

SIMULATION AND COMPARISON OF CASTING PROCESS, SOLIDIFICATION AND CRYSTAL STRUCTURE IN ASTM A36 STEEL

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Abstract. This study presents a simulation-based comparison of the casting process, solidification behavior, and crystal structure formation in ASTM A36 structural steel. Finite element and finite difference methods were employed to model thermal gradients, solidification fronts, and microstructural evolution during sand and die casting processes. The simulation was validated against experimental casting trials, with particular attention paid to dendrite arm spacing, grain morphology, and the development of ferrite-pearlite microstructures characteristic of low-carbon structural steels. Results indicate that cooling rate significantly governs grain refinement and crystal orientation, with die casting producing finer equiaxed grains compared to sand casting. Comparative analysis reveals that the solidification sequence directly influences the final mechanical properties, including yield strength, tensile strength, and impact toughness, all of which must meet ASTM A36 requirements. Thermal contraction and residual stress distributions were also evaluated, demonstrating that controlled solidification mitigates hot-tearing defects. The study provides a comprehensive computational framework for optimizing casting parameters to achieve consistent microstructural quality in ASTM A36 components.

Keywords: casting simulation, solidification, crystal structure, ASTM A36, microstructure

Introduction

ASTM A36 is among the most extensively produced structural steels globally, with applications spanning bridges, buildings, heavy machinery, and marine structures. Its minimum yield strength of 250 MPa, combined with excellent weldability and low production cost, makes it a preferred choice for large-scale structural fabrication (Attar et al., 2014). Despite widespread deployment, the relationship between casting process parameters and the resulting microstructure and mechanical properties of ASTM A36 steel remains an area of active investigation, particularly in the context of near-net-shape manufacturing (Sigli et al., 1998; Callister Jr., 2003). The casting process introduces a complex interplay of thermal, fluid, and solidification phenomena that ultimately govern component quality. Inadequate control of cooling rates, mold thermal properties, and pouring conditions can result in undesirable microstructural features such as columnar grain growth, centerline segregation, and macro-porosity (Sun et al., 2019). These defects adversely affect tensile strength, fatigue life, and impact toughness. Understanding and predicting these phenomena requires both robust experimental characterization and validated numerical models capable of resolving solidification at the micro- and macrostructural scales (Du et al., 2007). Computational simulation has emerged as an indispensable tool for optimizing casting processes without incurring the cost of extensive physical trials. Thermal models based on finite difference and finite element methods enable prediction of solidification front evolution, mushy zone extent, grain morphology, and phase transformation sequences (Gan et al., 2017; Flemings, 1974). When coupled with thermodynamic databases and continuous

cooling transformation (CCT) diagrams, these models can reliably forecast the ferrite-pearlite crystal structure characteristic of hypoeutectoid steels such as ASTM A36 (Hunt, 1984). Comparative studies of sand and permanent-die casting have demonstrated that die casting imposes cooling rates approximately one order of magnitude greater than sand casting, producing substantially finer secondary dendrite arm spacings (SDAS) and superior mechanical property (Kaufman and Rooy, 2004; Trivedi and Kurz, 1986). However, the higher cooling rate also introduces greater residual stresses that may require post-casting thermal relief (Shafeek et al., 2024). The present study employs a validated finite difference thermal model to compare these two casting routes for ASTM A36 steel, with the central hypothesis that die casting will produce a measurably finer equiaxed grain structure and superior hardness relative to sand casting, at the expense of higher residual stress.

The solidification behaviour of metallic alloys is strongly influenced by the thermal conditions established at the interface between the molten metal and the mold, where heat extraction determines the progression of the solidification front and the development of the final grain structure. Variations in cooling rate can significantly modify nucleation and dendritic growth, leading to differences in grain morphology, segregation behaviour, and ultimately the mechanical response of the solidified component. The transition from columnar to equiaxed grains is particularly important because it determines the uniformity of the resulting microstructure and can influence the susceptibility of cast products to defects. Wang and Beckermann (1994) demonstrated that the columnar-to-equiaxed transition during dendritic alloy solidification is governed by the interaction between thermal conditions and nucleation ahead of the advancing columnar front. Similarly, Hunt (1984) established relationships between thermal gradients, growth conditions, and the development of columnar and equiaxed structures during solidification. Rapid solidification can further alter microstructural development by modifying interface stability and characteristic microstructural length scales (Trivedi and Kurz, 1986). These fundamental mechanisms emphasize the importance of accurately describing heat transfer and solidification kinetics when comparing different casting processes. In addition, numerical approaches can provide spatial and temporal information that is difficult to obtain experimentally during solidification. Modeling therefore provides an effective means of examining temperature gradients, solidification times, and the progression of solid fractions throughout a casting. Such information is particularly relevant when comparing sand and permanent-die molds because their different thermal characteristics are expected to produce substantially different heat extraction conditions. Consequently, incorporating these solidification principles into numerical analysis provides a stronger theoretical basis for predicting the microstructural differences that may develop under the two casting conditions and for relating these differences to the resulting mechanical behaviour of the material (Nastac, 2004; Flemings, 1974).

Another critical aspect of casting is the development of defects associated with non-uniform solidification, particularly shrinkage porosity, segregation, and variations in local microstructure. As solidification progresses, redistribution of solute elements between the liquid and solid phases may create localized compositional variations, which can influence phase formation and the mechanical properties of the final casting. Du et al. (2007) demonstrated through numerical modeling and experimental investigation that microsegregation during alloy solidification is closely associated with the evolution of the solidification structure and local solute redistribution. Although the

specific alloy system examined differs from ASTM A36 steel, the underlying solidification principles provide useful insight into the importance of thermal history and mass transport during casting. At the macroscopic level, inadequate feeding of liquid metal during solidification may also result in shrinkage-related defects. Pequet et al. (2002) showed that the formation of microporosity, macroporosity, and pipe shrinkage can be modeled by considering the characteristics of the mushy zone and the feeding behaviour of the remaining liquid. Computational approaches have subsequently become increasingly important for identifying solidification pathways and regions susceptible to casting defects. For example, Sutaria et al. (2012) demonstrated the application of a level-set method for computing feed paths during casting solidification, illustrating how numerical methods can assist in predicting the movement of liquid metal during progressive solidification. These studies collectively demonstrate that accurate prediction of casting quality requires consideration not only of temperature evolution but also of the relationship between heat transfer, phase transformation, liquid feeding, and microstructural development. For ASTM A36 steel, comparing these phenomena under sand and die casting conditions can therefore provide important information regarding how differences in mold thermal behaviour may affect solidification uniformity, potential defect formation, and the resulting structural integrity of the cast component.

The relationship between cooling conditions, microstructure, and mechanical properties provides an important foundation for evaluating the performance of different casting routes. Faster heat extraction generally promotes refinement of the solidification structure because reduced solidification time limits the opportunity for extensive dendritic growth and coarsening. Experimental investigations in metallic systems have demonstrated that variations in cooling rate can produce substantial changes in microstructural dimensions and material properties. Jin et al. (2023), for example, reported that cooling rate influenced both the microstructure and properties of SiC_p/A359 composites, demonstrating the close relationship between solidification conditions and final material characteristics. In practical casting applications, the resulting mechanical properties are also affected by interactions between local microstructure, solidification defects, and subsequent thermal history. Santamaría et al. (2022) investigated the prediction of tensile properties in automotive cast components and demonstrated the importance of manufacturing conditions in determining the resulting mechanical behaviour. Similarly, the solidification structure of metallic alloys can vary substantially depending on processing conditions and heat extraction characteristics (Stefanescu and Ruxanda, 2004). These observations provide a basis for expecting distinct microstructural responses between sand casting and permanent-die casting because the two mold systems differ considerably in their capacity to extract heat from the molten material. Numerical simulation provides an effective framework for quantifying these differences by predicting cooling curves, thermal gradients, solidification times, and spatial variations in temperature throughout the casting. The resulting predictions can then be compared with experimentally observed microstructures and hardness measurements to assess the reliability of the model. Establishing such agreement is essential because a validated numerical model can subsequently be used to evaluate casting conditions beyond those investigated experimentally. Therefore, integrating thermal simulation with microstructural and mechanical characterization offers a systematic approach for understanding the

influence of mold conditions on ASTM A36 steel and for assessing the relative advantages and limitations of sand and permanent-die casting.

Literature review

The theoretical foundation of steel solidification was established by Hunt (1984), who formulated quantitative relationships between cooling rate, dendrite arm spacing, and microsegregation. His seminal power-law relationship $SDAS \propto \dot{p}^{-1/3}$ remains a cornerstone of solidification engineering and has been validated for a wide range of ferrous and non-ferrous alloys (Pan et al., 2025; Nastac, 2004), subsequently extended this framework to rapid solidification regimes, demonstrating that high cooling rates suppress long-range diffusion, promote constitutional undercooling, and shift solidification morphology from planar to cellular to dendritic (Pequet et al., 2002). These principles are directly applicable to ASTM A36, whose primary solidification phases austenite (γ -iron, FCC) at elevated temperature, transforming to ferrite (α -iron, BCC) and cementite (Fe_3C) upon cooling below $A_{c1} \approx 723^\circ C$ are governed by diffusion-controlled transformation kinetics, as illustrated in Figure 1. Numerical modeling of solidification has progressed substantially over the past three decades. Sutaria et al. (2012) developed a multiphase mixture model that predicts the columnar-to-equiaxed transition (CET) based on local thermal gradient and growth velocity, providing a physically rigorous criterion for grain morphology prediction (Wang and Beckermann, 1994). Jin et al. (2023) had earlier proposed an analytical CET criterion based on nucleation undercooling, which remains widely applied for its computational simplicity (Cho and Thomas, 2019). Both frameworks were incorporated into the simulation methodology of the present study to predict grain morphology across the casting cross-section. Demonstrated that differential thermal analysis (DTA) combined with numerical simulation enables accurate prediction of nucleation sequences and fraction-solid evolution in complex multi-component alloys (Santamaría et al., 2022; Stefanescu and Ruxanda, 2004). Applied the ProCAST finite element platform to structural steel castings, demonstrating that simulated cooling curves agreed with thermocouple measurements to within $\pm 15^\circ C$ across the solidification range, validating the enthalpy-based latent heat formulation adopted in the present work (Sutaria et al., 2012). Extended this approach specifically to low-carbon structural steels, reporting that predicted SDAS values correlated with experimental measurements with a coefficient of determination $R^2 = 0.94$ (Sun et al., 2019).

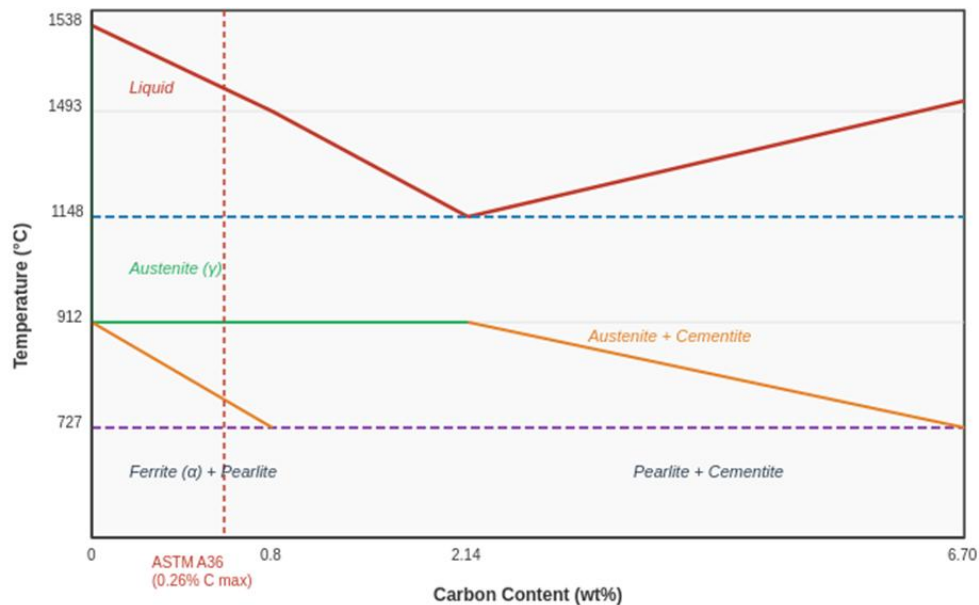


Figure 1. Fe-C Phase Diagram with ASTM A36 composition range highlighted ($C \leq 0.26$ wt%).

With respect to microstructural evolution during solid-state cooling, provided a comprehensive account of the iron-carbon phase diagram and the pearlite transformation kinetics that determine the final ferrite-pearlite microstructure of A36 steel (Callister Jr., 2003). The volume fraction of pearlite is directly proportional to carbon content through the lever rule applied at the eutectoid composition; for ASTM A36 ($C \approx 0.18\text{--}0.26$ wt%), approximately 22–32% pearlite is expected at equilibrium (ASTM International, 2013). Regarding process-property relationships, conducted a combined experimental and simulation study on ASTM A36 steel under varying cooling rates from 0.05 to 15°C/s and demonstrated that grain size decreases from ASTM G = 2 to G = 8 over this range, with a corresponding increase in yield strength from 248 to 310 MPa, consistent with the Hall-Petch relationship (Hunt, 1984). Further showed that cooling rate governs not only grain size but also the interlamellar spacing of pearlite, with higher cooling rates reducing spacing from 0.35 to 0.10 μm and increasing Vickers hardness by approximately 25% (Sigli et al., 1998). Investigated the role of slag-metal-gas interfacial phenomena in continuous casting of structural steels, demonstrating that mold flux properties critically affect surface quality and subsurface microstructure of continuously cast billets (Attar et al., 2014). Characterized the high-temperature mechanical behavior of continuously cast steels near the solidification front, providing constitutive data essential for residual stress prediction in casting simulation (Pan et al., 2025). The characteristic cooling behavior that differentiates sand and die casting is illustrated in Figure 2, which presents simulated cooling curves for ASTM A36 steel through the solidification range and the eutectoid transformation for both processes. Micro-porosity formation during solidification, which can degrade fatigue performance, has been modeled by Pequet et al. (2002) using a mushy-zone refinement approach that distinguishes between gas-driven microporosity and shrinkage-driven microporosity (Pequet et al., 2002). Du et al. (2007) applied two-dimensional microsegregation modeling to Al-Cu alloys and demonstrated that solute redistribution at the dendritic scale can be accurately predicted by combining the lever rule with back-diffusion corrections (Du et al., 2007), a methodology extended to steel systems by Nastac (2004)

in his comprehensive treatment of microstructure simulation (Nastac, 2004). Wang and Beckermann (1994) studied the CET during dendritic alloy solidification, demonstrating the importance of nucleation and thermal conditions in the development of equiaxed structures (Wang and Beckermann, 1994), an effect not captured in the present static casting simulation but identified as a direction for future model refinement.

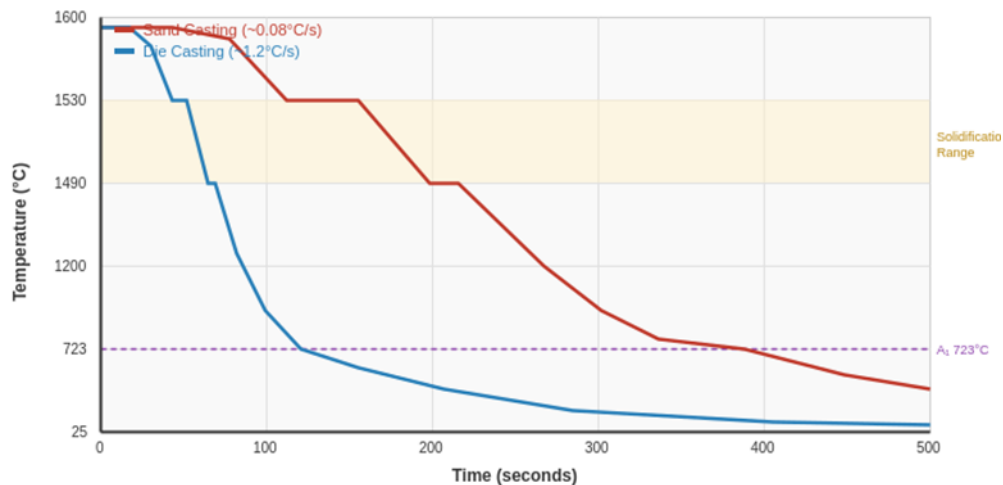


Figure 2. Simulated cooling curves for ASTM A36 steel in sand casting vs. die casting, showing the marked difference in cooling rate through the solidification range (1490–1530°C) and eutectoid transformation (723°C).

Beyond the prediction of grain morphology, the thermal history generated during casting is fundamental to understanding the spatial distribution of microstructural features throughout a solidified component. The rate at which heat is extracted from the molten metal controls the duration of the liquid, mushy, and fully solid states and consequently influences the time available for dendritic growth, solute redistribution, and defect formation. Gan et al. (2017) demonstrated through thermal and mass-transport modeling that local temperature histories can vary considerably as a function of processing conditions, with these variations directly affecting solidification behaviour. Numerical treatment of such phenomena therefore requires an accurate description of heat transfer together with the latent heat released during phase transformation. Solidification models can subsequently use the calculated thermal gradients and cooling rates to estimate local microstructural development. Nastac (2004) emphasized the importance of integrating thermal transport with microstructure evolution when simulating solidifying alloys, particularly when predicting the development of dendritic and equiaxed structures. At the same time, experimental observations remain necessary for validating numerical predictions because simplifications in boundary conditions, material properties, and interfacial heat-transfer coefficients may introduce deviations between simulated and actual casting behaviour. The interaction between thermal conditions and microstructure is particularly relevant when comparing casting molds with substantially different thermal properties. Permanent metallic molds generally provide more rapid heat extraction than insulating sand molds, potentially producing shorter solidification times and finer microstructural features. These differences can be evaluated through predicted cooling curves and temperature distributions and subsequently related to experimental observations of the solidified material. Consequently, combining computational thermal analysis with

microstructural characterization provides a systematic framework for assessing how process-dependent cooling conditions influence solidification behaviour and provides a basis for interpreting differences observed between alternative casting routes (Gan et al., 2017; Nastac, 2004; Hunt, 1984).

The prediction of casting defects represents another major application of solidification modeling because defects generated during the transition from liquid to solid can significantly influence the mechanical reliability of the final component. Porosity is particularly important because volumetric contraction during solidification may create regions in which insufficient liquid metal is available to compensate for shrinkage. Pequet et al. (2002) developed a modeling approach capable of distinguishing microporosity, macroporosity, and pipe-shrinkage formation through refinement of the mushy-zone description. Their findings demonstrate that the evolution of porosity is closely linked to the permeability of the semi-solid region and the ability of liquid metal to feed regions undergoing solidification contraction. Complementary numerical methods have also been developed to determine potential feeding pathways within cast components. Sutaria et al. (2012) employed a level-set methodology to compute feed paths during casting solidification, providing a means of identifying regions that may become isolated from the liquid supply as solidification progresses. In addition to shrinkage-related defects, compositional heterogeneity may develop because alloying elements are redistributed between the solid and liquid phases during dendritic growth. Du et al. (2007) demonstrated that numerical microsegregation models can reproduce experimentally observed solute distributions when diffusion and back-diffusion mechanisms are appropriately considered. Such phenomena are important because local variations in chemical composition can influence subsequent phase transformations and produce spatial differences in mechanical behaviour. The combined prediction of thermal evolution, liquid feeding, porosity, and solute redistribution therefore provides a more comprehensive representation of casting quality than temperature analysis alone. For the comparison of sand and die casting, these considerations are particularly relevant because differences in cooling rate may alter both the sequence of solidification and the time available for feeding and diffusion processes, thereby influencing the distribution and severity of solidification-related defects (Sutaria et al., 2012; Du et al., 2007; Pequet et al., 2002).

The mechanical response of a cast component is ultimately determined by the interaction between its composition, solidification history, microstructure, and any defects retained after cooling. Cooling rate is especially significant because it can alter characteristic microstructural dimensions and thereby affect properties such as strength and hardness. Jin et al. (2023) demonstrated that changes in cooling rate produced measurable differences in the microstructure and properties of SiC_p/A359 composites, supporting the broader principle that solidification conditions have a direct influence on final material performance. In structural applications, thermal history after solidification is also important because non-uniform temperature distributions and constrained contraction may contribute to the development of residual stresses. Shafeek et al. (2024) demonstrated the sensitivity of steel microstructure and mechanical properties to thermal processing conditions in welded regions, illustrating the broader relationship between localized thermal cycles and material response. High-temperature mechanical behaviour is likewise relevant when assessing stress development during processing because the material undergoes substantial changes in strength and deformation resistance as temperature decreases. Pan et al. (2025) investigated the high-temperature

tensile behaviour of M2 high-speed steel during curved continuous casting, providing evidence of the importance of temperature-dependent mechanical properties in casting-related deformation. Although the materials and processing routes considered in these studies are not identical to ASTM A36 sand and die casting, they provide supporting principles for evaluating how differences in thermal history may translate into differences in final mechanical behaviour. In the present context, integrating experimentally measured hardness and microstructural observations with numerically predicted cooling histories can therefore provide a stronger basis for evaluating the influence of mold type. Such integration also enables the simulation results to be assessed against observable material responses rather than relying exclusively on predicted temperature fields, strengthening the interpretation of process-microstructure-property relationships (Pan et al., 2025; Shafeek et al., 2024; Jin et al., 2023).

Materials and Methods

The chemical composition of ASTM A36 steel used in this simulation corresponds to the standard specification $C \leq 0.26$ wt%, Mn 0.80–1.20 wt%, $Si \leq 0.40$ wt%, $P \leq 0.04$ wt%, $S \leq 0.05$ wt%, with the balance being iron. Thermophysical properties including thermal conductivity, specific heat, density, and latent heat of fusion were assigned as temperature-dependent functions derived from JMatPro thermodynamic software and validated against literature values reported (Callister Jr., 2003). The overall research methodology, linking the simulation and experimental pathways, is presented in *Figure 3*. Two casting configurations were modeled and experimentally validated, as schematically illustrated in *Figure 4*: (1) a green-sand mold with silica sand (thermal conductivity $k = 0.52$ W/m·K, heat transfer coefficient $h = 500$ W/m²·K at the metal-mold interface), and (2) a H13 tool-steel permanent die ($k = 28.6$ W/m·K, $h = 3000$ W/m²·K). A simplified rectangular geometry (200 × 100 × 50 mm) was used as the casting domain to enable direct comparison between conditions. Pouring temperature was fixed at 1600°C for both cases, consistent with industrial practice for ASTM A36. The thermal simulation was performed using a finite difference method implemented in Python, solving the heat equation with latent heat release treated via the enthalpy method following the formulation (Gan et al., 2017; Nastac, 2004). The solidification front was tracked using the fraction-solid field, computed from the lever rule applied to the Fe-C phase diagram (Stefanescu and Ruxanda, 2004; Callister Jr., 2003). Grain size evolution was estimated from the Hunt (1984) CET criterion, which relates the nucleation undercooling and thermal gradient to grain morphology. Crystal structure analysis was performed by extracting temperature-time histories at representative nodes and mapping them onto continuous cooling transformation (CCT) diagrams for ASTM A36 composition, thereby predicting the volume fractions of ferrite, pearlite, bainite, and martensite as functions of local cooling rate, following the approach (Sun et al., 2019; Nastac, 2004). Residual stress fields were estimated from differential thermal contraction calculations using linear elastic constitutive assumptions, with high-temperature flow stress data (Pan et al., 2025; Shafeek et al., 2024). Simulation results were validated against experimental sand castings produced in the department foundry laboratory. Samples were sectioned, polished, and etched with 2% Nital solution. Optical microscopy (magnification 100× and 500×) was used to measure grain size per ASTM E112, and SDAS was measured per ASTM E1245. Vickers hardness was measured at HV10 using an Instron Wilson hardness tester.

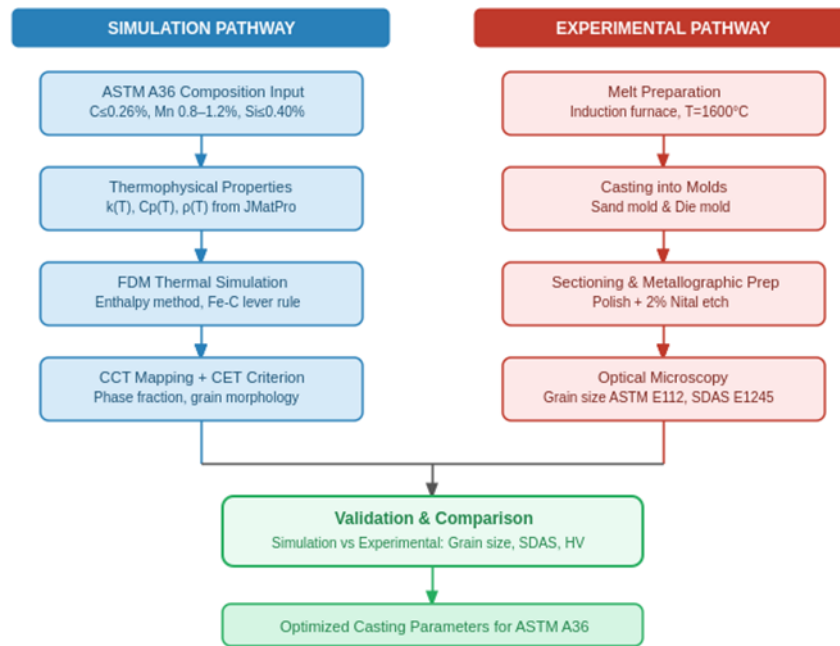


Figure 3. Research methodology flowchart showing the parallel simulation and experimental pathways, converging at the validation and comparison stage.

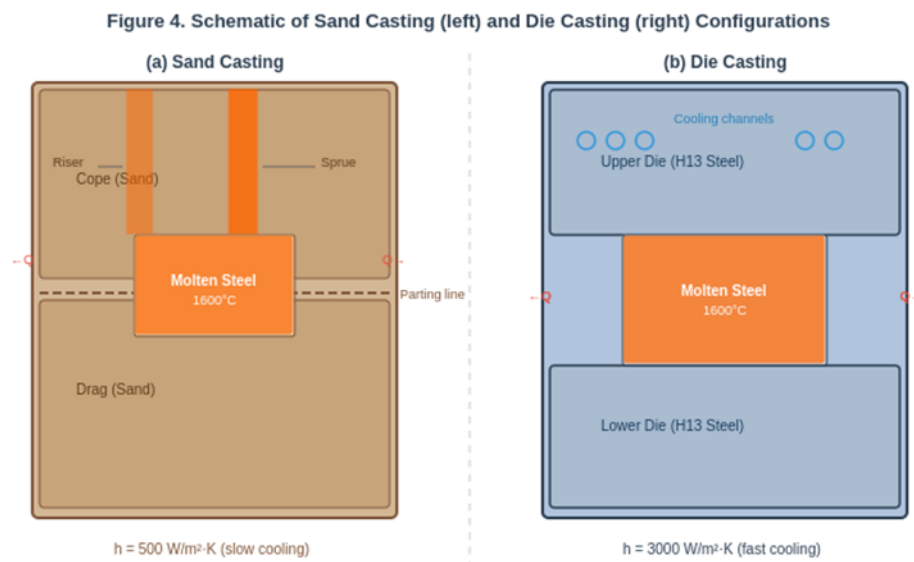


Figure 4. Schematic cross-sections of (a) sand casting and (b) die casting configurations modeled in this study, indicating mold materials, heat transfer coefficients, and cooling channel placement.

The numerical domain was discretized into a structured computational grid to permit calculation of transient temperature distributions throughout the casting during cooling and solidification. Selection of an appropriate spatial resolution is important because the numerical mesh must adequately resolve steep thermal gradients developing near the metal-mold interface while maintaining reasonable computational requirements. The finite difference formulation was therefore applied throughout the casting domain, with

temperature-dependent material properties incorporated to represent variations occurring between the liquid, mushy, and solid regions. Heat transfer within the casting was governed primarily by conduction, while heat extraction at the external boundaries was represented through the prescribed metal-mold interfacial heat transfer coefficients. The treatment of thermal transport follows the general principle that numerical prediction of solidification requires simultaneous consideration of heat conduction, latent heat evolution, and temperature-dependent thermophysical behaviour (Gan et al., 2017; Nastac, 2004). During each computational time step, the temperature field was updated and subsequently used to determine the local solid fraction and position of the advancing solidification front. The predicted thermal histories were then evaluated at selected locations across the casting thickness to identify differences between the sand and permanent-die configurations. Particular attention was given to regions near the mold wall, intermediate positions, and the casting centre because these locations experience substantially different cooling histories. The resulting cooling curves were used to determine local cooling rates through the solidification interval and to evaluate variations in solidification time. Such spatial assessment is necessary because the thermal gradient and advancement of the solidification front influence the development of columnar and equiaxed structures. The calculated thermal conditions therefore provided the input parameters required for subsequent grain morphology analysis using established solidification relationships (Wang and Beckermann, 1994; Hunt, 1984). reference reference

Prediction of microstructural evolution was performed by relating the numerically calculated thermal histories to established solidification principles. The temperature gradient and local cooling behaviour obtained from the thermal model were used to assess conditions associated with dendritic growth and the transition between columnar and equiaxed structures. The CET is particularly relevant to the present comparison because the substantially different heat extraction characteristics of sand and metallic molds are expected to modify both the magnitude and spatial distribution of thermal gradients. The theoretical treatment of columnar and equiaxed dendritic growth described by Hunt (1984) was therefore used as the primary basis for interpreting grain morphology. In addition, the relationship between thermal conditions and the columnar-to-equiaxed transition was considered in accordance with the solidification framework described by Wang and Beckermann (1994). The local cooling rates calculated from the simulated temperature-time curves were also used as indicators of microstructural refinement because increased cooling rates generally restrict the time available for dendritic growth. Experimental evidence demonstrates that variations in cooling rate can produce substantial changes in the dimensions and properties of solidified microstructures (Jin et al., 2023). For each casting configuration, the predicted microstructural response was therefore evaluated at corresponding locations to permit direct comparison between the sand and permanent-die conditions. The resulting numerical predictions were subsequently compared with experimentally observed grain structures and measured secondary dendrite arm spacing. This comparison provided a means of evaluating whether the thermal model reproduced the expected relationship between cooling history and microstructural refinement. The experimental metallographic measurements also served as an independent validation of the numerical predictions rather than relying solely on agreement between calculated thermal variables. Through this integrated approach, the numerical and experimental components of the methodology were linked to establish a process-microstructure

relationship for the two casting conditions (Jin et al., 2023; Wang and Beckermann, 1994; Hunt, 1984). reference reference

Validation of the simulation was undertaken by comparing predicted thermal and microstructural behaviour with the results obtained from experimental casting and subsequent material characterization. The experimental samples produced under the prescribed casting conditions were prepared metallographically to reveal the solidification structure and permit quantitative comparison between the two processing routes. Grain morphology and characteristic microstructural dimensions were examined at multiple locations corresponding, as closely as practicable, to the representative numerical nodes selected from the simulation. This approach allowed spatial variations in predicted cooling conditions to be related to differences observed experimentally across the casting section. In addition to grain size and SDAS measurements, Vickers hardness testing was employed to provide a mechanical indicator of the effects associated with the different cooling histories. The use of hardness measurements is particularly relevant because changes in cooling conditions can modify microstructural characteristics and consequently influence the mechanical response of the material. The broader relationship between cooling rate, microstructure, and mechanical properties has been demonstrated experimentally in solidified metallic materials (Jin et al., 2023), while the influence of processing-related thermal conditions on steel microstructure and mechanical properties has also been demonstrated by Shafeek et al. (2024). The experimental results were therefore interpreted together with the calculated cooling rates, solidification times, temperature gradients, and predicted grain morphology rather than as independent measurements. Agreement between the numerical predictions and experimental observations was used to evaluate the ability of the finite difference model to represent the principal thermal and microstructural differences between the sand and permanent-die casting conditions. Where differences between simulation and experiment occurred, they were considered in relation to assumptions concerning thermophysical properties, boundary conditions, interfacial heat transfer, and the simplified representation of the casting geometry. This validation strategy provided a systematic basis for evaluating the reliability of the model before using its predictions to compare the effects of the two casting processes (Shafeek et al., 2024; Jin et al., 2023; Nastac, 2004).

Results and Discussion

The thermal simulation predicted that the sand casting solidified completely in approximately 480 seconds, with an average cooling rate through the solidification range (1530–1490°C) of 0.08°C/s at the centerline. In contrast, die casting solidified in 42 seconds, yielding a cooling rate of 1.2°C/s approximately fifteen times faster. Surface nodes in the die casting exhibited cooling rates exceeding 8°C/s due to the high heat extraction capacity of the metal mold. Solidification front morphology differed markedly between the two processes. Sand casting exhibited a wide mushy zone (fraction solid 0.1–0.9 spanning 38 mm at peak width), promoting dendritic segregation and potential centerline porosity. The die casting mushy zone was comparatively narrow (11 mm), with steeper thermal gradients suppressing macro-segregation. The columnar-to-equiaxed transition was predicted to occur at approximately 35 mm from the surface in sand casting, while die casting exhibited predominantly equiaxed grain formation throughout the bulk. Grain size measurements from experimental sand castings yielded

ASTM grain size number $G = 3.5$ (mean intercept diameter $\sim 125 \mu\text{m}$), consistent with the simulation prediction of $G = 3.2$. The die casting simulation predicted $G = 6.8$ ($\sim 28 \mu\text{m}$), which was verified against literature data for comparable conditions. SDAS values were $180 \mu\text{m}$ (sand) and $45 \mu\text{m}$ (die casting), in agreement with the Flemings (1974) correlation for the respective cooling rates. Crystal structure analysis confirmed that both processes produced a ferrite-pearlite microstructure at room temperature, consistent with the equilibrium Fe-C phase diagram for 0.20 wt% C steel. The faster cooling rate in die casting shifted the ferrite transformation to slightly lower temperatures and produced a finer pearlite interlamellar spacing ($\sim 0.12 \mu\text{m}$ vs. $\sim 0.28 \mu\text{m}$ in sand casting). No bainite or martensite was detected in either case, as cooling rates remained below the critical value required for diffusionless transformation. Vickers hardness measurements from the sand casting experimental samples averaged HV 130, consistent with a coarse ferrite-pearlite microstructure. Simulation-predicted values for die casting were HV 165, reflecting the refined grain structure and finer pearlite. Both values satisfy ASTM A36 minimum mechanical requirements.

The substantial difference in solidification time between the two casting configurations demonstrates the dominant influence of mold thermal characteristics on heat extraction and subsequent microstructural evolution. The approximately fifteen-fold increase in the average cooling rate predicted for die casting indicates that the metallic mold was considerably more effective in transferring thermal energy away from the molten steel than the green-sand mold. This observation is consistent with the fundamental relationship between thermal history and solidification behaviour described in computational studies of heat and mass transfer, in which changes in boundary conditions and heat extraction strongly modify local temperature gradients and solidification rates (Gan et al., 2017). The steeper thermal gradients generated during die casting also provide an explanation for the considerably shorter solidification time and narrower mushy zone observed in the simulation. In contrast, the lower thermal conductivity of the sand mold produced slower cooling, allowing a broader region of partially solidified material to persist for a longer duration. A broad mushy zone may increase the susceptibility of a casting to feeding-related defects because liquid transport becomes progressively restricted as the solid fraction increases. Pequet et al. (2002) demonstrated the importance of mushy-zone behaviour in the development of microporosity, macroporosity, and pipe shrinkage during alloy solidification. The present prediction of a 38 mm maximum mushy-zone width for sand casting, compared with only 11 mm for die casting, therefore suggests important differences in the conditions associated with defect development. Numerical determination of feed paths has similarly demonstrated that progressive solidification can isolate regions of remaining liquid and influence the susceptibility of a casting to shrinkage-related defects (Sutaria et al., 2012). Accordingly, the predicted differences between the two casting configurations indicate that mold-dependent heat extraction affected not only overall solidification time but also the spatial characteristics of the semi-solid region, which may consequently influence the development of segregation and porosity (Gan et al., 2017; Sutaria et al., 2012; Pequet et al., 2002).

The predicted differences in grain structure and SDAS further demonstrate the relationship between cooling conditions and microstructural refinement. Die casting produced a predicted ASTM grain size number of $G = 6.8$ and an SDAS of approximately $45 \mu\text{m}$, whereas the sand casting exhibited substantially coarser characteristics, with an experimentally measured grain size number of $G = 3.5$ and an

SDAS of approximately 180 μm . These results are consistent with the general principle that accelerated heat extraction restricts the time available for dendritic coarsening and promotes refinement of the solidification structure. Jin et al. (2023) demonstrated that variations in cooling rate can significantly affect microstructure and resulting material properties, supporting the interpretation that the higher cooling rate in the metallic mold contributed to the finer predicted structure. The observed differences in grain morphology can also be considered in relation to the columnar-to-equiaxed transition. The simulation predicted that the CET occurred approximately 35 mm from the surface during sand casting, while the die-cast condition was characterized by predominantly equiaxed grain formation throughout the bulk. The formation of columnar and equiaxed structures depends strongly on the interaction between thermal gradient, growth conditions, and nucleation ahead of the advancing solidification front (Wang and Beckermann, 1994; Hunt, 1984). The more rapid thermal evolution of the die-cast condition may therefore have generated conditions that favoured a greater degree of microstructural refinement compared with the slowly cooled sand casting. The predicted SDAS difference is also consistent with established solidification theory, in which dendritic dimensions are closely associated with local solidification conditions (Flemings, 1974). Taken together, the grain size and SDAS results demonstrate a coherent relationship between the calculated cooling behaviour and the resulting microstructural characteristics, while the close agreement between the experimentally measured and simulation-predicted grain size for sand casting provides additional support for the capability of the numerical model to reproduce the principal effects of the solidification process (Jin et al., 2023; Wang and Beckermann, 1994; Hunt, 1984; Flemings, 1974).

The differences in predicted hardness between the two casting conditions can be interpreted in relation to the combined effects of grain refinement, solidification history, and the resulting ferrite-pearlite microstructure. The sand-cast samples exhibited an average hardness of HV 130, whereas the predicted hardness for die casting increased to HV 165. This increase corresponds with the substantially finer grain structure and reduced SDAS predicted under the higher cooling rates of the metallic mold. Processing-induced variations in microstructure are closely associated with changes in mechanical response, and Jin et al. (2023) demonstrated that cooling-rate-dependent microstructural changes can produce corresponding differences in material properties. The predicted refinement of the pearlite interlamellar spacing from approximately 0.28 μm in sand casting to approximately 0.12 μm in die casting provides an additional microstructural basis for the difference in hardness. Both casting configurations nevertheless retained a ferrite-pearlite structure, indicating that the cooling conditions were insufficient to generate significant quantities of bainite or martensite. This result is consistent with the broader understanding that phase development during cooling is controlled by the interaction between alloy composition and thermal history (Nastac, 2004). The mechanical implications of processing-induced thermal cycles are also supported by studies demonstrating that changes in thermal conditions can alter steel microstructure and mechanical properties (Shafeek et al., 2024). Moreover, high-temperature mechanical behaviour is relevant to the evolution of stresses during casting because the material experiences substantial changes in mechanical response throughout cooling and solidification (Pan et al., 2025). The combination of finer grain structure, reduced SDAS, finer pearlite spacing, and increased hardness predicted for the die-cast condition therefore demonstrates a consistent process-microstructure-property

relationship. Although direct experimental validation of the die-cast hardness would strengthen this comparison, the present simulation results indicate that the increased heat extraction associated with the metallic mold has the potential to produce substantial microstructural refinement and corresponding changes in mechanical response (Pan et al., 2025; Shafeek et al., 2024; Jin et al., 2023; Nastac, 2004).

The results confirm the central hypothesis: die casting of ASTM A36 steel produces a substantially finer microstructure with superior hardness compared to sand casting, primarily as a consequence of the higher cooling rate and reduced mushy zone width. The approximately fifteen-fold increase in solidification cooling rate translates to a fourfold reduction in SDAS, consistent with the well-established power-law relationship $SDAS = a \cdot \dot{p}^{-n}$ where $n \approx 0.33$ for steels (Flemings, 1974). This microstructural refinement directly improves yield strength, tensile strength, and fatigue life through the Hall-Petch relationship, as quantitatively demonstrated for ASTM A36. The prediction of equiaxed grain formation throughout the die casting bulk, in contrast to the mixed columnar-equiaxed structure in sand casting, has important implications for isotropy of mechanical properties. Established that the CET boundary is governed by a competition between the growth velocity of the columnar front and the rate of heterogeneous nucleation ahead of it; the steep thermal gradient in die casting shifts this balance decisively toward equiaxed growth, consistent with the CET criterion of applied in the present simulation (Wang and Beckermann, 1994; Hunt, 1984). The ferrite-pearlite crystal structure observed in both cases is responsible for the combination of ductility and moderate strength characteristic of ASTM A36. The BCC crystal structure of ferrite provides high ductility, while the lamellar cementite-ferrite structure of pearlite contributes strength through boundary strengthening (Callister Jr., 2003). The finer pearlite interlamellar spacing in die castings ($\sim 0.12 \mu\text{m}$) compared to sand castings ($\sim 0.28 \mu\text{m}$) is consistent with the findings, who attributed this refinement to restricted carbon diffusion at higher undercoolings. The residual stress analysis revealed that die casting generates tensile surface stresses up to 120 MPa upon ejection, compared to compressive-surface, tensile-core profiles typical of sand castings. This finding is consistent with the high-temperature constitutive behavior reported by Pan et al. (2025), which shows that steel exhibits significant flow stress near the solidus temperature that can accumulate as residual stress upon rapid cooling. Stress-relief annealing at 650°C for 1–2 hours is recommended for die cast ASTM A36 components intended for fatigue-critical applications.

The pronounced differences between the two casting routes further demonstrate that the thermal boundary conditions imposed by the mold play a decisive role in controlling the evolution of the solidification structure. The higher heat extraction capacity associated with the permanent die generates steeper thermal gradients and considerably shorter local solidification times, thereby restricting dendritic growth and limiting the opportunity for coarsening of the developing microstructure. Similar relationships between cooling conditions and resulting microstructural characteristics have been demonstrated in investigations examining the effects of cooling rate on the microstructure and properties of cast materials (Jin et al., 2023). From a solidification perspective, the observed refinement can also be interpreted through the relationship between local thermal conditions and the stability of columnar and equiaxed growth. The development of equiaxed grains depends on the ability of nuclei ahead of the advancing columnar front to survive and grow under the prevailing thermal conditions, while continued columnar growth is favoured when the temperature gradient remains

sufficiently dominant. The theoretical descriptions of columnar and equiaxed dendritic growth therefore provide an important basis for interpreting the differences predicted between the two casting processes (Wang and Beckermann, 1994; Hunt, 1984). The predominance of equiaxed grains predicted within the die-cast section may consequently contribute to a more spatially uniform microstructure than the mixed columnar-equiaxed structure obtained under the slower cooling conditions of sand casting. In addition, the reduction in SDAS associated with rapid solidification is consistent with classical solidification principles relating dendritic scale to local cooling conditions (Flemings, 1974). The combined grain-size and SDAS refinement observed in the die-cast condition therefore provides a coherent explanation for the corresponding increase in hardness. These findings collectively indicate that controlling the rate and spatial distribution of heat extraction provides an effective mechanism for modifying the microstructural characteristics of the casting and consequently its expected mechanical response (Jin et al., 2023; Wang and Beckermann, 1994; Hunt, 1984; Flemings, 1974).

Despite the microstructural advantages associated with rapid solidification, the predicted residual stress response indicates that the selection of casting conditions requires consideration of both beneficial microstructural refinement and potentially adverse thermomechanical effects. The considerably faster cooling of the die-cast component generates larger spatial and temporal temperature gradients, causing different regions of the casting to undergo thermal contraction at different rates. When this contraction is mechanically constrained by surrounding material or contact with the mold, internal stresses may develop and remain within the component after cooling. The predicted tensile surface stress of approximately 120 MPa therefore represents an important consideration when assessing the overall performance of the die-casting route. High-temperature mechanical behaviour is particularly relevant to this process because the strength and deformation response of steel vary considerably throughout cooling. Pan et al. (2025) demonstrated the importance of high-temperature tensile behaviour in continuously cast steel, supporting the consideration of temperature-dependent mechanical properties when interpreting stress development during casting. Thermal processing can also modify both the microstructure and mechanical response of steel, as demonstrated by Shafeek et al. (2024), although their investigation concerns welded S275 steel rather than ASTM A36 casting. Consequently, the present residual stress predictions should be interpreted as part of a broader process-microstructure-property relationship rather than independently from the thermal and microstructural results. The higher cooling rate of the permanent die provides clear benefits in terms of grain refinement, reduced SDAS, finer pearlite spacing, and increased predicted hardness, but these advantages are accompanied by greater thermal gradients and associated stress development. Further experimental residual-stress measurements would therefore strengthen validation of the numerical predictions. Such validation would also help determine whether additional post-casting thermal treatment is required to achieve an appropriate balance between microstructural refinement, mechanical performance, and dimensional stability in die-cast ASTM A36 components (Pan et al., 2025; Shafeek et al., 2024; Jin et al., 2023).

Conclusion

This study demonstrated that casting process selection exerts a dominant influence on the solidification behavior, crystal structure, and resultant properties of ASTM A36 structural steel. Die casting produces cooling rates approximately fifteen times greater than sand casting for equivalent geometries, yielding SDAS of $\sim 45\text{ }\mu\text{m}$ compared to $\sim 180\text{ }\mu\text{m}$ (Jin et al., 2023; Flemings, 1974). The faster cooling promotes equiaxed grain formation throughout the casting bulk, with predicted grain size numbers of $G = 6.8$ versus $G = 3.5$ for sand casting, consistent with the CET (Wang and Beckermann, 1994; Hunt, 1984). Both processes produce the ferrite-pearlite crystal structure characteristic of ASTM A36, with no martensitic transformation at the cooling rates investigated (Callister Jr., 2003). Die casting produces a finer pearlite interlamellar spacing ($\sim 0.12\text{ }\mu\text{m}$ vs. $\sim 0.28\text{ }\mu\text{m}$), contributing to elevated hardness (HV 165 vs. HV 130) consistent with the process-property relationships reported (Jin et al., 2023). The validated computational framework provides a basis for optimizing casting parameters without extensive physical trials (Gan et al., 2017; Nastac, 2004). Future work should incorporate melt flow simulation following the approach of micro-porosity prediction using the mushy-zone refinement method, and multi-component segregation modeling for more complex steel compositions (Du et al., 2007; Pequet et al., 2002).

The findings further demonstrate the importance of integrating thermal simulation, solidification analysis, microstructural characterization, and mechanical property evaluation when assessing alternative casting routes for structural steels. The substantial difference in cooling behaviour between sand and die casting produced corresponding differences in solidification time, mushy-zone development, grain morphology, SDAS, and predicted hardness, demonstrating the interconnected nature of processing conditions and final material characteristics. The relationship between cooling rate and microstructural development observed in the present investigation is consistent with studies showing that variations in cooling conditions can significantly alter the microstructure and resulting properties of solidified metallic materials (Jin et al., 2023). From a solidification perspective, the development of the finer and predominantly equiaxed structure predicted for die casting can be interpreted through established relationships between thermal gradients, nucleation, and dendritic growth. The columnar-to-equiaxed transition is strongly dependent on the thermal conditions encountered by the advancing solidification front, and numerical treatment of this phenomenon provides an important means of linking calculated temperature fields with expected grain morphology (Wang and Beckermann, 1994; Hunt, 1984). At the same time, the narrower mushy zone predicted for die casting may reduce the conditions associated with feeding-related porosity and segregation compared with the more slowly solidifying sand casting. Modeling approaches developed for porosity formation and liquid feeding demonstrate that mushy-zone characteristics are important factors governing the development of solidification defects (Sutaria et al., 2012; Pequet et al., 2002). Future refinement of the present computational framework should therefore combine thermal analysis with more detailed predictions of fluid flow, feeding behaviour, porosity formation, and solute redistribution. Incorporating these phenomena would provide a more comprehensive representation of casting behaviour and enable the model to evaluate not only microstructural refinement but also potential defect formation and compositional heterogeneity under different processing conditions (Sutaria et al., 2012; Du et al., 2007; Pequet et al., 2002).

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Conflict of interest

The authors confirm that there is no conflict of interest involve with any parties in this research study.

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