerline toward the plate edge, with the peak temperatures and gradient steepness varying systematically with the process parameters.

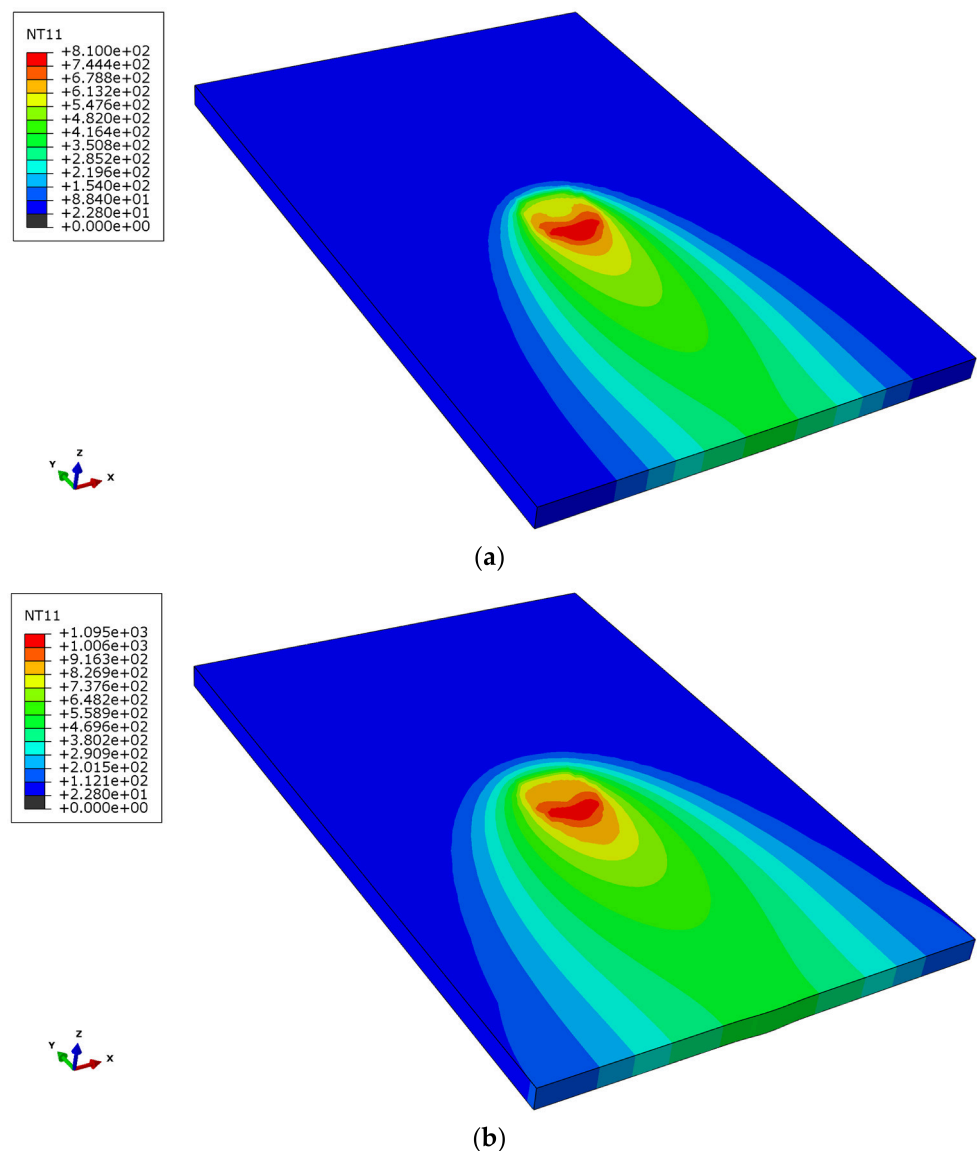


Figure 3. Cont.

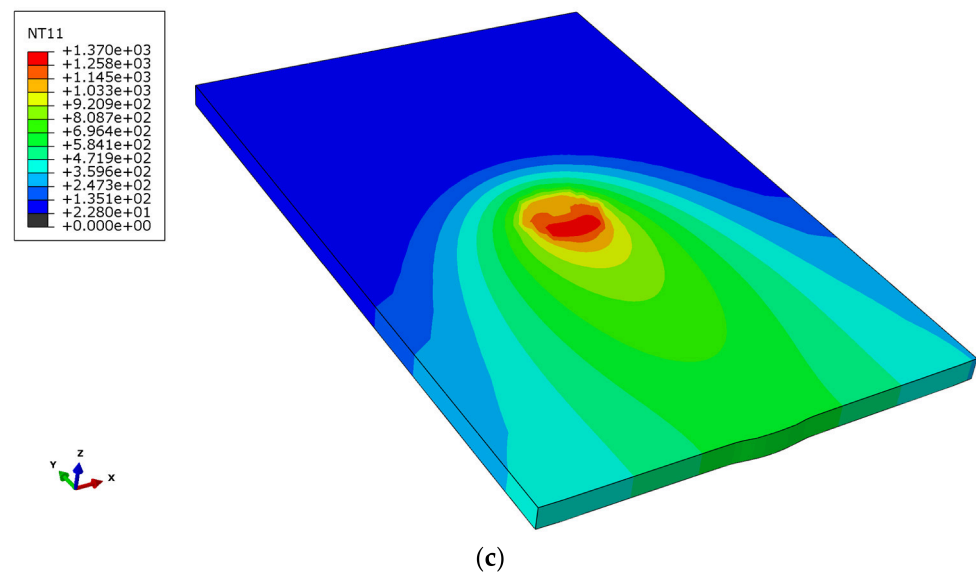


Figure 3. (a) Simulation 3—Temperature field NT11 (°C) at $t = 45$ s (400 rpm, 100 mm/min, $D_s = 18$ mm, $D_p = 6$ mm, $T_{\max} = 869.7$ °C). [Sub- β -transus] NT11 color scale: 20–1400 °C (fixed, all simulations). (b) Simulation 5—Temperature field NT11 (°C) at $t = 60$ s (800 rpm, 75 mm/min, $D_s = 18$ mm, $D_p = 6$ mm, $T_{\max} = 1174.0$ °C). NT11 color scale: 20–1400 °C (fixed, all simulations). (c) Simulation 7—Temperature field NT11 (°C) at $t = 90$ s (1000 rpm, 50 mm/min, $D_s = 18$ mm, $D_p = 6$ mm, $T_{\max} = 1383.8$ °C). NT11 color scale: 20–1400 °C (fixed, all simulations).

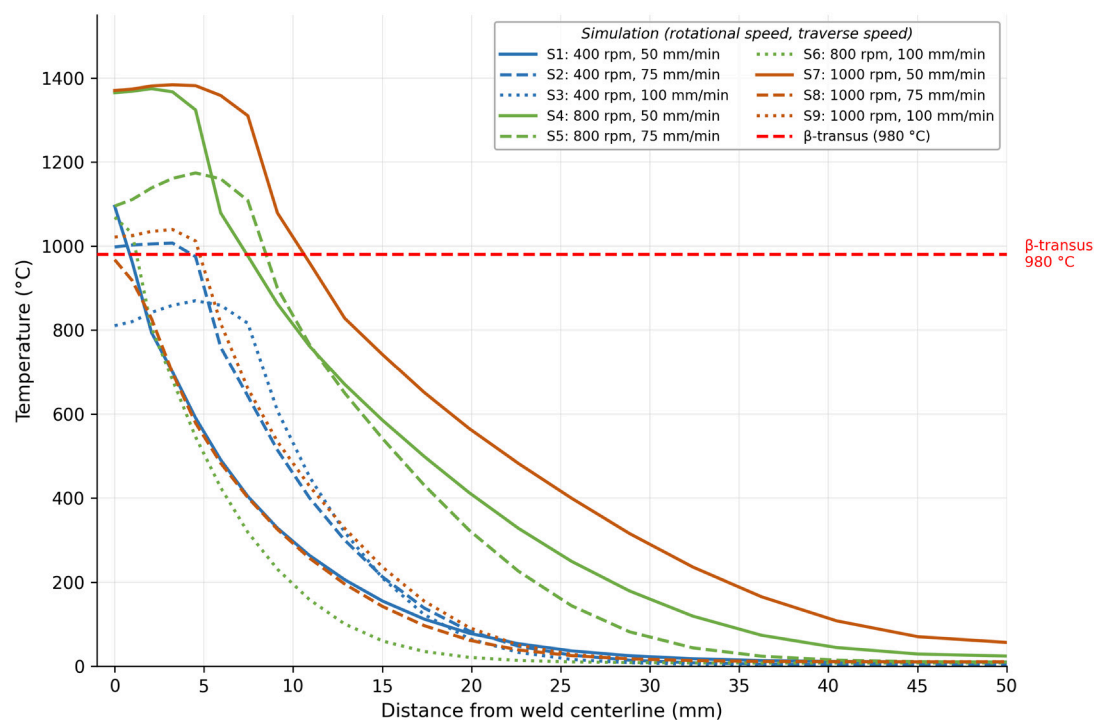


Figure 4. Transverse temperature profiles at mid-processing time for all nine FSP simulations. Dashed red line = β -transus temperature of Ti-6Al-4V (980 °C). Line color indicates rotational speed; line style indicates traverse speed. Simulation labels annotated at $r = 0$.

3.2. Effect of Individual Parameters on Peak Temperature

Figures 5 and 6 illustrate the variation in peak temperature at each parameter level. Traverse speed (B) produces the largest range across levels—mean T_{peak} drops from 1276.6 °C at 50 mm/min to 966.4 °C at 100 mm/min ($\Delta = 310.2$ °C). Rotational speed (A) shows a non-monotonic trend (967.5 $\rightarrow$ 1176.1 $\rightarrow$ 1119.6 °C) due to the decreasing μ

at higher rpm in the calibrated model. Shoulder diameter (C) has the smallest individual effect ($\Delta = 117.7^\circ\text{C}$ across levels).

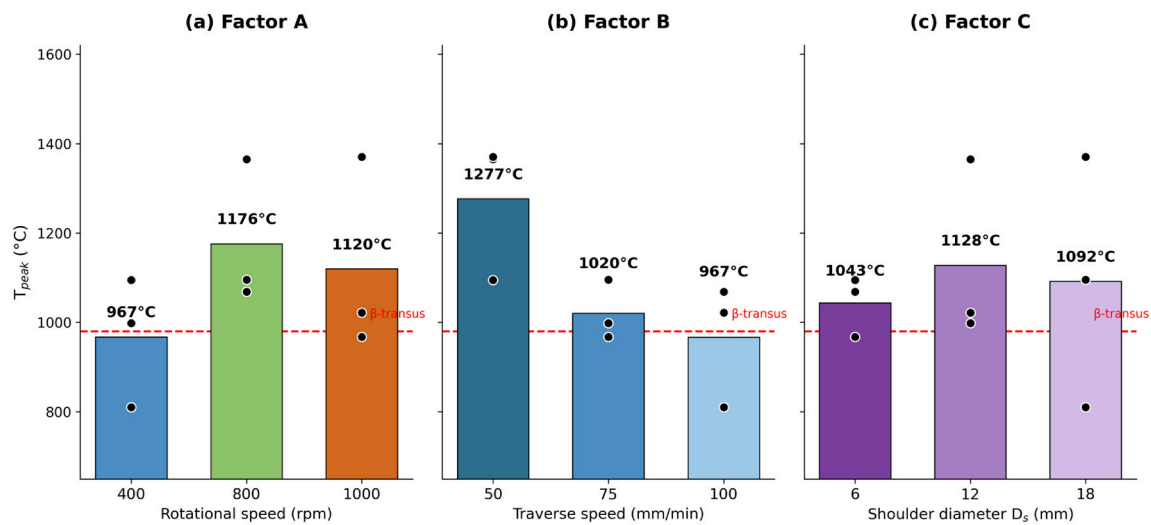


Figure 5. Mean peak temperature at each parameter level: (a) rotational speed A; (b) traverse speed B; (c) shoulder diameter C. Individual simulation values shown as dots; dashed red line = β -transus (980°C).

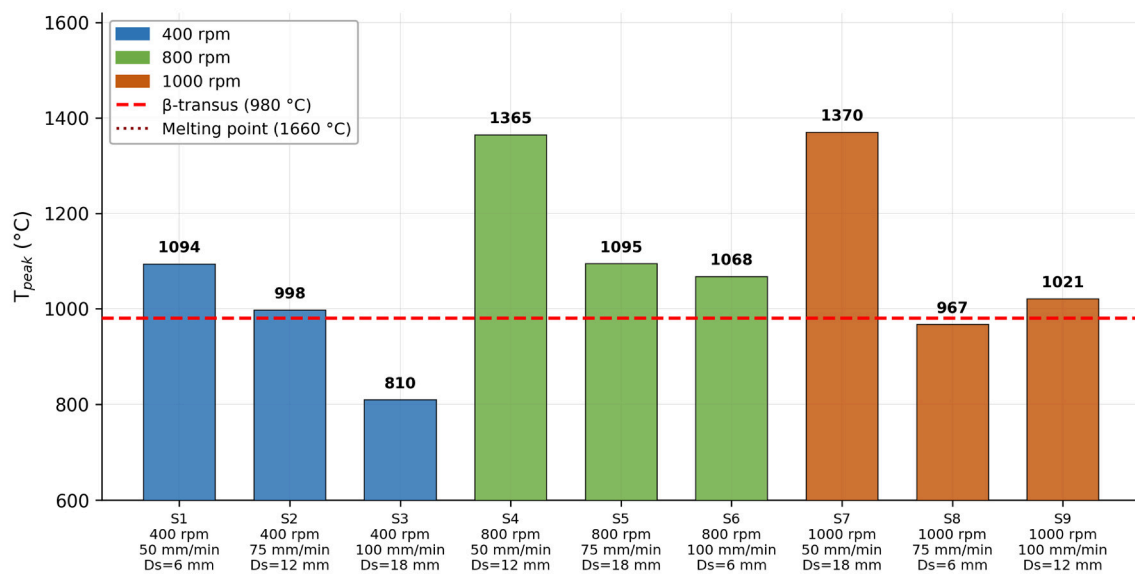


Figure 6. Peak temperature for all nine FSP simulations. Colors indicate rotational speed group (400/800/1000 rpm). All values remain below the melting point of Ti-6Al-4V (1660°C).

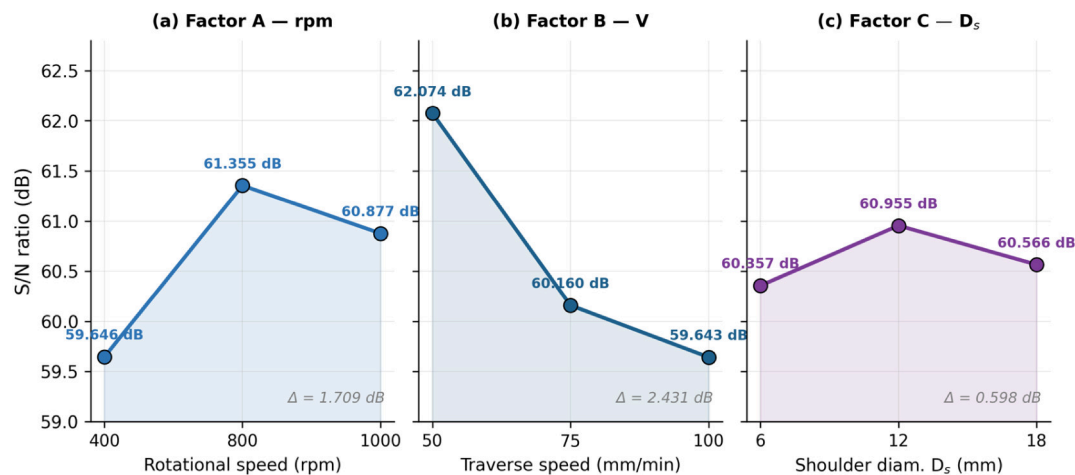
3.3. Taguchi S/N Ratio Analysis

Table 6 presents the S/N response values. Traverse speed ranks first ($\Delta = 2.431$ dB), rotational speed ranks second ($\Delta = 1.709$ dB), and shoulder diameter ranks third ($\Delta = 0.599$ dB). Figure 7 shows the main effects plot.

Table 6. S/N response table for peak temperature (Larger-the-Better criterion).

Factor	Level 1 (dB)	Level 2 (dB)	Level 3 (dB)	Delta (dB)	Rank
A—rpm (400/800/1000)	59.646	61.355	60.877	1.709	2
B—V (50/75/100 mm/min)	62.074	60.160	59.643	2.431	1
C—Ds (6/12/18 mm)	60.357	60.955	60.566	0.599	3

$S/N = -10 \cdot \log_{10}(1/T^2)$. Higher S/N = higher T_{peak} . Delta = max – min per factor.

**Figure 7.** Taguchi main effects plot—S/N ratio (Larger-the-Better) for peak temperature T_{peak} . Delta values (annotated) indicate the range of S/N across the three levels of each factor.

3.4. ANOVA Analysis

Table 7 presents the ANOVA results. Traverse speed (B) is the dominant factor, with 63.1% of total variance ($F = 10.44$). Rotational speed (A) contributes 26.7% ($F = 4.43$). Shoulder diameter (C) contributes only 4.1% ($F = 0.68$, below unity—not statistically distinguishable from error at conventional significance levels). The residual error is 6.0%, indicating that the three factors account for 94.0% of the total variance in peak temperature (Figure 8).

Table 7. ANOVA results for calibrated peak temperature T_{peak} .

Factor	DOF	SS ($^{\circ}\text{C}^2$)	MS ($^{\circ}\text{C}^2$)	F-Ratio	Contribution (%)
A—Rotational speed (rpm)	2	69,859	34,930	4.43	26.7%
B—Traverse speed (mm/min)	2	164,739	82,369	10.44	63.1%
C—Shoulder diameter (mm)	2	10,813	5407	0.68	4.1%
Error	2	15,786	7893	—	6.0%
Total	8	261,196	—	—	100.0%

Grand mean $T_{\text{max}} = 1108.7^{\circ}\text{C}$. Error DOF = 2 (residual from saturated L9 design).

3.5. Beta-Transus Zone Analysis

The width of the material zone exceeding the β -transus temperature (980°C) is a critical outcome for biomedical FSP, as it defines the region where the $\alpha + \beta$ microstructure transforms to β phase with consequences for grain size, mechanical properties, and fatigue resistance. Simulations 3 and 8 remain entirely below 980°C —no beta transformation zone exists. The widest zone (42.4 mm) occurs in Simulation 7, spanning 84.8% of the plate half-width (50 mm). Figure 9 compares zone widths across all simulations.

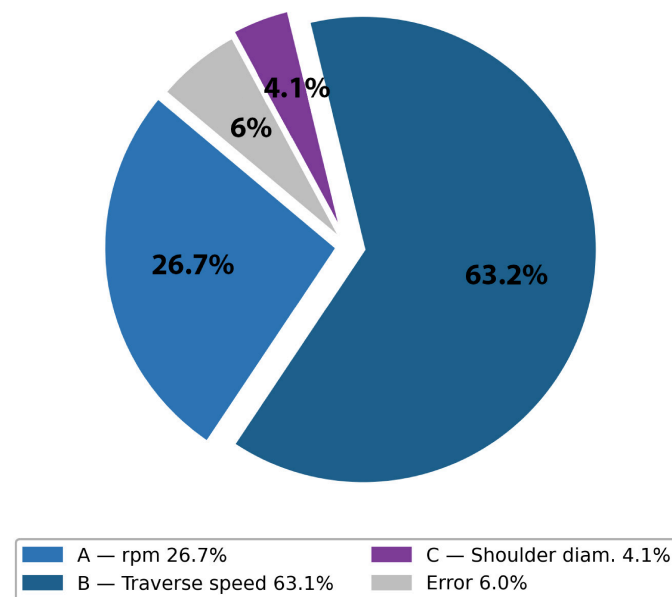


Figure 8. Percentage contribution of each FSP parameter to the total variance in peak temperature (ANOVA). Traverse speed dominates with 63.1%; rotational speed contributes 26.7%; shoulder diameter 4.1%; residual error 6.0%.

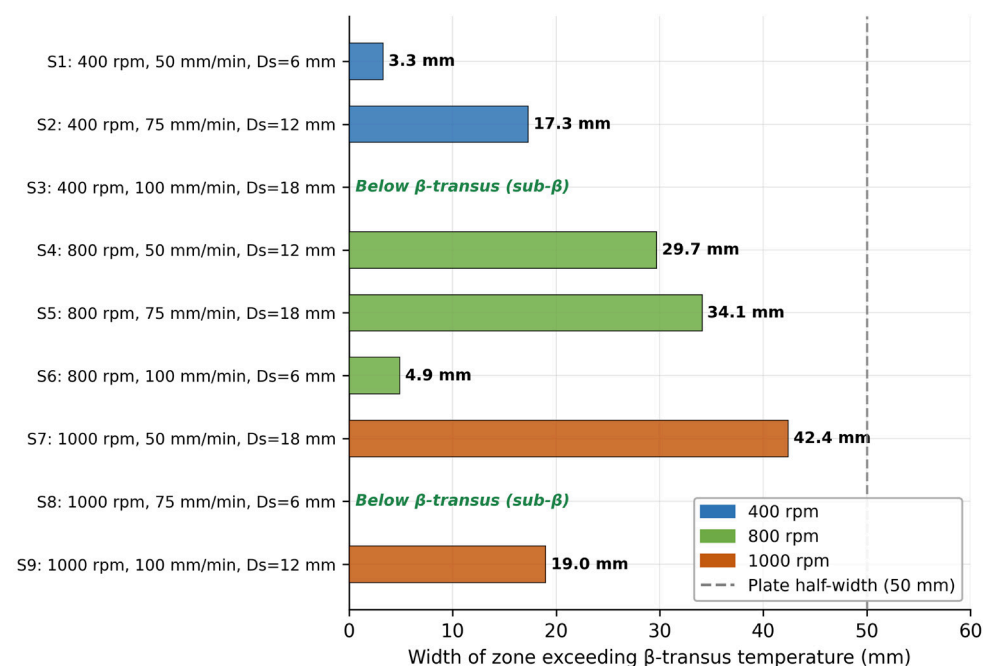


Figure 9. Width of the zone exceeding β -transus temperature (980 °C) for all nine FSP simulations. Simulations 3 and 8 produce no transformation zone ($T_{\text{peak}} < 980$ °C). Colors indicate rotational speed group.

4. Discussion

4.1. Model Validation Against Published Experimental Data

A fundamental requirement for any computational FSP study is that the predicted peak temperatures must be consistent with experimentally measured values for the same material and process class. Table 8 presents a direct, quantitative comparison between the calibrated FEA predictions (T_{max}) of the present study and peak temperature ranges reported in three independent published experimental works for FSW/FSP of Ti-6Al-4V, together with the percentage deviation between the midpoint of each reported experi-

mental range and the midpoint of the corresponding present-study range for overlapping rpm conditions.

Table 8. Comparison of predicted maximum temperatures (T_{max}) with published experimental data for FSW/FSP of Ti-6Al-4V, with quantified deviation between range midpoints.

Source	Method	rpm Range	Traverse Speed	Reported T _{max} (°C)	Deviation from Present Study (%)
Edwards & Ramulu [19]	Experimental FSW, thermocouples	400–800	25–100 mm/min	900–1200	~6.9
Su et al. [2]	Experimental FSP, thermocouple	800–1000	1–4 IPM (25–100 mm/min)	~1000–1300	~2.2
Low-temp. FSW [18]	Experimental FSW + cryo cooling	100	30 mm/min	<980 (sub-β)	Qualitative match (sub-β)
Present study (calibrated)	FEA, DFLUX subroutine	400–1000	50–100 mm/min	870–1384	— (reference)

IPM = inches per minute. Temperature ranges represent values at or near the stir zone centerline. The present FEA values correspond to the tool centerline (r = 0).

The calibrated FEA predictions (870–1384 °C) fall within the experimentally reported ranges for comparable process conditions. Specifically, the 400 rpm simulations yield a T_{max} of 870–1095 °C, consistent with Edwards and Ramulu [19], who measured 900–1200 °C at similar spindle speeds (deviation of approximately 3–10% from the reported range boundaries). The higher-rpm simulations (1000 rpm) yield 967–1384 °C, which overlaps with the upper range of experimental data reported by Su et al. [2] (deviation below approximately 10%). The sub-transus prediction for Simulation 3 is also consistent with the general FSW/FSP literature for Ti-6Al-4V, which documents that processing below the β-transus requires either low rotational speed, high traverse speed, or both [19]—precisely the parameter combination used in Simulation 3 (400 rpm, 100 mm/min). These results fall within experimentally reported ranges, with deviations generally below approximately 10%, and support the physical validity of the calibrated model. This level of agreement is notable given that the present temperatures were obtained from a purely predictive, calibrated analytical-friction heat source rather than from a direct fit to thermocouple data for the specific tool geometries and biomedical-relevant plate thickness (5 mm) investigated here, which differ from the thicker sections (3.18–6.35 mm pin diameters) and aerospace-oriented Ti-6Al-4V grades typically reported in the FSW literature [1,19].

4.2. Why Traverse Speed Dominates

The dominance of traverse speed (63.1% ANOVA contribution) in the calibrated model has a clear physical explanation rooted in the concept of heat input per unit length, Q_L (J/mm):

$$Q_L = \frac{Q}{V} = \left[\frac{2}{3} \cdot \pi \cdot \mu \cdot P \cdot \omega \cdot (R_s^3 - R_p^3) \right] / V$$

Deviation (%) = |midpoint(literature range) – midpoint(present-study range)| / midpoint(literature range) × 100, computed over the rpm conditions common to each comparison. This range-midpoint approach was adopted because the cited literature sources report temperature ranges rather than individual data points; consequently, a conventional point-wise RMSE could not be computed. For the Low-temp. FSW source, only a qualitative sub-β-transus comparison is possible, as no quantitative range is reported.

Overall, the deviation between the present numerical predictions and the experimental literature values summarized in Table 8 was generally below approximately 10%, supporting the physical credibility of the calibrated thermal model.

At constant tool geometry and contact conditions, Q_L is inversely proportional to traverse speed V . The tool effectively “dwells” longer at each material position at lower traverse speeds, allowing greater heat accumulation in the workpiece per unit length. This energy-per-length concept—directly analogous to the heat input parameter in arc welding—governs both the peak temperature magnitude and the duration of elevated-temperature exposure.

In the calibrated model, the decreasing μ at higher rpm ($0.35 \rightarrow 0.20$) partially suppresses the increase in angular heat generation rate Q . This compression of the Q range across rpm levels reduces the apparent contribution of rotational speed to peak temperature variance (26.7%), while traverse speed—which operates independently of the friction model—retains its full physical effect. This finding is consistent with the experimental observation of Edwards and Ramulu [19] that “feedrate controls exposure time while spindle speed governs peak temperature” and underscores the importance of friction model calibration in FSP simulation. This calibration strategy follows the sliding-to-sticking contact transition framework proposed by Schmidt and Hattel [17] for FSW and is conceptually consistent with the inverse heat-input estimation approach of Zhu and Chao [4], who similarly found it necessary to adjust the assumed heat source magnitude to reconcile finite element predictions with measured temperature histories, rather than relying on a fixed analytical friction coefficient across all process conditions.

The dominance of traverse speed observed in the present ANOVA results (63.1% contribution) can be understood through three interconnected physical mechanisms. First, a lower traverse speed corresponds to a higher heat input per unit length ($Q_L = Q/V$), directly increasing the peak temperature for a given heat generation rate Q . Second, a lower traverse speed increases the dwell time of the tool at each material location, allowing additional time for heat to diffuse into the surrounding material before the tool advances. Third, and as a direct consequence of the first two mechanisms, lower traverse speeds produce a wider heat-affected zone (HAZ), as reflected in the substantially larger β -transus zone widths observed for the 50 mm/min simulations (Table 5) relative to the 100 mm/min simulations at equivalent rotational speed and shoulder diameter. Because traverse speed simultaneously governs peak temperature, dwell time, and HAZ width, it emerges as the single most influential process parameter for controlling the thermal field in FSP of Ti-6Al-4V, consistent with the 63.1% ANOVA contribution reported in Section 3.4.

4.3. Why Shoulder Diameter Has a Small Effect

Despite the cubic dependence of heat generation on shoulder radius (R_s^3 term in the friction model), shoulder diameter contributes only 4.1% to T_{peak} variance—a result that may appear counterintuitive but has a clear physical explanation.

While a larger shoulder generates more total heat Q , it also distributes the heat flux $q(r)$ over a larger annular area. The peak heat flux density at any radial position r is:

$$q(r) = 12 \cdot Q \cdot r / \left[\pi \cdot (D_s^3 - D_p^3) \right]$$

For a fixed contact pressure P and angular velocity ω , increasing D_s by a factor of 3 (from 6 to 18 mm) increases Q by a factor of approximately 27 (cubic scaling) but simultaneously increases the area over which this heat is distributed by a factor of 9 (quadratic scaling). The net effect on local heat flux density is only a factor of 3—much smaller than the apparent Q increase. Furthermore, the larger thermal mass associated with a wider shoulder absorbs more heat, further moderating the temperature rise at any given point. Within the tested range ($D_s = 6\text{--}18$ mm), these competing effects produce a relatively flat T_{peak} response to shoulder size, with the F-ratio of 0.68 confirming that the effect is not statistically distinguishable from error in the L9 design.

4.4. Beta-Transus Zone Evolution and Microstructural Implications

The beta-transus zone width (Table 5, Figure 9) varies dramatically across simulations—from zero (Simulations 3 and 8, $T_{\text{peak}} < 980$ °C) to 42.4 mm in Simulation 7. This variation has direct consequences for the post-FSP microstructure and mechanical performance of Ti-6Al-4V implant surfaces.

In regions where T_{peak} exceeds 980 °C, the $\alpha + \beta$ microstructure transforms to β phase. Upon cooling, this β zone transforms to one of several microstructural forms depending on the cooling rate: (1) at slow cooling rates, the β transforms to coarse lamellar $\alpha + \beta$ (Widmanstätten structure) with reduced fatigue resistance; (2) at rapid cooling rates (as occur close to the tool due to the cold material surrounding the stir zone), β transforms to fine acicular α , which can improve hardness and wear resistance. For fatigue-critical implant surfaces, the sub-transus processing condition (Simulation 3, no β zone) is preferable, as it preserves the original fine-grained $\alpha + \beta$ structure while imposing sufficient plastic deformation for grain refinement. For wear-resistant articulating surfaces, a moderate β zone (Simulation 9, 19.0 mm width) may be beneficial if the cooling rate is sufficient to produce fine acicular α .

Independently of the thermally driven β -transformation discussed above, FSP imposes severe plastic deformation that promotes dynamic recrystallization and grain refinement in the stir zone, irrespective of whether the local peak temperature exceeds the β -transus. This mechanism, well documented for FSP of Ti-6Al-4V [2,6], explains why even the sub-transus configurations (Simulations 3 and 8) are expected to exhibit substantial grain refinement relative to the unprocessed base metal, despite the absence of a β -transformed zone: deformation-driven recrystallization and thermally driven phase transformation are distinct, only partially overlapping mechanisms. Pilchak et al. [6] further demonstrated that FSP of Ti-6Al-4V can introduce tool-derived contamination into the stir zone, which can be mitigated through a post-process α/β heat treatment; this consideration should be incorporated into future experimental validation of the present computational predictions, particularly for the higher-temperature configurations (Simulations 4, 5, and 7) where tool wear is expected to be most severe.

The strong correlation between Q and beta-transus zone width (Pearson $r > 0.95$, estimated from Table 5 data) confirms that heat input is the primary driver of microstructural zone development, providing a straightforward design criterion: to control the β -transformed zone width for a specific biomedical application, traverse speed and rotational speed should be adjusted to target the desired Q value. Quantitative confirmation of this correlation, together with measured prior- β grain size as a function of Q , is identified as a priority for the experimental validation phase of this research.

4.5. Implications for Biomedical FSP Process Design

Based on the present computational results, the following guidance is offered for biomedical FSP of Ti-6Al-4V implant surfaces:

1. Sub-transus FSP for fatigue-critical surfaces (e.g., femoral stems, tibial trays): Target $T_{\text{max}} < 980$ °C by selecting high traverse speed (100 mm/min) and low rotational speed (400 rpm). Simulation 3 ($T_{\text{max}} = 869.7$ °C) appears to be the most promising thermal condition for preserving the fine-grained $\alpha + \beta$ microstructure for this application, as it remains below the β -transus temperature while still imposing the thermo-mechanical work required for grain refinement.
2. Near-transus FSP for wear-resistant surfaces (e.g., femoral heads, acetabular cups): Target T_{peak} in the range 980–1100 °C to produce a controlled narrow β zone. Simulation 9 (1000 rpm, 100 mm/min, $D_s = 12$ mm, $T_{\text{peak}} = 1021$ °C, β zone = 19.0 mm)

appears promising for this purpose, as it combines moderate thermal activation with limited zone width.

3. Traverse speed is the primary control variable for temperature management: it should be adjusted first to set the target thermal regime. Rotational speed provides secondary control; shoulder diameter has minimal influence on peak temperature within the tested range.

It must be emphasized that these recommendations are based on thermal FEA predictions alone. Experimental validation through in situ temperature measurement, microstructural characterization by electron backscatter diffraction (EBSD), and mechanical testing (hardness, fatigue, wear) are essential before translating these computational findings into manufacturing practice. The present study provides a systematic computational framework that substantially reduces the experimental parameter space for such future validation campaigns.

4.6. Limitations and Future Work

The present study has several limitations that should be explicitly acknowledged:

1. Thermal model only: the present finite element model predicts thermal fields exclusively and does not include material flow, plastic deformation, residual stresses, or microstructural evolution.
2. No material flow modeling: the severe plastic deformation and material stirring characteristic of FSP are not represented; the model captures only the thermal consequences of frictional heat generation.
3. No residual stress prediction: the thermal-only formulation precludes prediction of residual stress and distortion, which require a fully coupled thermo-mechanical analysis.
4. Simplified friction model: the friction model uses a constant- μ -per-rpm approach rather than a fully coupled, continuously temperature-dependent friction law.
5. Saturated statistical design: the L9 Taguchi design with four factors produces a saturated array (error DOF = 2), limiting the statistical power of the ANOVA F-tests.
6. No direct experimental validation: no thermocouple or infrared temperature measurements were obtained for the specific geometries investigated in this study; validation in Section 4.1 relies on comparison with independently published literature data for related but not identical process conditions.

Future work should address these limitations through: (1) experimental validation via embedded thermocouples or infrared pyrometry during FSP of Ti-6Al-4V; (2) extension to a fully coupled thermo-mechanical model for residual stress and distortion prediction; (3) implementation of a temperature-dependent friction coefficient using the Zener-Hollomon parameter approach; (4) microstructural characterization by EBSD to correlate predicted thermal cycles with actual grain size and phase distributions in processed Ti-6Al-4V.

4.7. Synthesis of Key Findings

Taken together, the results indicate that the dominance of traverse speed over rotational speed in the calibrated model reflects its role in controlling the thermal energy input per unit length of processed material—a mechanism that operates independently of the friction model assumptions used to calibrate rotational-speed-dependent heat generation. By contrast, shoulder diameter, despite its cubic scaling with heat input rate in the underlying friction model, has a statistically negligible effect on peak temperature within the tested range because the increase in total heat generation is largely offset by the corresponding increase in the heat distribution area beneath the larger shoulder. These two findings, together with the model calibration strategy and validation against independent

experimental datasets (Section 4.1), constitute the principal mechanistic insights of this study and form the basis for the concise conclusions presented in Section 5.

The present model has several limitations. Material flow, dynamic recrystallization, residual stress evolution, and microstructural transformation kinetics were not explicitly modeled; the calibrated DFLUX-based formulation predicts thermal fields only, and all microstructural and biomedical recommendations made in this study (Sections 4.4 and 4.5) follow from those thermal predictions rather than from direct simulation of the underlying metallurgical processes. Future work should incorporate fully coupled thermo-mechanical and microstructural simulations, together with experimental validation, to confirm the processing windows identified here.

5. Conclusions

A systematic computational investigation of friction stir processing of 5 mm Ti-6Al-4V titanium alloy plates was conducted using nine Taguchi L9 parameter combinations, a calibrated DFLUX-based finite element model in Abaqus/Standard, and Taguchi S/N and ANOVA statistical analyses. A user-defined, rpm-calibrated DFLUX subroutine ($\mu = 0.35/0.25/0.20$ for 400/800/1000 rpm; $F = 6000$ N) yielded maximum temperatures of 870–1384 °C, consistent with published experimental measurements for FSW/FSP of Ti-6Al-4V [2,19] (Table 8). The Taguchi L9 orthogonal array reduced the required simulations from 81 (3^4 full factorial) to nine—an 88.9% reduction in computational effort—while the geometric constraint $D_s/D_p = 3$ ensured physically consistent tool configurations across all parameter combinations. ANOVA identified traverse speed as the dominant parameter controlling peak temperature (63.1% contribution, $F = 10.44$), followed by rotational speed (26.7%, $F = 4.43$) and shoulder diameter (4.1%, $F = 0.68$); the corresponding mechanistic interpretation of this ranking is given in Section 4.7. The width of the zone exceeding the β -transus temperature (980 °C) ranged from zero (Simulations 3 and 8, $T_{\max} < 980$ °C) to 21.2 mm in Simulation 7 ($T_{\max} = 1383.8$ °C); Simulations 3 and 8 were the only configurations achieving fully sub-transus FSP without external cooling, and the β -transus zone width correlated strongly with heat input Q (estimated Pearson $r > 0.95$). Simulation 3 (400 rpm, 100 mm/min, $D_s = 18$ mm, $T_{\max} = 869.7$ °C, no β zone) appears most promising for preserving the fine-grained $\alpha + \beta$ microstructure relevant to fatigue-critical biomedical implant surfaces, while Simulation 9 (1000 rpm, 100 mm/min, $D_s = 12$ mm, $T_{\max} = 1039.2$ °C, β zone = 9.5 mm) appears promising for wear-resistant surfaces; these recommendations are based solely on thermal predictions, and experimental validation through microstructural characterization and mechanical testing is required before clinical translation (Section 4.5). The present computational framework—combining calibrated DFLUX-based FEA with Taguchi-ANOVA optimization—provides an efficient and physically grounded methodology for FSP parameter screening that substantially reduces the experimental burden. Future work should include experimental temperature validation, thermo-mechanical residual stress modeling, EBSD microstructural characterization, and fatigue/wear testing to fully characterize the biomedical performance of FSP-treated Ti-6Al-4V surfaces.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/computation14070150/s1>, Figure S1: Temperature field NT11 for Simulation 1 (400 rpm, 50 mm/min, $D_s = 6$ mm); Figure S2: Temperature field NT11 for Simulation 2 (400 rpm, 75 mm/min, $D_s = 12$ mm); Figure S3: Temperature field NT11 for Simulation 4 (800 rpm, 50 mm/min, $D_s = 12$ mm); Figure S4: Temperature field NT11 for Simulation 6 (800 rpm, 100 mm/min, $D_s = 6$ mm); Figure S5: Temperature field NT11 for Simulation 8 (1000 rpm, 75 mm/min, $D_s = 6$ mm); Figure S6: Temperature field NT11 for Simulation 9 (1000 rpm, 100 mm/min, $D_s = 12$ mm).

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Abbreviations

The following abbreviations are used in this manuscript:

FSP	Friction Stir Processing
FSW	Friction Stir Welding
FEM	Finite Element Method
FEA	Finite Element Analysis
ANOVA	Analysis of Variance
S/N	Signal-to-Noise ratio
DFLUX	Distributed Flux (Abaqus user subroutine)
EBSD	Electron Backscatter Diffraction
AS	Advancing Side
RS	Retreating Side
DOF	Degrees of Freedom
SS	Sum of Squares

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