

FINAL REPORT

Developing Smart Agile Manufacturing System for Improved Sustainability: From Waste Steel to Materiel

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Executive Summary

This project aimed to establish an additive manufacturing (AM) enabled investment casting process using ferrous scrap from forward operating bases (FOBs). Ferrous waste materials were first characterized, and a waste material database was created to store critical information about scrap for sorting and recycling. A blending model was created to select scrap for remelting and making target steel alloys in the fields.

In the investment casting process, stereolithography (SLA) printed patterns were used to replace the traditional wax patterns, which significantly increased the versatility and flexibility of the manufacturing process. Two types of SLA printers were studied and compared. Both printers were proven feasible in the established procedure. Zirconium silicate-based primary slurry and Zircon sand were used in the ceramic shell-making process. A dipping-stucco process was established to fabricate ceramic shells, and a burnout process was designed and optimized for SLA pattern removal. MagmaSoft was utilized to assist with the casting tree design. Three demonstrative components were successfully made using a similar compact casting system in the foundry at Worcester Polytechnic Institute.

To satisfy the need of the FOBs, a three-container-based mobile foundry was designed which enabled rapid manufacturing of urgently needed parts in the fields. Casting facilities and inspection equipment were configured into three standard-size shipping containers. Thermal simulations were conducted in ANSYS to ensure a safe operating environment. A list of commercially available microgrid systems and instruments needed in the mobile foundry was compiled with supplier information.

Data-driven tools have been established and studied for post-treatment after casting. An artificial neural network (ANN) model was created and applied to study the relationship between a wide range of steel chemical compositions and multiple mechanical properties. The model used alloying element concentrations in steel and basic heat treatment information as inputs. The model outputs included mechanical properties, including yield strength (YS), ultimate tensile strength (UTS), Brinell hardness number (BHN), and elongation (EL).

Overall, this project successfully established an AM-enabled investment casting process that utilizes ferrous scrap from FOBs, designed a mobile foundry system to meet urgent manufacturing needs and created data-driven tools for post-treatment after casting. The findings of this project provide a solid foundation for future work in this area.

Publications and Conferences

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2. Yutao Wang, Jianyu Liang, Diran Apelian, Brajendra Mishra, Richard Sisson, Jian Yu, Brandon McWilliams. From Waste Steel to Material: Agile production enabled by additive manufacturing. SERDP and ESTPC Symposium. Dec. 2022
3. Wang W, Yang Z, Ge X, Sisson RD, Mishra B, Varde A, Liang J, Machine learning tools to predict mechanical properties of steel alloys based on compositions, heat treatments and microstructures, MS&T, Columbus, Ohio. Oct. 2021.
4. Wang W, Yang Z, Ge X, Sisson RD, Mishra B, Varde A, Liang J. Machine learning tools to predict mechanical properties of steel alloys based on compositions, heat treatments and microstructures, 2021 DoD Steels Research Summit, Nov. 2021 (virtual).
5. Wang W, Yang Z, Sisson RD, Mishra B, Apelian D, Liang J. From Waste Steel to Matériel: Additive Manufacturing Enabled Agile Manufacturing. SERDP Symposium. Dec. 2021 (virtual)
6. The undergraduate project as part of this project was presented at the ASEE NE 2021, IEEE MIT Undergraduate Research Conference 2021 and Sigma Xi Student Research Conference 2021. Title: “Outfitting a Compact Steel Casting System for Mobile Foundry for Department of Defense (DoD) Rapid Equipping Force (REF)”
7. Raymond Monroe and Jianyu Liang. Predicting Cast Steel Alloy Properties Based on Composition and Heat Treatment. Steel Founders' Society of America. The National Technical & Operating (T&O) Conference, Dec. 2020.
8. Karl Sundberg, Raymond Monroe, Yutao Wang, Jianyu Liang, Diran Apelian, Richard Sisson, Brajendra Mishra, Jian Yu, Brandon McWilliams, From Waste Steel to Material: Agile Production Enabled by Additive Manufacturing, Scrap Supplements and Alternative Ironmaking. March 2020. Orlando, USA

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16. Sundberg, K., Kelly, S., Apelian, D., Sisson, R., and Liang, J. (March 2019). "From Waste Steel to Weapons: Agile Production Enabled by Additive Manufacturing," Symposium on Recycling, Waste Treatment and Clean Technology

Media Coverage

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2. WPI Website: <https://www.wpi.edu/news/wpi-helps-us-military-optimize-mobile-manufacturing-labs>
3. Modern Casting, June 2021: <https://www.qgdigitalpublishing.com/publication/?m=55001&i=708682&p=34&ver=html5>

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Chapter 1: Introduction and Background

1.1 Need for This Project.

Based on research conducted by the US Army Research Laboratory (ARL) and the US Natick Soldier Research, Development and Engineering Center (NSRDEC), iron waste is the most prevalent category of metals in solid waste generated from forward operating bases (FOB). From April 2014 to May 2015, a recommended breakdown of metal waste that simulates the waste generated by force provider expeditionary camps is shown in Figure 1. This breakdown suggests that ferrous waste comprises 60% of the total, while aluminum waste comprises 36%, and the remaining 4% is composed of other metals [1, 2].

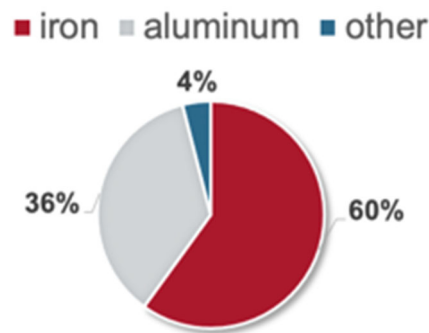


Figure 1 Recommended breakdown of metal waste recipe at FOBs.

Currently, the proper disposal of solid waste by deployed military forces is heavily reliant on three factors: the duration of a campsite, the security situation at the site, and the capacity and willingness of local infrastructure to handle waste [3]. The Strategic Environmental Research and Development Program (SERDP) aims to reduce the logistics tail by establishing in-theater manufacturing using recycled and reclaimed waste materials. Specifically, the program aims to demonstrate that waste streams generated at FOBs and battlefield scrap can be repurposed using field-capable manufacturing processes to produce replacement parts or repair equipment in the field. As a result, an agile manufacturing process that reuses ferrous waste is highly desirable.

In response to this need, a 3D printing-enabled investment casting manufacturing process was proposed to repurpose iron waste, which is the most abundant metal waste generated at FOBs.

1.2 The Need to Control Composition of Steel Remelts for High-Quality Parts

Recovering steel not only saves money but is also friendlier to the

environment, significantly reducing energy consumption and greenhouse gas emissions compared to manufacturing steel from raw materials. Iron scrap recycling has a rich history spanning over 150 years. In the United States, more than 83% of steel is recycled as of 2008[4]. Recycling steel is more cost-effective than mining virgin ore for the production of new steel. Recovering steel not only saves money but also significantly reduces energy consumption and greenhouse gas emissions compared to manufacturing steel from raw materials. Currently, all steel products contain between 25% and 100% recycled material[5].

In the steel-making industry, iron scrap is typically classified into three categories: home scrap from steel mills and rolling mills, process scrap from steel processing lines, and obsolete scrap from consumer goods[5].

Obsolete scrap is made up of iron or steel products that have reached the end of their useful life. This scrap is often mixed or coated with other materials such as copper, tin, glass, and polymers. The content of harmful elements in obsolete scrap is often high, and it serves as a primary source of elements like copper and tin that can have negative effects on the mechanical properties of recycled steel products. For example, tinplate from food and beverage cans and other packages typically contributes between 2 to 8 kg of pure tin for every 1 ton of steel plate, depending on the thickness of the plate and the tin layer. This means that the steel melt can contain between 0.2% to 0.8% tin after smelting the tinplate scrap, which is an unacceptably high level of tin for every steel grade[6, 7]. Scrap from higher copper-containing steels, such as concrete reinforcing steels or stainless steels, contains copper and other impurity elements. Table 1 illustrates the wide range of tramp element content in obsolete scrap.

Table 1 Typical composition of the obsolete scrap from varied sources, wt.%.

Source	Shredded scrap	Urban incinerator	Cryo shredded
Cu	0.230-0.430	0.304-0.980	0.169-0.275
Sn	0.027-0.042	0.032-0.140	0.022-0.033

The ferrous (iron) wastes typically observed at Forward Operating Bases (FOBs) include food cans, nails and cleats, ammunition boxes, banding material for pallets, and scrap metal from furniture, vehicles, or buildings. In other words, these are considered to be obsolete scrap. The

recommended ferrous (iron) waste simulation is composed of 75% steel cans and 25% non-coated steel nails[1]. An analysis of the combined chemical composition of steel cans and steel nails reveals a similarity to Chromium-Molybdenum alloy steel, which has good tensile strength but is not easily welded[8]. It is crucial to note that any effective reuse and recycling of ferrous (iron) wastes in theater must be based on a clear understanding of their chemical composition and the implementation of techniques to monitor, adjust, and control the composition of the waste metal.

1.3 Investment Casting of Steel Alloy

1.3.1 Introduction

According to the American Foundry Society, 90% of all manufactured goods contain metal casting components. The United States is the global leader in casting applications and ranks second in production[7]. A study commissioned by the U.S. International Trade Commission titled “Foundry Products: Competitive Conditions in the U.S. Market, Investigation No. 332-460” [9] notes that “Steel castings are produced in a wide range of chemical compositions and physical properties. Steel castings are, in general, of higher strength and ductility than cast iron. Castings of alloy steel have high strength, and those of stainless steel are highly resistant to corrosion. Steel castings are used extensively in the agricultural, construction, manufacturing, power generation, processing, and transportation industries. Typical products made from steel castings include bridge and building supports, compressors, mechanical components, pumps, tools, and valves. Because of their high strength and low cost, highly engineered lightweight steel castings are increasingly used in high-volume automotive chassis and drive-train applications.” In 2002, cast iron, steel, aluminum, and copper accounted for 92% of the value of metal casting produced in the United States, with cast iron accounting for around 38%, steel for 17%, aluminum for 32%, and copper for 5%[9].

Investment Casting (IC), also known as “lost wax casting,” is a well-established and widely used process for producing metal parts with excellent surface finish, accuracy, repeatability, versatility, and integrity. Almost any intricate shape, thin walls, and tiny delicate components can be cast using IC [10-12]. As shown in Figure 2, wax patterns are usually handcrafted or

created by injecting wax into a die or metal mold. These patterns are attached to a sprue, also known as a “casting tree”. The casting tree assembly is then dipped into a liquid slurry, and refractory sand is applied to the wet surface to form a multi-layer shell. The wax patterns are removed by a burnout process, and molten metal is poured to fill the mold. After pouring, the ceramic shell is removed by shaking or high-pressure water blasting, and the parts are cut off from the casting tree[13].

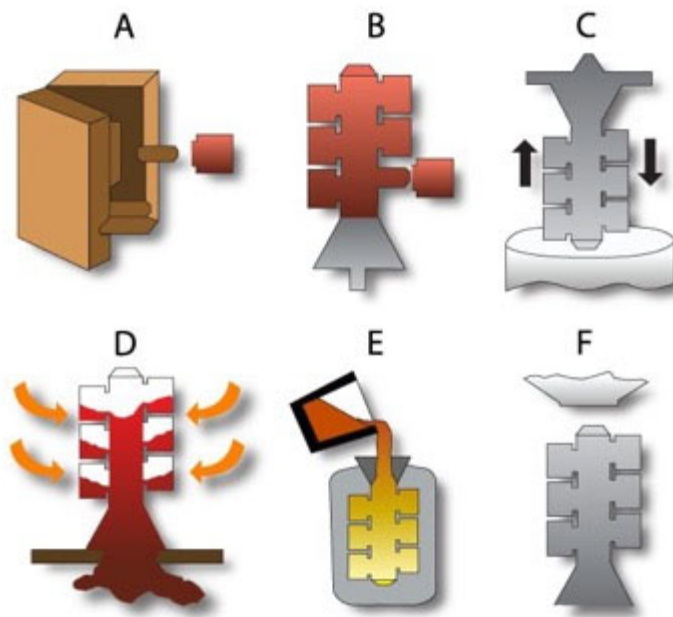


Figure 2 Production of components by investment casting. (a)Creating wax pattern, (b)Mounting the wax patterns and creating casting tree assembly, (c)Making the mold shell, (d)Wax Removal, (e)Melt and cast, (f)final operations [13].

Archaeological evidence indicates that as early as 5000 BC, humans used a similar process to manufacture jewelry and ornaments from beeswax patterns[14]. Modern investment casting technology evolved during World War II when the demand for precision components with complex geometries significantly increased. Traditional tooling processes were unable to meet the needs due to excessive time and material consumption, as well as manufacturability limitations. As a result, investment casting was applied to industrial manufacturing as an alternative process. The IC process not only provided a direct, efficient, and economical route to the manufacture of a finished part but also contributed to the conservation of materials and energy. The investment casting industry has continued to expand over the past few decades [15].

While die casting cannot cast ferrous metals such as carbon steel and stainless steel, investment casting allows for the casting of both ferrous and non-ferrous metals such as aluminum, brass, and bronze. The investment casting process enables the economic manufacture of intricate parts with high geometric accuracy and good surface finish, making it especially preferred for hard-to-machine metals like stainless steels and superalloys used in aerospace, defense, and medical applications. Investment casting of steels accounts for 35% of the total investment casting output value globally, with superalloys accounting for 50% and aluminum accounting for 10% [16].

However, investment casting suffers from long lead times and high tooling costs, making it less desirable for producing single castings or small and medium production units. These shortcomings can be overcome by using 3D printing applications to shorten the lead time for creating IC patterns.

1.3.2 Investment Casting Pattern Material

Various materials have been used to make patterns in the investment casting process, including plastic, wax, and frozen mercury. However, wax has been the most commonly used pattern material in industrial production due to its low melting point, high machinability, and the absence of harmful gas production during burnout.

The critical requirements of an investment casting pattern wax are as follows:

- (1) It should have the lowest possible thermal expansion to form a shape with high dimensional accuracy.
- (2) Its melting point should not be much higher than ambient temperature to prevent distortion of thick sections and surface cavitations.
- (3) It should be resistant to breakage, have sufficient strength, and be hard enough at room temperature to be handled without damage.
- (4) It should have a smooth and wettable surface to obtain a finished cast part with a smooth surface.
- (5) It should have a low viscosity when melted to fill the thinnest sections of the die.
- (6) It should be easily released from the die after formation.

- (7) It should have a very low ash content to prevent ash from being left inside the ceramic shell.
- (8) It should be environmentally safe and not lead to the formation of environmentally hazardous or carcinogenic materials upon combustion [17].

In recent years, with the popularization and development of 3D printing technology, multiple polymer additive manufacturing technologies have been applied to the pattern making of investment casting [18-20]. The use of additive manufacturing in investment casting will be further discussed in Section 1.4.

1.3.3 Ceramic Shell

An investment casting ceramic shell is composed of multi-layer refractory material and is commonly fabricated using dipping and stucco coating processes. The wax pattern is first dipped into a ceramic slurry to form a fine primary coating. Then, the wet pattern is sprinkled with coarse ceramic stucco. The coarse stucco minimizes drying stresses in the coatings by presenting several stress concentration centers that distribute and reduce the magnitude of the local drying stress. The stucco also provides a rough surface, increasing the mechanical bond between primary coating and secondary investment [21].

The key requirements of an investment casting ceramic shell are as follows:

- (1) It should have sufficient green (unfired) strength to withstand wax removal without failure.
- (2) It should have sufficient fired strength to withstand the weight of the cast metal.
- (3) It should be sufficiently weak to prevent hot tearing in susceptible alloys.
- (4) It should have high thermal shock resistance to prevent cracking during metal pouring.
- (5) It should have high chemical stability.
- (6) It should have low reactivity with the metals being cast to improve the surface finish.
- (7) It should have sufficient permeability and thermal conductivity to maintain adequate thermal transfer through the wall and allow the metal to cool.
- (8) It should have low thermal expansion to limit dimensional changes within the ceramic shell and ultimately the casting [21].

Various combinations of materials have been used to produce the ceramic shell. Among those material combinations, the silicon-water-based binder system is mostly used and has been proven to be the most environmentally friendly [22]. In this system, a colloidal binder provides enough fired strength to withstand the weight of the cast metal during casting. Liquid polymer additions, such as latex or polyvinyl alcohol, are added to provide enough green strength, which prevents cracking during burnout and handling. In recent years, fiber materials such as carbon fibers have also been used to reinforce the green strength of the ceramic shell, especially for the investment casting of large components [23].

1.4 Rapid Prototyping Enabled Rapid Investment Casting

1.4.1 Stereolithography Apparatus Additive Manufacturing

Metal additive manufacturing (metal AM), also known as 3D printing of metal parts, offers various advantages over traditional manufacturing methods. However, it also has some disadvantages. For example, material selection is limited for metal AM. Although the range of available metal materials for additive manufacturing is expanding, it is still relatively limited compared to the wide variety of metals available in traditional manufacturing. This can restrict the choice of materials for specific applications, especially when dealing with unique or specialized alloys. The mechanical properties of metal parts produced through additive manufacturing can be different from those of conventionally manufactured parts. The layer-by-layer deposition process can introduce anisotropic behavior, leading to variations in strength, fatigue resistance, and other mechanical properties in different directions within the part. Another disadvantage of metal AM is the metal powder hazard. Metal powders, especially fine particles, are highly reactive and can ignite or explode when exposed to an ignition source, such as a spark or open flame. Some metal powders, like aluminum and titanium, are particularly prone to combustion. Therefore, appropriate precautions must be taken to prevent fire and explosion hazards in the handling, storage, and processing of metal powders. In this study, a polymer AM assisted metal investment casting process is developed, which can effectively avoid the above-mentioned disadvantages brought about by direct metal AM.

Stereolithography Apparatus (SLA) was the first rapid prototyping technique invented in 1986 and remains a successful and relatively simple process. In SLA, layers of liquid resin are

successively cured by a laser until the final shape is obtained. SLA machines can run with unattended operation, and the parts have very good detail and surface finish, with accuracy often within 0.1 mm [24]. The apparatus for this highly automated technology demands modest energy, is relatively easy to operate and maintain, and comes in various dimensions depending on the size of the desired build plate.

The Army's Rapid Equipping Force (REF) has supplied a Stratasys Fortus 250 3D printer to the battlefield in the Expeditionary Laboratory (ExLab), but the equipment is limited to only ABS plastic. This is a Fused Deposition Modeling (FDM) driven 3D printer.

Compared to FDM and other prevailing rapid prototyping (RP) technologies, SLA is generally considered the technology that provides the greatest accuracy and best surface finish. In IC, the surface quality of patterns and castings are directly related. The relatively rough surfaces of untreated RP patterns are due to stair-stepping caused by layered building, building method (laser scanning, binder spraying, etc.), and feedstock material. SLA instruments provide just as much mobility as FDM and can be deployed similarly to FDM instruments (Figure 3).

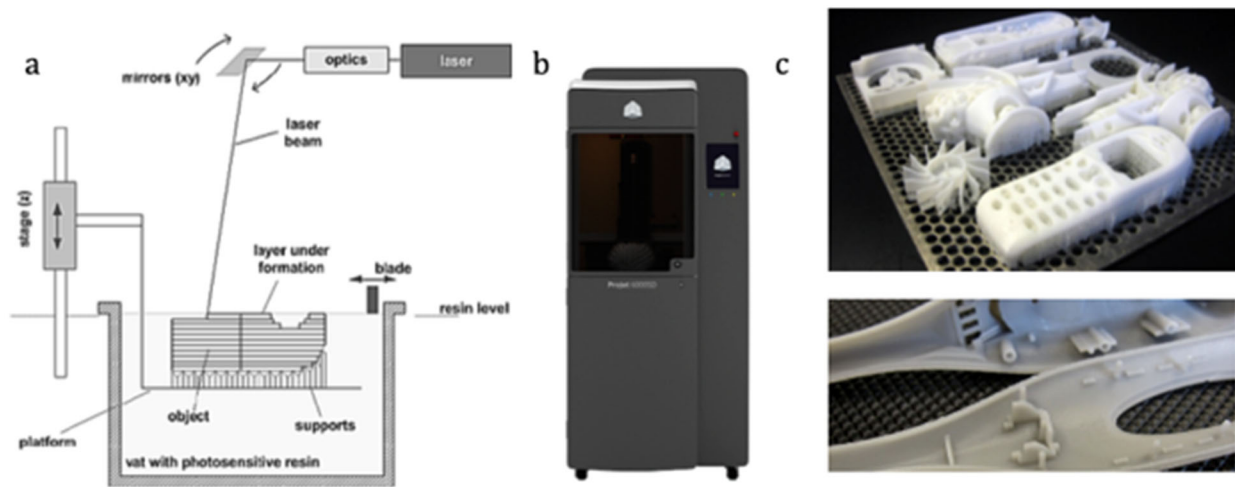


Figure 3(a) Schematic of SLA process (b) the ProJet® 6000 HD SLA machine in ARL Additive Manufacturing Lab that will be employed for this study (c) examples of structures and surfaces printed by ProJet 6000HD SLA.

In SLA printing, a CAD model can be divided into cross-sections between 0.002 and 0.006 in (about 0.05 and 0.15 mm). Studies have demonstrated that SLA is capable of producing patterns

with the required tolerance range (± 0.05 – ± 0.254 mm) and surface quality (16–20 μ m Ra) for IC applications [25].

The honeycomb-like makeup of SLA parts can make material use very efficient, with the structure being up to 85% hollow. The build rate for SLA parts is among the fastest available, at approximately 1 cu. in./hour (2.54 cu. cm/hour). Additionally, SLA is capable of building the largest parts available, with a maximum envelope of 25 x 30 x 22 in. (63.5 x 76.2 x 55.9 cm).

SLA resins are rated 2 out of 4 (moderate hazard to health) in National Fire Protection Association (NFPA) ratings. However, proper personal protection equipment such as safety glasses, gloves, and lab jackets can mitigate the risk of exposure. The consolidated parts (printed parts) are biocompatible and are used in medical models and devices. A study has shown that SLA has a lower total energy indicator compared to Selective Laser Sintering (SLS) and Fused Deposition Modeling (FDM) [26]. Thus, SLA is a desirable rapid casting mold creating method from the perspectives of quality, speed, cost, safety, and energy consumption.

1.4.2 Benefit of Integrating SLA with IC

The integration of SLA with IC provides the opportunity for rapid investment casting in theater, significantly shortening lead times from several months to just a few days and eliminating the need for high-cost tooling. This approach is particularly suitable for manufacturing custom parts and hard-to-machine parts that require fast turnaround time [27]. Previously, the U.S. Army in collaboration with key industrial partners has developed the Tactical Metal Fabrication program (TacFab) to enable metal sand casting capability through a mobile platform. Developing a mobile manufacturing platform to provide SLA enabled rapid investment casting capability will complement the TacFab by enabling reliable in theater rapid manufacturing of complex and detailed components that require tight dimensional tolerances.

Investment casting is a cost-effective method for manufacturing intricate parts with high geometric accuracy and good surface finish, especially for hard-to-machine metals such as alloy/stainless steels and superalloys used in aerospace, defense, and medical applications. While the traditional investment casting method uses wax to mold a net shape object, SLA plastic

printing enables the direct printing of casting patterns without the need for wax pattern tooling. The mold is printed in almost any 3D geometry, and molten metal is poured directly into the mold, burning out the plastic. SLA investment casting generally provides higher accuracy (0.001-0.002-inch tolerance) and surface finish than other casting processes, with minimum to no machining required on the finished product.

The main benefits of SLA-enabled investment casting include:

Low initial tooling costs and fast turnaround time: SLA-enabled investment casting is capable of repairing or replacing war materiel at or near the point of need at a turnaround time much faster than many other metal manufacturing methods. Depending on the size and complexity of the part, it may only demand a few days to produce a product.

Elimination of material waste: Investment castings are essentially cast to size, thus decreasing the amount of machining required.

Design flexibility and capability: Infinite choice of alloys and design flexibility for internal and external configurations is an advantage.

Design enhancements: There are no draft requirements in the investment casting process.

Consistency: The process gives a reliable and consistent product order to order.

Close Tolerances: Consistently produces close tolerances over other processes.

Surface Finish Improvement: SLA investment casting typically provides a surface finish of about 75 RMS.

While rapid investment casting has found various applications such as creating implants [28, 29], dental replacements [30, 31], jewelry [32], turbine blades [33], cylinder heads [34], etc., rapid investment casting using steel wastes on FOBs has not been done and faces many uncertainties, unknowns and challenges. For example, there is a large variation in the steel waste source and composition. The impact of composition variation on the castability and properties of the cast product needs to be assessed. Limitation imposed by the source material needs to be understood. In addition, agile manufacturing capability demands a complete manufacturing process that integrates the collection and sorting of the steel wastes, the computer-aided design (CAD) and modeling of patterns, the SLA enabled IC, quality control and product inspection, post process treatment, and recycling of materials.

To address these challenges, this study aims to develop a complete rapid investment casting process that utilizes typical steel wastes from FOBs to produce the needed parts for the warfighter. The process includes waste sorting and chemical composition adjustment, SLA-enabled investment casting, post-process treatment, characterization, and inspection of the manufactured parts.

1.5 Chemical Composition of Steel Alloy

Table 2 Common element additions and their functions in steel alloy [22].

Element	Symbol	wt. %	Function
Aluminum	Al	0.95–1.30	Alloying element in nitriding steels
Bismuth	Bi	–	Improves machinability
Boron	B	0.001–0.003	Improves hardenability
Chromium	Cr	0.5–2.0	Improves hardenability
		4–18	Corrosion resistance
Copper	Cu	0.1–0.4	Corrosion resistance
Lead	Pb	–	Improves machinability
Manganese	Mn	0.25–0.40	Prevents brittleness in combination with sulfur
		>1	Increases hardenability
Molybdenum	Mo	0.2–0.5	Inhibits grain growth
Nickel	Ni	2–5	Increases toughness
		12–20	Improves corrosion resistance
Silicon	Si	0.2–0.7	Increases strength and hardenability
		2	Increases yield strength (spring steel)
		Higher %	Increases magnetic properties
Sulfur	S	0.08–0.15	Improves machinability (free-machining steel properties)
Titanium	Ti	–	Reduces martensitic hardness in Cr steels
Tungsten	W	–	Increases hardness at high temperatures
Vanadium	V	0.15	Increases strength while maintaining ductility, promotes fine grain structure

Steel alloys typically contain a wide range of elements that are added to adjust their mechanical, thermal, and corrosion resistance properties. Each element addition has different contributions to specific properties. Table 2 below lists some of the most commonly used element additions and their functions in steel alloys [35]:

According to the different alloy compositions, steel can be classified into various types, including stainless steel, tool steel, and alloy steel, among others. Each type of steel has significant differences in performance. For a specific steel type, mechanical properties such as strength, toughness, hardness, and ductility can be adjusted within a certain range via heat treatment [36]. In fact, most steel alloys must undergo heat treatment before they can be used in practical applications, especially for critical applications. The heat treatment of steel and the mechanisms that occur during heat treatment will be further discussed in the next section.

It is worth noting that hardenability is a property that is solely determined by the chemical composition of an alloy. The hardenability of ferrous alloys refers to the ability of steel to form a martensitic microstructure when quenched from its austenitizing temperature. By knowing the hardenability of steel, it is possible to choose the appropriate heat treatment procedure.

1.6 Heat Treatment and Mechanical Properties Prediction in Steel Production

1.6.1 Heat Treatment of Steel Alloy

There are usually residual stresses in cast parts as-fabricated due to rapid cooling during the steel manufacturing process. In order to remove defects and achieve desired mechanical properties, heat treatment is required for steel products. Four commonly used heat treatment processes in steel production are annealing, normalizing, hardening, and tempering [37]. The phase transformation of steel alloys during heat treatment can be well explained in a Continuous Cooling Transformation (CCT) diagram, as shown in Figure 4 [38].

Annealing of steel involves heating it above its critical temperature and letting it cool slowly to room temperature, which helps remove residual stress and improves ductility while decreasing hardness. The cooling process is usually performed in the furnace or an insulated environment. During annealing, steel recrystallizes and converts pearlite and other low-temperature phases into

austenite, and then, by cooling it at a low rate, the austenite transforms into homogeneous ferrite and pearlite.

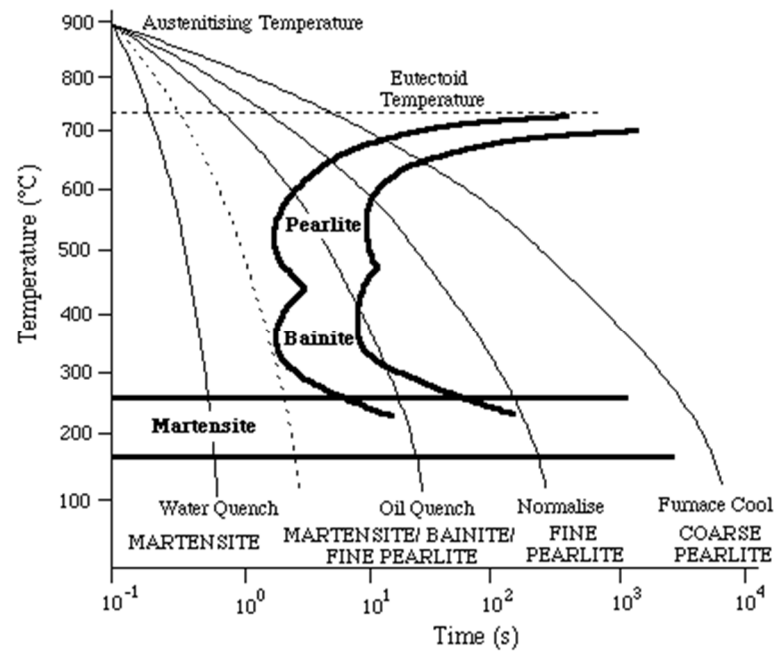


Figure 4 A continuous cooling transformation (CCT) phase diagram.

Normalizing is a similar process to annealing, but the cooling rate is higher, leading to the formation of pearlite and ferrite. The shift of the eutectoid composition to a lower value and the formation of cementite lead to more pearlite in normalizing than annealed steel with the same carbon content.

Quenching is the most commonly used process for hardening steel. It involves heating steel above its critical temperature, holding it for a certain period, and then rapidly cooling it using water, oil, or polymer. This process results in maximum hardness and strength, with a full quenching leading to martensite microstructure.

Tempering is a process commonly used after quenching to reduce brittleness and improve toughness. During tempering, carbides precipitate in martensite, forming tempered martensite. The hardness and other mechanical properties of steel alloys can be controlled by tempering at

$$H_p = \frac{(273.15 + T)}{1000} \cdot (C + \log(t)) \quad \text{Equation 1}$$

different temperatures. The relationship between temperature, time, and the effect of the tempering treatment has been studied by Holloman and Jaffe [39]. They established the Holloman-Jaffe equation (Equation 1) to describe the response of steel under different tempering conditions. In the steel casting industry, tempering is also performed on normalized parts to increase ductility and machinability.

*Where H_p is Hollomon–Jaffe parameter,
 T is tempering temperature in degrees Celsius,
 C is a parameter unique to the material used,
 t is tempering time in hour.*

1.7 Approaches for Mechanical Properties Prediction and Composition Design

1.7.1 Hardenability, Critical Diameter and Carbon Equivalent

The hardenability of an alloy is a crucial factor in designing its composition. One traditional method involves selecting the appropriate carbon content to achieve the target hardenability and then adding the necessary alloying elements to attain the desired mechanical properties through heat treatment. The hardenability of a steel alloy is typically measured by its critical diameter (DI), which can be calculated based on its chemical composition [40].

DI is defined as the diameter of a steel sample that would produce 50% martensite at the center when quenched in a coolant of infinite cooling rate [36]. The ideal critical diameter for a particular steel can be obtained from the experimental critical diameter, as shown in Figure 5. The Grossmann Quenching Intensity Factor (H) in Figure 5 is a constant determined by the coolant type. In an ideal situation, $H=\infty$, which means the coolant can instantaneously reduce the surface temperature of the sample to the coolant temperature without affecting the coolant temperature itself. Experiments have shown that the DI of a particular steel can also be measured as the distance along the Jominy bar at which the hardness equivalent to 50% martensite occurs[41].

Grossmann also proposed the following equation to calculate the ideal critical diameter:

$$D_{ig} = f(N_A) * f_C * f_{Si} * f_{Mn} * f_P * f_S * f_{Cu} * f_{Ni} * f_{Cr} * f_{Mo} \quad \text{Equation 2}$$

This equation of DI was optimized for different alloy types and more specific applications.

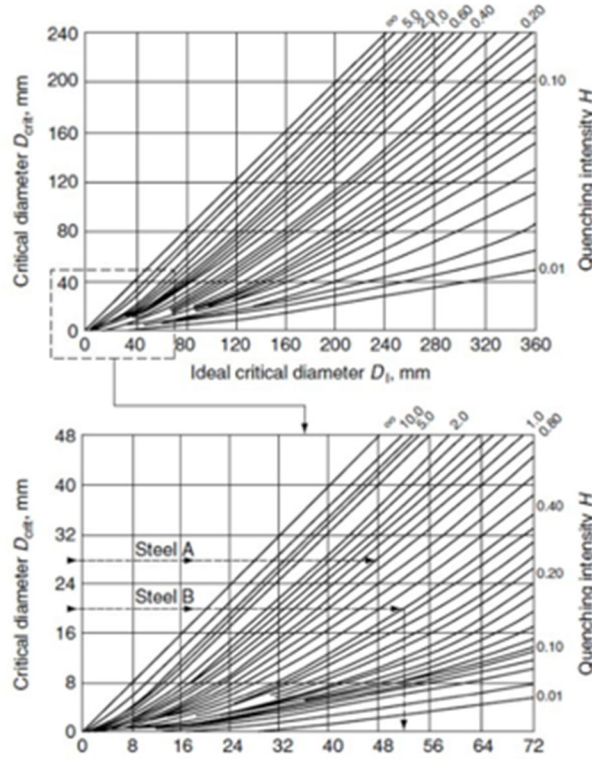


Figure 5 The chart for converting the values of the critical diameter D_{crit} into the ideal critical diameter D_I , or vice versa for any given quenching intensity H , according to Grossmann and coworkers.

Similar to DI, another method for determining the hardenability of steels is through the use of the Carbon Equivalent (CE) factor. The concept of CE was first introduced by Dearden in 1940[42], and it is used to represent the combined effects of various alloying elements contained in carbon steels as an equivalent amount of carbon. CE is proposed to explain the hardness of the Heat Affected Zone (HAZ), and it can be expressed as a linear combination of the concentration of each alloying element present in a steel sample in Eq. 3:

$$CE = C + Si/6 + P/0.8 + Mn/5. \quad \text{Equation 3}$$

Dearden and O'Neil predicted the ultimate tensile strength as a function of CE using Eq. 4 :

$$UTS(\text{tons/in.}^2) = 16 + 40CE \pm 2 \text{ tons/in.}^2 \quad \text{Equation 4}$$

This equation was used as a mathematic model to determine the coefficients in CE equation. By using this process, the equation of carbon equivalent is expanded to include other alloying elements as in Eq. 5:

$$CE = C + Si/6 + Mn/8 + Cr/7 + Ni/16 + Mo/4 + Co/16 + P/0.8 \quad \text{Equation 5}$$

Two important applications of the CE equations are the prediction of the maximum HAZ hardness and the ultimate tensile strength as in Eqs. 6 and 7.

$$H_v = 120CE - 200 \quad \text{Equation 6}$$

$$UTS = 16 + 40CE \quad \text{Equation 7}$$

Many studies have attempted to optimize the use of CE in predicting hardness, strength, and martensite transformation start time [43-45]. As a result, updated equations for CE have been proposed for different steel types and applications [46].

1.7.2 Linear Regression Analysis

Predicting the mechanical properties of steels can be a complex task. Various factors, including chemical composition, heat treatment process, and manufacturing process, can affect the properties of the final product. Over the past century, metallurgists have developed numerous linear regression equations to calculate the properties of steel. These equations are used to determine whether the alloy composition and production process will achieve the desired performance. Some of these equations are specific to a small group of steel alloys or products fabricated using a particular manufacturing process.

One of the earliest linear regression equations (Eq. 8) for predicting ultimate tensile strength (UTS) from chemical composition was proposed by McWilliam in 1918 [47]:

$$UTS_{o1} = 38,000 + 800 * C + 100 * Mn + 100 * P \quad \text{Equation 8}$$

Equation 8 is used for C-Mn-P steel. For C-Mn-P steel with silicon, an optimized equation (Eq. 9) is proposed as follows:

$$UTS_{o2} = 38000 + (800 + 4 * (C - 20)) + 120 * Si + (100 + 2 * (C - 20)) * Mn + 100 * P \quad \text{Equation 9}$$

In 1965, Soboslay & Dukelow proposed equations to predict the mechanical properties including UTS, yield strength (YS) and Elongation percentage (EL%) [48]:

$$UTS_{sd} = 476.1 + 581.9 * C + 83.4 * Mn + 535.2 * P + 129.5 * Si - 0.117 * T_f \quad \text{Equation 10}$$

$$YS_{sd} = 533.1 + 249.1 * C + 56.8 * Mn + 268.7 * P + 72.45 * Si - 0.186 * T_f \quad \text{Equation 11}$$

$$El(\% \text{ 8in.})_{sd} = -0.138 - 31.8 * C - 3.10 * Mn - 78.09 * P - 13.3 * Si + 0.020 * T_f \quad \text{Equation 12}$$

Eqs. 10, 11, and 12 are used for rolled steel products. Soboslay & Dukelow took into account the effect of the finish temperature (T_f) of rolling on final mechanical properties.

Custer also proposed equations to predict multiple mechanical properties form chemical composition for alloy steels in 1978:

$$UTS_{cu} = 142 + 774.9 * C + 170 * Mn + 370.9 * P - 226.4 * S + 216.5 * Si + 50.97 * Cu + 71.5 * Ni + 204 * Cr + 1776 * V + 48.2 * Mo \quad \text{Equation 13}$$

$$YS_{cu} = 120 + 319.2 * C + 127.7 * Mn + 131.7 * P + 34.5 * S + 196.9 * Si + 37.6 * Cu + 92.0 * Ni + 174.3 * Cr + 2426 * V + 5.24 * Mo \quad \text{Equation 14}$$

$$El_{cu} = 33.35 - 31.75 * C - 3.6 * Mn - 0.79 * P + 6.11 * S - 2.36 * Si - 2.90 * Cu - 0.10 * Ni - 7.42 * Cr + 14.22 * V + 4.68 * Mo \quad \text{Equation 15}$$

In 1979, Seyffart & Kasatkin [49] classified the microstructure of steels and proposed equations for mechanical properties prediction. By using the established equations for steel with different microstructures, prediction of UTS, YS, EL and RA (reduction of area) can be calculated more accurately.

For ferrite-pearlite steel:

$$YS_{fp} = 187 + 92 * C + 47 * Mn + 90 * V \quad \text{Equation 16}$$

$$UTS_{fp} = 297 + 1360 * C + 60 * Mn + 140 * V \quad \text{Equation 17}$$

$$El_{fp} = 36.5 - 127 * C + 135 * C^2 - 1.16 * Mn + 8.0 * V + 0.66 * \ln(t_{8/5}) \quad \text{Equation 18}$$

$$RA_{fp} = 65.4 - 88 * C - 82 * C^2 - 6.7 * Mn + 18 * V + 0.6 * \ln(t_{8/5}) \quad \text{Equation 19}$$

For martensite steel:

$$YS_m = 602 + 2150 * C + 500 * Mo \quad \text{Equation 20}$$

$$UTS_m = 798 + 3215 * C \quad \text{Equation 21}$$

$$El_m = 12.267 * C^2 - 1.5 * Mn + 0.76 * \ln(t_{8/5}) \quad \text{Equation 22}$$

$$RA_m = 48.5 - 158 * C + 116 * C^2 - 0.98 * \ln(t_{8/5}) \quad \text{Equation 23}$$

For bainite steel:

$$UTS_b = 590 + 960 * C + 39.7 * Mn + 200 * V \quad \text{Equation 24}$$

$$YS_b = 500 + 460 * C - 120 * C^2 + 150 * V + 360 * Mo \quad \text{Equation 25}$$

$$El_b = 21.3 - 35.6 * C - 4.0 * Mn - 5.0 * V + 1.84 * \ln(t_{8/5}) \quad \text{Equation 26}$$

$$RA_b = 53.3 - 132 * C + 103 * C^2 - 5.1 * Mn - 10 * V + 3.4 * \ln(t_{8/5}) \quad \text{Equation 27}$$

Where $t_{8/5}$ is Beckert time to cool from 800°C (1472°F) to 500°C (932°F) (s).

Hardness represents the ability to resist deformation. For most of metallic materials, there is a close relationship between hardness and tensile strength properties (UTS, YS). Therefore, effort has been made to calculate strength properties from hardness value, as hardness can be measured much more easily. In 2008, Pavlina&Vantyne proposed equations for calculating UTS and YS from Vickers hardness (HV) [50]. In their study, they proposed equations that are widely applicable for all types of steel alloys. In addition, they proposed equations subdivided according to the microstructure and strength level.

For all steel:

$$YS_{PVa} = -90.7 + 2.876 \cdot HV \quad \text{Equation 28}$$

$$UTS_{PVa} = -99.8 + 3.734 \cdot HV \quad \text{Equation 29}$$

For martensitic steel:

$$YS_{PVm} = 110.9 + 2.507 \cdot HV \quad \text{Equation 30}$$

$$UTS_{PVm} = -273.6 + 4.279 \cdot HV \quad \text{Equation 31}$$

For non-martensitic steel:

$$YS_{PVnm} = -84.8 + 2.646 \cdot HV \quad \text{Equation 32}$$

$$UTS_{PVnm} = 2.5 + 3.339 \cdot HV \quad \text{Equation 33}$$

For low strength steel:

$$YS_{PVls} = 15.3 + 2.860 \cdot HV \quad \text{Equation 34}$$

$$UTS_{PVls} = 10.9 + 3.150 \cdot HV \quad \text{Equation 35}$$

For medium strength steel:

$$YS_{PVms} = -70.5 + 2.736 \cdot HV \quad \text{Equation 36}$$

$$UTS_{PVms} = -99.8 + 3.800 \cdot HV \quad \text{Equation 37}$$

For high strength steel:

$$YS_{PVhs} = -94.8 + 2.466 \cdot HV \quad \text{Equation 38}$$

$$UTS_{PVhs} = -205.7 + 4.410 \cdot HV \quad \text{Equation 39}$$

1.7.3 Database Method

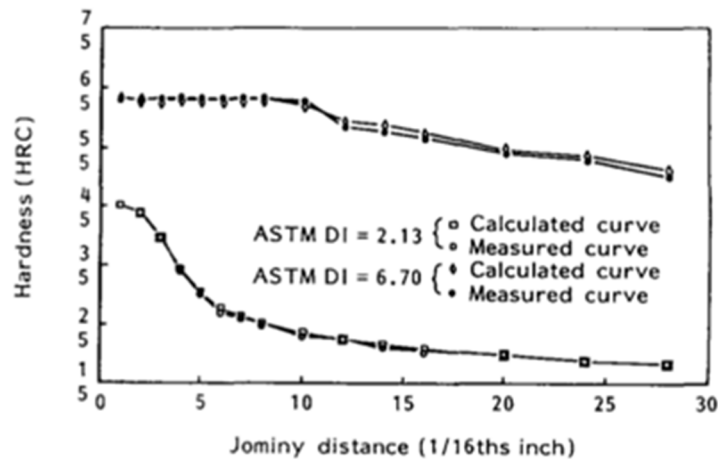


Figure 6 Jominy profile measured and calculated by database method [51].

Another method to predict the mechanical properties of steels from chemical composition is called the "Database method" [51]. Jominy end-quench test is a standard method of measuring steel's hardenability. Jominy hardness provides a measure of the ability of a steel to harden by transforming into martensite under set conditions [52]. To determine the Jominy profile of steel with certain chemical composition, the query data is compared with the records that are stored in a database. The Jominy hardness profile is calculated based on the record that has the closest chemical composition and DI value. As shown in Figure 6, the hardness at Jominy positions is predicted by using the database method with an average error of less than 0.1. Compared with the regression method, the database method could be used for a wider range of compositions. Moreover, the database method is able to make relevantly accurate predictions based on a smaller volume of experimental data, while the regression method required an extensive amount of data to determine the constant factors in the equation. However, both the regression method and the database method are found to have large prediction variations. These methods also lacked the ability to generalize from trained chemical composition data to a wide steel range. Therefore, other prediction methods are desired in industrial production.

1.7.4 Application of ANNs in Steel Chemical Composition Design

Artificial Neural Network (ANN) is a mathematical computing method used to establish a quantitative relationship for complex problems with a large number of variables. The inspiration

for ANN comes from biological neural networks, and its history can be traced back to the 1940s [53]. The first fundamental modeling of neural nets as a computational model of "nervous activity" was proposed by McCulloch and Pitts [54]. The basic unit in an artificial neural network is called an artificial neuron or node. Multiple neurons form multiple layers, and each layer is connected by complex algorithms [55]. An artificial neuron is described as a linear threshold computing unit with multiple inputs and a single output of either 0 if the neuron stays inactive or 1 if the sum of the inputs exceeds a specific threshold. A single neuron can receive input signals from neurons in the previous layers or external data. These values are delivered to neurons in the next layers as results. A typical ANNs structure, as shown in Figure 7, consists of the input layer, output layer, and one or multiple hidden layers [56].

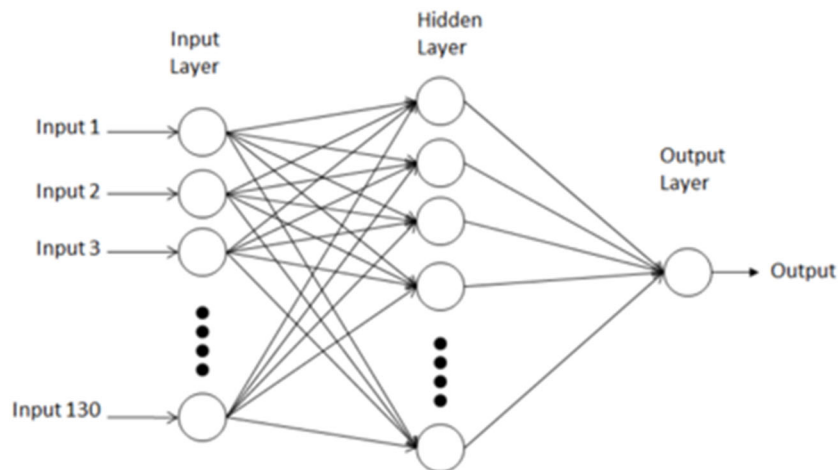


Figure 7 Artificial Neural Network structure.

ANNs, as well as other technologies derived from ANNs, such as deep learning, have been widely applied in various fields, including image classification, handwriting recognition, and natural language processing. In material research, data-driven tools like ANNs have been used to enable rapid prediction based on past data rather than experiments [57]. In some materials, the molecular or microstructure can be very complex, and the constituent elements can also be very diverse. The use of data-driven tools can reduce the human effort required to discover new materials with better functional abilities and more suitable combinations. However, applying ANNs to materials research requires researchers to have knowledge of the material structure and a good understanding of the manufacturing process. For instance, in 1974, Adamson and Bush proposed a method for relating the structure and properties of chemical compounds based on

serum binding percentage [58]. Unlike previous research, this conclusion was obtained more easily through data regression. In industrial production, the performance of materials can also vary greatly due to their microstructure or manufacturing process. There are numerous influencing factors, and the principles can be very complicated. With the help of modern industrial big data systems, a vast amount of data is collected during industrial production. Hence, ANNs could be used to predict product performance and improve industrial processes. This article will focus on the application of ANNs in steel products.

L. A. Dobrzanski et al. [59] reported on a steel chemical composition design tool that can select and calculate the chemical composition in steel based on the required hardenability curve to achieve desirable mechanical properties. As shown in Figure 8, a general method for selecting

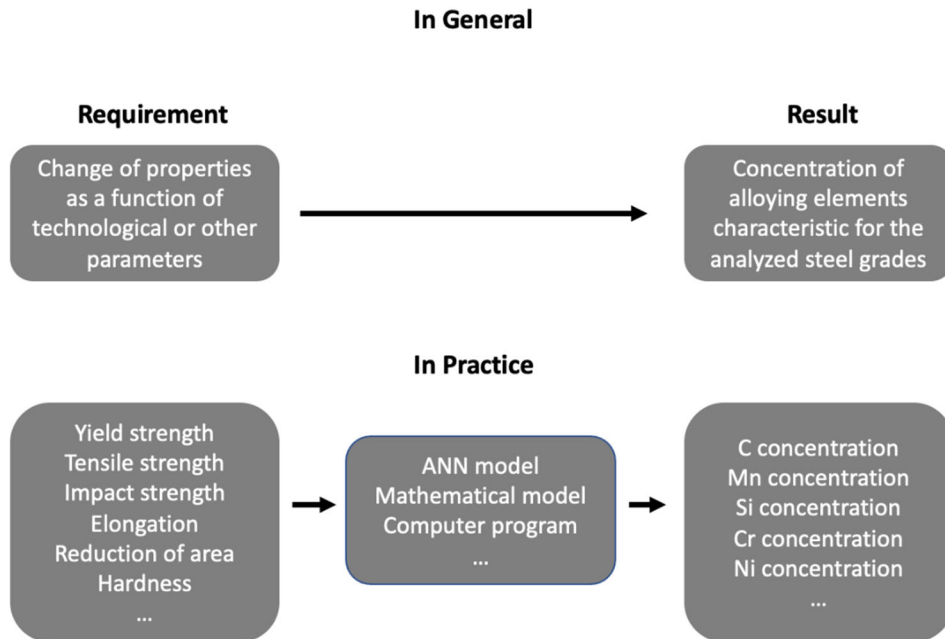


Figure 8 Flow diagram of modelling the steel chemical composition depending on the defined requirements.

steels for machine parts is to choose a grade. In this study, the ANN model was used as a tool that enabled the precise determination of the chemical composition in steels to match the required Jominy hardness profile.

Unidirectional multi-layer ANNs were employed with the error backpropagation algorithm as the learning method to calculate the chemical composition of steel. The input parameters for this model consisted of 15 hardness values measured by the Jominy test, while the output values were

6 basic alloy elements that affect the hardenability of steels (C, Mn, Si, Cr, Ni, Mo). The model was trained individually for each steel class using a data set obtained from experiments. To verify this model, the researchers conducted Jominy tests on steels with selected chemical compositions. As shown in Figure 9, the experimental curve matched the required curve, with a difference between experimental Jominy hardness and the required Jominy hardness of less than 2.5 HRC. This research accurately calculated the chemical composition of steel required for achieving the desired hardenability.

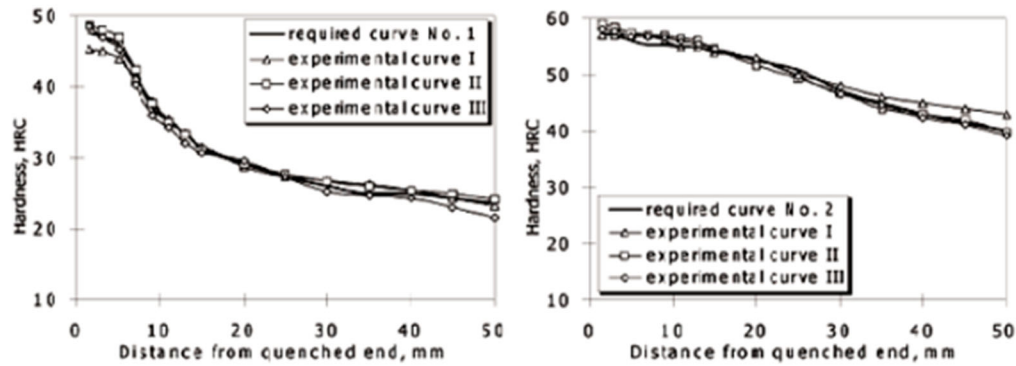


Figure 9 Comparison of the required hardenability curves and the experimental ones of the steels' heats of the designed chemical composition [59].

Chapter 2: Approach and Objectives

2.1 Ferrous Waste Material Recycling and Agile Manufacturing

The first objective of this project is to develop an agile manufacturing process that allows for the reuse of ferrous (iron) waste, which is the most abundant metal waste, at FOBs to produce necessary parts for the warfighter.

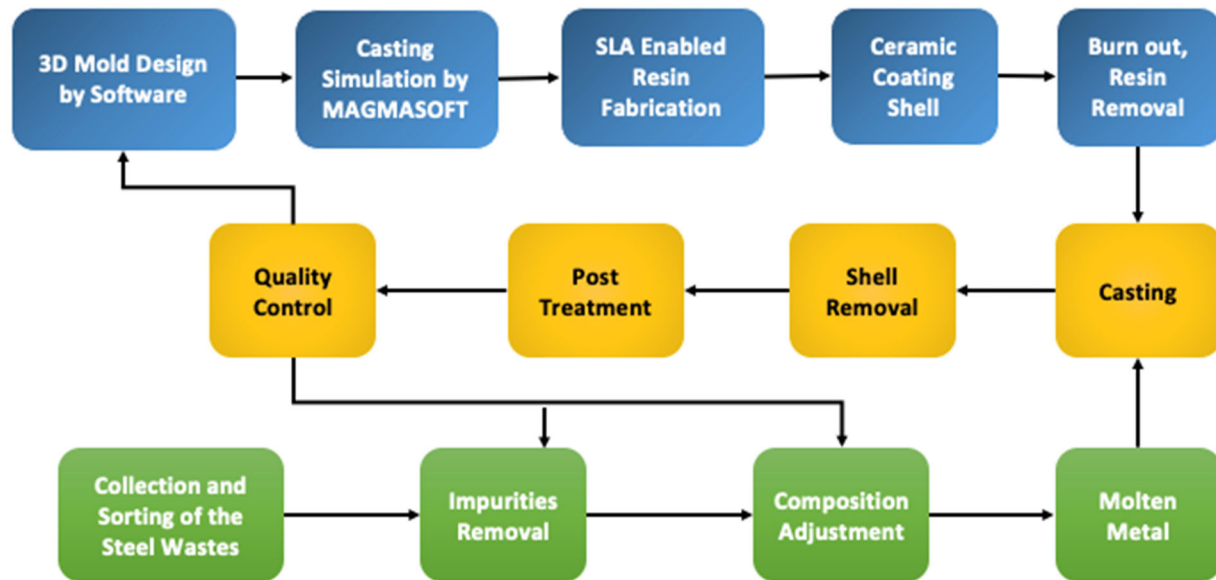


Figure 10 The schematic of SLA enabled investment casting, from metal scrap to parts.

As shown in Figure 10, there are three major tasks involved in achieving Objective 1:

Task 1: Create an effective sorting, chemical composition monitoring, and composition adjustment process for ferrous (iron) waste at FOBs to ensure quality control of the material for subsequent rapid investment casting.

Task 2: Establish additive manufacturing (AM) technology of stereolithography apparatus (SLA) enabled investment casting (IC) using ferrous waste from FOBs as the cast material.

Task 3: Develop post-processing treatments for upgrading the quality of cast parts.

2.2 Data-driven Tool for Mechanical Properties Prediction and Heat-treatment Design

Additionally, to assist in formulating heat charges that meet desired mechanical properties, an ANN machine learning model has been developed using the extensive database provided by the Steel Founders' Society of America (SFSA). The SFSA database contains over 20,000 entries with common alloy properties, including composition, heat treatment, and mechanical properties. As shown in Figure 11, this database is used to train the ANN model, which can also be used in reverse to formulate steel chemical composition and design heat treatment schedules to achieve desired mechanical properties including tensile strength, yield strength, hardness and elongation.

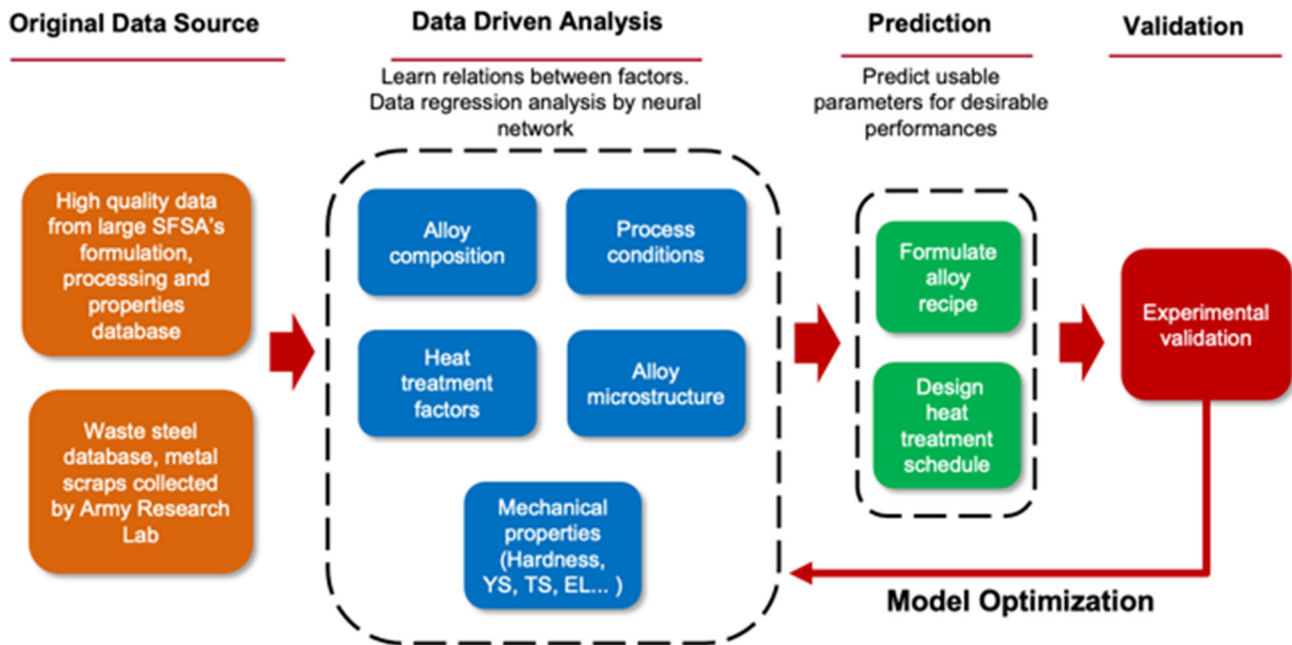


Figure 11 Schematic overview of data driven tools for steel alloy production.

There are three major tasks involved in this project:

Task 1: Data classification, cleaning, and pre-processing.

Task 2: Establish ANN model, use chemical composition and heat treatment as inputs to determine the mechanical properties of steel alloys based on the developed model.

2.3 Shipping-container-housed Casting Foundry Design

The WPSON-18-C4 Statement of Need aims to develop "an agile, novel expeditionary battlefield manufacturing process using recycled and reclaimed materials." To achieve this goal, a mobile foundry system has been designed, which can complement the previously deployed

Expeditionary Laboratory (ExLab). This compact steel casting system will be housed in standard-sized shipping containers and effectively repurpose reclaimed materials from the battlefield into value-added products while maintaining an environmentally responsible waste cycle.

There are two major tasks involved in this project:

Task 1: Design a compact steel casting system that can be housed in standard-sized shipping containers and repurpose reclaimed materials from the battlefield into value-added products.

Task 2: Using thermal simulation to select effective ventilation.

Chapter 3: Additive Manufacturing Enabled Rapid Casting from Waste Steels

3.1 Waste Metal Scrap Database and Blending Model

A total of 2567.08 lbs. of waste metal from the Army Research Laboratory was received and characterized. Pictures of the waste parts were taken, and their sizes were recorded. After removing rust, paint, and surface contamination from the scrap, their chemical composition was determined using Optical Emission Spectroscopy (OES). The obtained information was stored in a database, as shown in Figure 12. This data assists in the classification and management of waste material and the selection of waste inventory based on needs during remelting.

Numerical Order	Picture of Scrap	Categorization	Dimensions (Approximate, Overall Size)	Contamination	Weight (lbs.)
3-1		Star End Piece	30.0" x 6.25" x 12.0"	Coating, Little Rust	43.55
3-2		Red Cane	1.0" x 28.0"	Coating	0.99
3-3		Brake Rotor 1	13.0" x 2.25"	Partial Rust	24.29
3-4		Brake Rotor 2	12.0" x 3.0"	Partial Rust	17.81

Figure 12 Waste metal database.

A blending model was developed using MATLAB to guide the selection and mixing of waste materials to create the targeted steel alloy. Additionally, a document containing instructions on how to effectively use the blending model was created to teach new users. The blending model has been shared with the research team members at WPI and ARL and will be readily available to any person instructed by our funding agency to access the tool.

The blending model can generate a spreadsheet similar to Figure 13, which specifies the targeted composition and mechanical properties, the selected waste materials and their weights, their corresponding compositions, and the expected composition range for the newly formulated alloy from these selected waste materials. The blending model also includes tools such as the ideal critical diameter (DI) as a measure of hardenability and carbon equivalent (CE) to indicate the alloy's response to avoid cracking during welding for improved control of mechanical properties. The formulated alloy from waste metals must meet both the composition range and the targeting DI and CE to ensure high confidence in obtaining the desirable hardness.

Steel 1 Carbon Steel 45 ksi YS																		
			CE	DI	% C	% Si	% Mn	% P	% S	% Cr	% Mo	% Ni	%Al	%Co	%Cu	%V	%Sn	
	Recovery				0.9	0.95	0.95	1.0	1.0	0.97	0.99	0.99	1.0	1.0	1.0	1.0	1.0	
	Target Composition	Aim	0.40	0.80														
		Min		0.60	0.15	0.40	0.50			0	0	0						
		Max	0.50	0.90	0.30	0.60	1.20	0.035	0.035	0.50	0.20	0.50						
Heat Composition			0.43	0.89	0.147	0.506	0.768	0.021	0.013	0.190	0.054	0.343	0.015	0.005	0.180	0.009	0.011	
	Heat Size (lb.)	70																
Waste Parts	Name	Remain	Added (lb.)	Fraction	Dimensions	% C	% Si	% Mn	% P	% S	% Cr	% Mo	% Ni	%Al	%Co	%Cu	%V	%Sn
#3-35	Plate with Square Hole Big	45.400	54.600	0.780	27.75" x 15.125" x 1.0"	0.136	0.050	0.809	0.017	0.008	0.077	0.014	0.084	0.019	0.003	0.188		0.009
#4-15	Thread Barrel 5	32.780	10.000	0.143	4.5" x 24"	0.355	0.320	0.739	0.055	0.022	0.879	0.284	1.870		0.017	0.090	0.052	0.020
#3-32	Big L Beam	27.810	5.000	0.071	3.0" x 3.0" x 64.0"	0.087	0.270	0.972	0.002	0.048	0.123	0.037	0.189		0.009	0.284	0.022	0.015

Figure 13 Blending Model.

The most widely used version of DI is reported in ASTM A255 [67]. Since multiple formulations for DI and CE and hardness are referred to and included in Appendix 2, a subscript was added to identify which DI or Ce was being referenced. This ASTM A255 DI formula is referred to as DI_{A255}. DI_{A255} is dominated by carbon and is a series of multiplicative factors for other alloying elements [67, 68]:

$$DI_{A255} = 0.54 * C * (1 + 3.333 * Mn) * (1 + 0.7 * Si) * (1 + 0.33 * Ni + 0.066 * Ni^{0.55} * Ni^3 + 0.18 * Ni^4) * (1 + 2.16 * Cr) * (1 + 3 * Mo) * (1 + 0.365 * Cu) * (1 + 1.73 * V) \quad \text{Equation 40}$$

The common form of CE used in ASTM casting standards such as ASTM A216 was developed by the International Institute of Welding (IIW). The formula used for CE_{IIW} is [69]:

$$CE_{IIW} = C + Mn/6 + (Cr + Mo + V)/5 + (Ni + Cu)/15.$$

Equation 41

Using the characterized waste metals and the blending model, multiple melting and casting experiments have been completed to validate the use of the blending model and to understand composition control during the remelting and casting processes.

3.2 8640, 4140, and 1025 Steels from Waste Materials

3.2.1 Creating New Alloys with the Help of the Blending Model

Based on the blending model, melting experiments were conducted to create 8640, 4140, and 1025 alloys using the received waste materials. Table 3 summarizes the target compositions and the compositions obtained from these melts.

Table 3 Target composition and obtained composition 8640, 4140 alloy steel and 1025 carbon steel melts.

		C	Mn	Si	Cr	Mo	Ni	S	P	DI	CE
Target: 8640	Min.	0.38	0.75	0.3	0.4	0.15	0.4	0	0	4.44	0.64
	Max.	0.43	1	0.6	0.6	0.25	0.7	0.04	0.035	8.38	0.81
As-cast Composition		0.43	0.7	0.57	0.75	0.19	0.66	0.016	0.019	8.06	0.78
Target: 4140	Min.	0.38	0.75	0.15	0.8	0.15	/	0	0	5.09	0.69
	Max.	0.43	1	0.3	1.1	0.25	/	0.04	0.035	8.15	0.87
As-cast Composition		0.414	0.805	0.153	1.12	0.215	0.527	0.039	0.023	7.05	0.81
Target: 1025	Min.	0.22	0.3	/	/	/	/	0	0	0.23	0.27
	Max.	0.28	0.6	/	/	/	/	0.05	0.04	0.45	0.38
As-cast Composition		0.25	0.65	0.32	0.34	0.11	0.43	0.016	0.029	0.43	0.36

The three melts resulted in compositions that closely matched the targeted compositions, validating the effectiveness of the developed blending model as a guiding tool for rationally formulating waste materials for remelting to obtain new alloys with desirable mechanical properties.

3.2.2 Correlation between UTS and Hardness

Steel tensile sample preparation is a time-consuming and challenging process. To address this, the team collaborated with the Steel Founders' Society of America (SFSA) to study the correlation of yield strength (YS), ultimate tensile strength (UTS), hardness, and chemical composition of steel materials. Over 30,000 data entries collected by SFSA from steel foundries all over the United States over many years were used to show that hardness can be used to

estimate YS and UTS of steel. The standard errors of the established correlation were 10.7 ksi for YS and 6.05 ksi for UTS. This result agrees with the previously reported linear correlation between steel tensile properties and hardness.

Linear regression analysis of the SFSA data obtained Eq. 42 and 43 that correlate UTS with HRCjE and HRCjE+TT:

$$\text{UTS} = 1.84 * \text{HRCjE} + 28.35 \quad \text{Equation 42}$$

$$\text{UTS} = 1.84 * \text{HRCjE} + 28.35 + 0.10 * (1170 - \text{TT}) \quad \text{Equation 43}$$

The comparison of the UTS estimations with the measurement data using hardness alone (Eq. 42) and using hardness adjustment with tempering temperature (Eq. 43) is shown in Figure 14. This result strongly agrees with the previous studies discussed in Section 1.7.2. Hence, the hardness measurement can be used as the primary mechanical property indicator of the products in this rapid manufacturing process since it is an easy measurement.

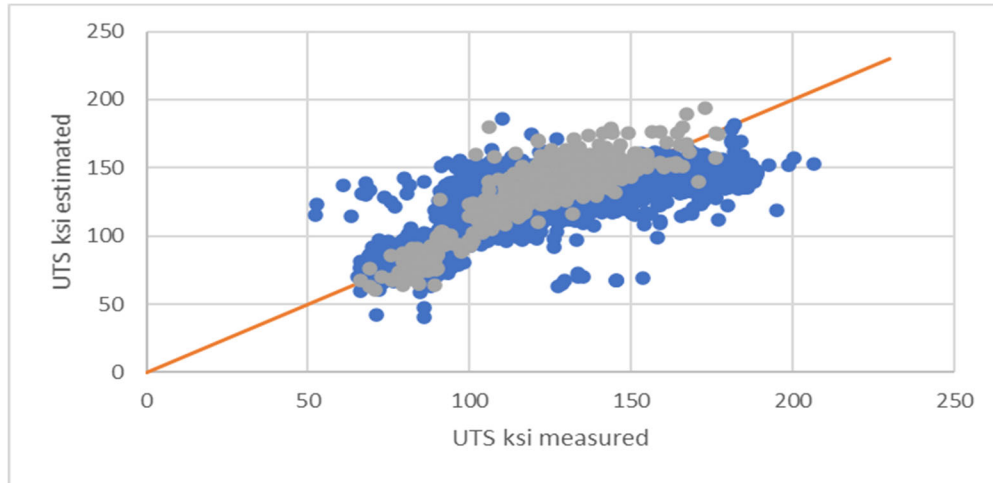


Figure 14 Correlation of estimated UTS from HRCjE for the SFSA data and HRCjE+TT with measured UTS.

Thus, The hardness of as-cast samples was characterized by microhardness indenter and used as the primary mechanical property indicator. The hardness values of as-cast products were measured in 10 different locations for each sample to reduce the influence of nonuniform microstructures. Vickers hardness test results of all three steel alloys are summarized in Table 4. Table 4 also shows the ranges of sparsely reported hardness values of these alloys from the

literature. The measured hardness of all three alloys appears to be in good agreement with the range of reported values. However, the variations in the reported values are very large. In addition, heat treatments significantly alter the mechanical properties of the steel alloys. In the later section of this report, the heat treatments applied to the three demonstration components and the hardness of the heat-treated final products are discussed.

The successful melts using the blending model that incorporates useful tools such as DI and CE in addition to individual alloy element composition confirm the feasibility of composition monitoring and adjustment of waste steel melts using the waste material database.

3.3 Additive Manufacturing Enabled Investment Casting Process

Table 4 Hardness measured and expected of as-cast 1025, 8640 and 4140 steel.

	As-cast 1025	As-cast 8640	As-cast 4140
Reported hardness range (HV)	131 -- 150	174 -- 286	180 --332
Measured hardness (HV)	139	292	303

3.3.1 Stereo Lithography Apparatus (SLA) Printers

Three SLA printers were used in this project: the 3D Systems ProJet 6000 HD, which is positioned in industrial applications and mass production; Formlabs Form 2, which is a low-cost desktop printer; and Formlabs Form 3+, the upgraded version of Form 2. Figure 15 shows the three SLA printers side by side. The ProJet 6000 HD takes up more space, but it is more reliable and suitable for batch manufacturing with a higher printing speed. Form 2 and Form 3+ have a much smaller footprint and lighter weight. Currently, Formlabs Form 2 is discontinued, and Formlabs Form 3+ is available at a low price, less than one-sixth of the price of the 3D Systems ProJet 6000 HD. For the quality of the printed part, there is no significant difference between Formlabs Form 2 and Formlabs Form 3+. Technical specifications of the two printers are compared in Table 5 [15].

Table 5 Technical specifications comparison: 3D System ProJet 6000 HD, Formlabs Form 2 and Formlabs Form 3+.

Model (Brand)	ProJet 6000 HD (3D system)	Form 2 (Formlabs)	Form 3+ (Formlabs)
Dimensions (mm)	787×737×1829	350×350×520	570×510×690
Weight(kg)	181	13	17.2
Min.Layer Thickness(mm)	0.05	0.03	0.025
XY Accuracy(mm)	0.025	0.14	
Max. Build Size(mm)	250×250×250	145×145×175	145×145×185
Price (\$)	185,000	3499(Discontinued)	2499



Figure 15 Three SLA printers used in the project: 3D System ProJet 6000HD, Formlabs Form 2, and Formlabs Form 3+.

3.3.2 Designing Investment Casting Patterns for 3D Printing

The patterns used in investment casting must be printed in a hollow structure. The hollow structure of the patterns can reduce the amount of material used, avoid cracks in the ceramic shell caused by polymer expansion during the burnout process, and maintain sufficient strength of the patterns. In 3D System printing software, there is a built-in hollow function. Using this function, the parts can be meshed into honeycomb-supported, hollow structures. Figure 16 (c) and (d) shows Part 1 hollow pattern printed with 3D System Project 6000HD. However, there

isn't such a function in Formlabs' printing software. Therefore, in order to print out hollow structures with Formlabs printers, other software such as AutoMeshmixer was used to hollow the parts before printing. By using AutoMeshmixer, the original solid STL model can be meshed and hollowed as shown in Figure 16 (a) and (b). Figure 16 (e) and (f) are the printed patterns with and without hollow structure by Formlabs printers. Drain holes also can be created in AutoMeshmixer. The team has tried printing hollow structures with different thicknesses from 0.3mm to 0.6mm. Based on experiment results, defects on the surface were observed when printing the hollow pattern with a wall thickness thinner than 0.4mm. Therefore, printing hollow patterns with 0.4mm-0.6mm wall thickness is feasible. The hollow STL can be printed by Formlabs printer with a lattice support structure that can be automatically created by the Formlabs' printing software.

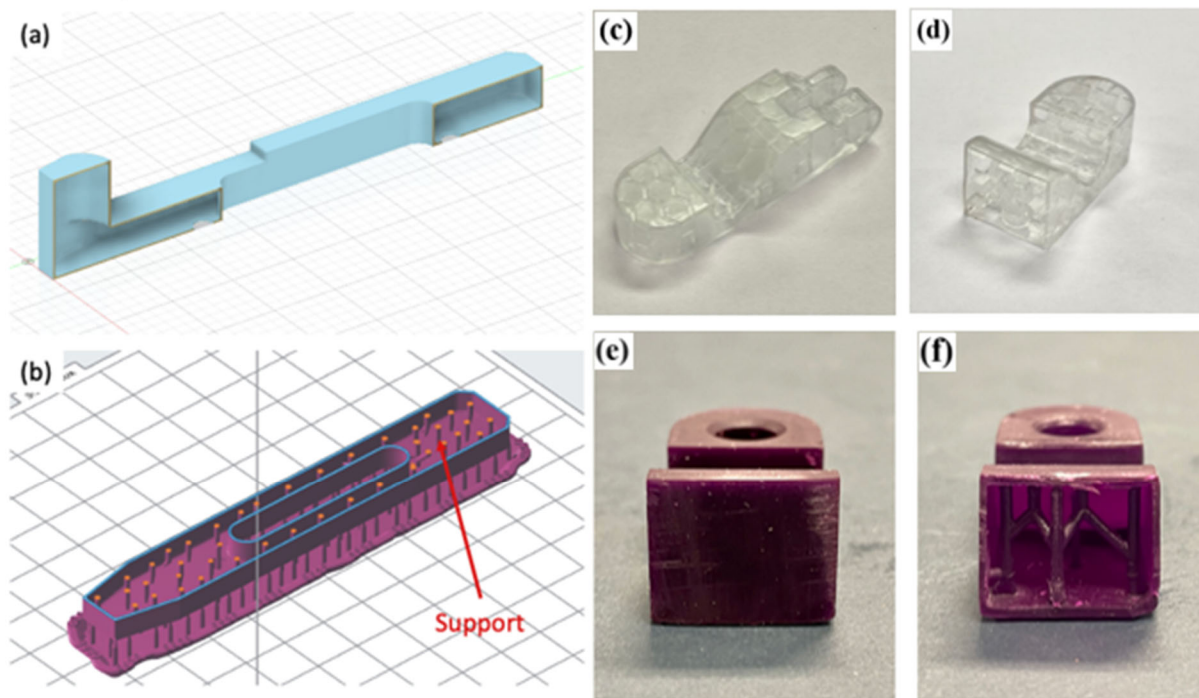


Figure 16 (a) Part2 hollow pattern cross-section view, (b) Internal supports created by Preform. (c) Part 1 hollow pattern printed with 3D System Project 600HD. (d) Cross-section of Part 1 hollow pattern with 3D System Project 600HD. (e) and (f) Cross-section of Part 1 hollow pattern with Formlabs.

3.3.3 Printing Investment Casting Patterns

To demonstrate the SLA-enabled investment casting process, three workpieces were selected, as provided by the U.S. Army DEVCOM Ground Vehicle System Center (DEVCOM-GVSC). Part

1 (Stop, Solenoid control) patterns were printed using VisiJet clear resin by the 3D Systems ProJet 6000HD printer, as shown in Figure 17(a). Part 2 (Link, input steer gain) and Part 3 (Arm, outer) patterns were printed using Castable Wax with the Formlabs printer as shown in Figure 17(b) and (c). However, the size of Part 3 exceeded the capacity of the furnace for burnout at WPI, which has a chamber size of 6 in.*5in.*5in. To demonstrate the process, the component was scaled proportionally by 50%.



Figure 17 (a) Part 1 hollow pattern printed with 3D System Project 600HD; (b) Part 2 hollow pattern printed with Formlabs Form 2; (c) Part 3 hollow pattern printed with Formlabs Form 2.

The design of the polymer patterns included a machine stock of 0.06 inches, which can be easily machined after casting. The holes on the workpieces are castable, but the tolerance requirements of these features still demand machining after casting. Therefore, different cast patterns were made with and without holes. For the design without holes, the cast piece was machined to create the required holes.

In investment casting, steel parts typically shrink by 1%~2.5% after solidification due to the melting of the wax mold, expansion of the ceramic shell, and shrinkage of the metal after cooling [61, 62]. In this project, shrinkage factors from 2% to 3% have been experimented with in SLA pattern designs. After trials, a shrinkage factor of 3% was used for the final SLA pattern design.

3.3.4 Investment Casting Tree Assembly Design and Simulation

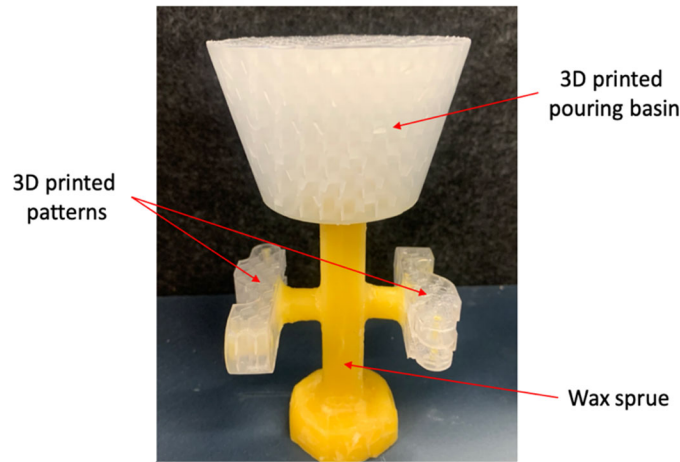


Figure 18 Casting tree assembly of Part 1.

Generally, in manufacturing settings, casting “trees” are not produced in a single step. Instead, delicate master patterns usually are made separately and then assembled onto a universal stem, as shown in Figure 18. Since the stem in a casting tree is only used as sprue and runners, it does not require high accuracy and can be made of wax at a lower cost.

Casting tree assemblies were designed for three demo parts, based on the MagmaSoft simulation results. MagmaSoft is one of the most commonly used finite-element analysis software in the metal casting industry. It can simulate temperature and flow during pouring and solidification. In the simulation, porosity and hot spots were special focused, which are two major defects in a cast part. Hot spots are sections of casting that cool down more slowly than the surrounding material. Any hot spot causes abnormal shrinkage in its vicinity, which can lead to porosity and cracking.

Multiple simulations were conducted. Based on the simulation results, optimized designs were created to avoid possible defects. For example, for Part 1, as shown in Figure 19 (a), runners had been added on the sides of the sprue to connect the parts. By doing so, metal flow would first fill the buffer zone at the bottom of the casting tree, and then fill the workpiece cavity at a gentle speed. As simulation results show in Figure 19 (b, c), no porosity or hot spots appeared in the workpieces. The defects were located in the pouring basin and sprue, which would not affect the quality of the final products. Figures 20 and 21 show the final cast tree design for the other two demo parts.



Figures 22 and 23 show the casting tree assembly of Part 3 and Part 2.



Figure 22 Casting tree assembly of Part 2.



Figure 23 Casting tree assembly of Part 3.

3.3.5 Ceramic Shell Making and Burnout

The ceramic shell was made by a 6-layer dipping and stucco process to ensure sufficient strength during burnout and casting as documented in our previous reports. All the refractory materials used to make ceramic shell were purchased from Remet. A completed ceramic shell is shown in Figure 24, the shell thickness was measured as 4.1mm.



Figure 24 Completed ceramic shell before burnout.

After the ceramic shell has been dried, it is placed in a burnout furnace. A 36-hour burnout schedule was developed and verified to be sufficient in fully removing the SLA printed polymer patterns. As per the TGA results presented in Figure 25, both VisiJet Clear Resin and Formlabs Castable Wax decompose completely at 650°C. After this stage, the ceramic shell is slowly cooled to room temperature at 60°C/h.

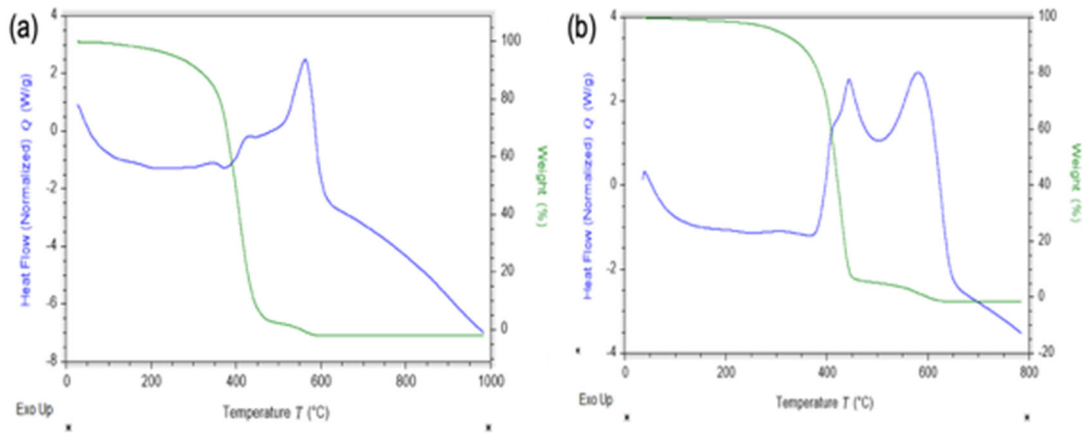


Figure 255 TGA results of (a) VisiJet castable resin and (b) FormLabs castable wax.

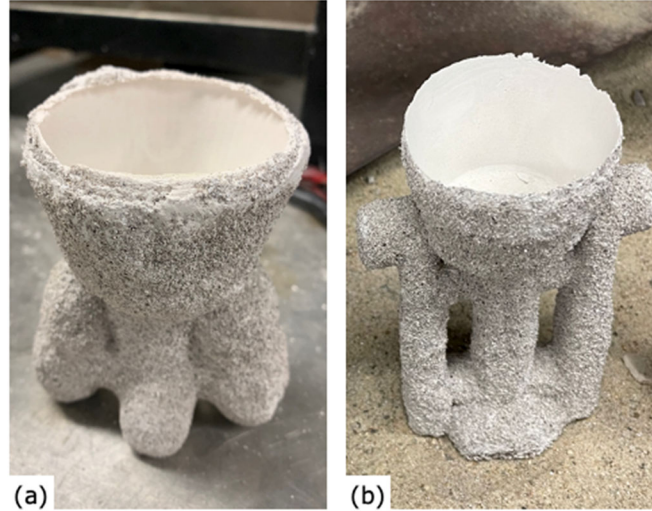


Figure 26 Ceramic shells after burnout (a) Part 1 casting tree assembly; (b) Part 2 casting tree assembly.

As depicted in Figure 26, no cracking was observed in the ceramic shell after the burnout process. The CT scan results shown in Figure 27 confirmed that the resin was completely decomposed, and a clean cavity was obtained. To ensure that there were no cracks or residual resin remaining in the ceramic shell, it was cut in half after burnout to carefully evaluate the

internal surface, as shown in Figure 28. No resin residue was found on the surfaces, in corners, or along the edges of the shell, and the overall geometry of the cavity was smooth and complete. This result confirms that the dipping, stucco, and burnout processes were effective for the required ceramic shell production, and the internal geometry of the ceramic mold replicated all the design features accurately.

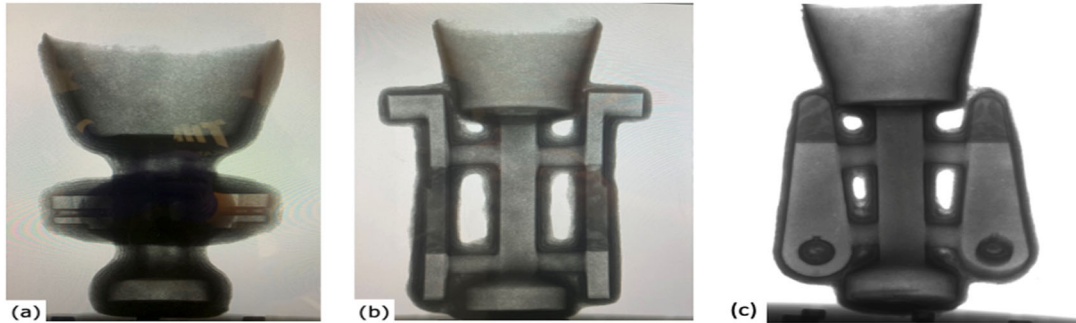


Figure 27 CT scan results of ceramic shells after burnout: (a) Part 1 casting tree assembly; (b) Part 2 casting tree assembly; (c) Part 3 casting tree assembly.



Figure 28 Cross-section view of ceramic shell after burnout.

3.3.6 Casting Process

Table 6 outlines the four stages of the melting process. First, the steel waste material was added to the crucible, and the furnace power was ramped up to 17 kW for preheating. This stage lasted at least 30 minutes until the waste metal pieces were heated to around 700°C and became red in color. The power was then increased to 30 kW for the melting stage, during which the materials were completely converted into molten metal. The melting time and crucible power were

adjusted based on the total amount of waste metal. A steel rod was used to stir the molten metal occasionally to ensure proper mixing, and a skimmer was used to remove slag formed during melting. Figure 29 shows some of the tools used during the melting process.

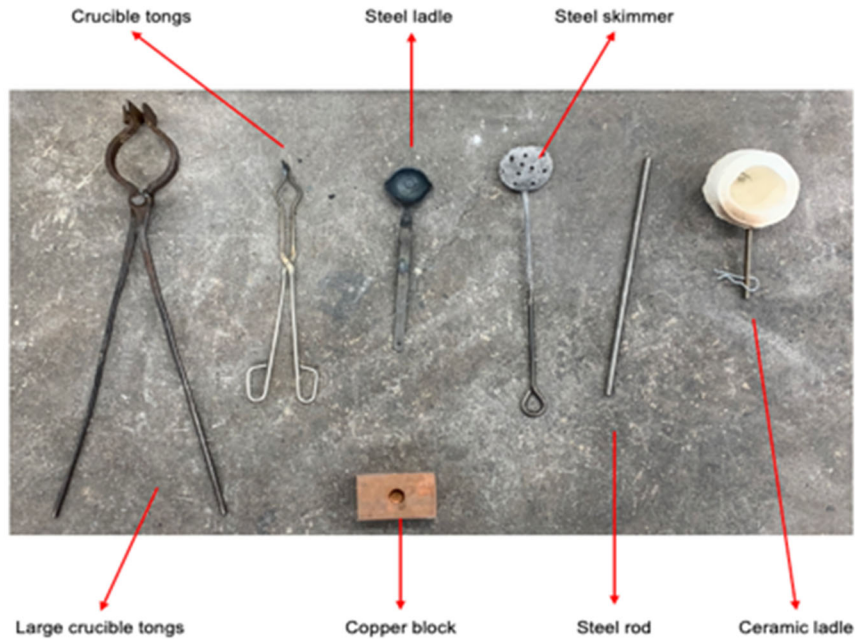


Figure 29 Tools utilized in melting and pouring process.

After the melting stage, the furnace power was reduced to 25 kW to conduct composition analysis using a portable optical emission spectroscopy (OES). A small amount of metal was scooped and poured into a copper mold with a 1-inch depth and 1-inch diameter cavity. The large difference in the thermal expansion coefficient between steel and copper makes it easy to remove the steel sample from the cavity for OES tests. Based on the OES test result and the alloy composition requirement, small amounts of additional materials were added to the crucible for chemical composition adjustment. The furnace power was then increased back to 30 kW to heat the molten metal to the target pouring temperature of 1650°C. An immersion pyrometer was used for temperature monitoring during the melting process. Once the temperature of the molten metal reached 1650°C uniformly, the metal melt was ready to be poured into ceramic shells.

Before pouring, the ceramic shell was preheated in a furnace at 1100°C and held for at least 2 hours, conducted in parallel with melting and completed before pouring. Once the molten metal reached the targeted pouring temperature uniformly, pouring had to be conducted immediately to avoid significant oxidation and loss of certain key alloying elements. The pouring spout of the crucible was also preheated using a propane blowtorch to avoid rapid cooling of the molten metal during pouring.

Table 6 Melting time using Inductotherm Mini-Melt furnace.

Time (Minutes)	Power (kW)	Action
0	0	Add waste material into crucible
0-30	17	Crucible preheat
30-90	30	Main melting stage
90-110	25	Conduct composition analysis, adjust composition
110-140	30	Temperature measuring, pouring

3.3.4 Post Treatment

After casting, the molds filled with metal were allowed to cool to room temperature in ambient air. The ceramic shell was then removed from the casting trees. Figure 30 shows the resulting as-cast trees, each of which produced multiple workpieces. The workpieces were cut off from the trees for cleaning and inspection. Figure 31 displays the as-cast parts that were cut from the cast

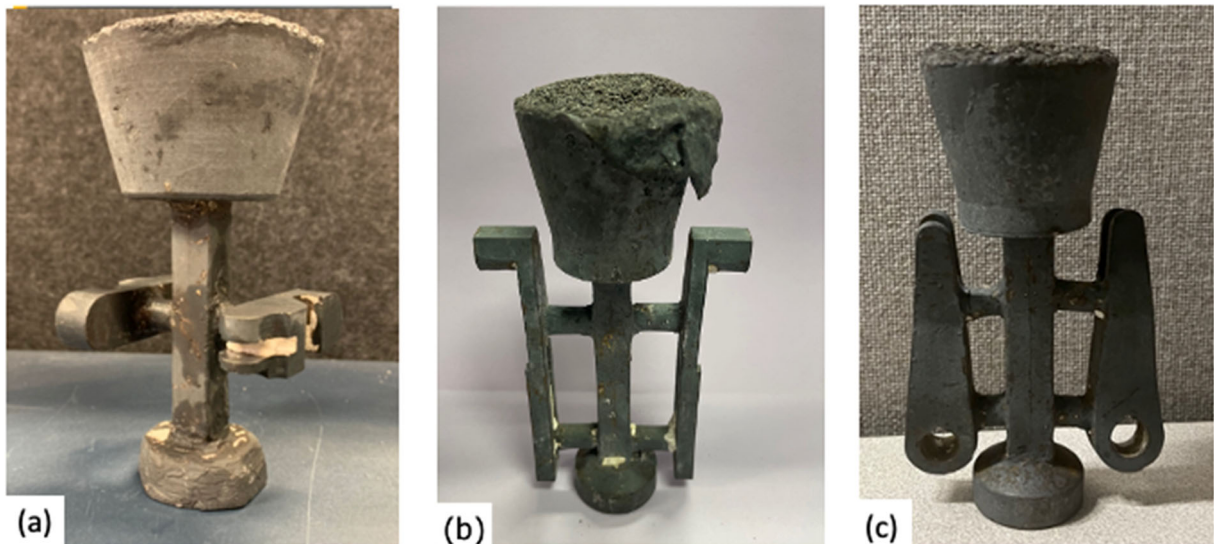


Figure 260 As-cast casting trees (a) Part 1 casting tree assembly; (b) Part 2 casting tree assembly; (c) Part 3 casting tree assembly.

trees shown in Figure 30. As previously mentioned, machining the holes in the parts is necessary to achieve the required tolerance. Thus, machining the holes is also a viable approach and has been used in the designs depicted in Figure 31 (a) and (b).



Figure 31 Parts cut from casting tree (a) Part 1; (b) Part 2; (c) Part 3.

The hardness of the as-cast Part 1 product was measured to be 36.1HRC. To reach the specified target hardness of 30-35HRC, and to eliminate residual stress in the as-cast product, a standard heat treatment process was conducted [36]. The heat-treatment process included normalization at 860°C for 1 hour, followed by quenching in water and tempering at 650°C for 1 hour. After heat treatment, the hardness of the final product became 33 HRC.

The hardness of the as-cast Part 2 product was measured to be 39.2HRC. To reach the specified target hardness of 32-38 HRC, Part 2 was quenched from 860°C and tempered at 450°C for 1 hour. After heat treatment, the hardness of the final product was 36 HRC.

It is worth noting that the heat-treatment process should be uniquely designed for a specific alloy and desired hardness.

The design of Part 3 does not specify the required hardness.

3.4 Characterizations

3.4.1 Chemical Composition and Microstructure Characterization

According to the part drawing and specification provided by DEVCOM-GVSC, Part 1 requires a material of 4140 or 8640 alloy steel. The waste materials were selected using the blending model developed from the waste metal database. During the melting process, in-situ composition

monitoring was performed using a portable OES. Based on the results, adjustments were made to the composition by adding 0.43 pounds of pure Mn flakes to increase the Mn concentration, 0.32 pounds of Ferrosilicon to increase the Si concentration, and 2.5 pounds of cast iron to increase the Carbon concentration. These elements are known to be easily lost during melting in steel making. As shown in Table 7, the chemical composition of the final product meets the required composition range for both AISI 4140 and AISI 8640 alloy steels.

Table 7 Chemical composition of fabricated parts and target composition range.

		C	Mn	Si	Cr	Mo	Ni	S	P	DI	CE
Part 1 Target composition	4140	0.38-0.43	0.75-1.0	0.15-0.3	0.8-1.1	0.15-0.25	/	0-0.04	0-0.0035		
	8640	0.38-0.43	0.75-1.0	0.15-0.35	0.4-0.6	0.15-0.25	0.4-0.7	0-0.04	0-0.0035	4.44-8.38	0.64-0.87
Product		0.41	0.805	0.15	1.12	0.215	0.53	0.039	0.023	8.26	0.85
Part 2 Target composition	4130	0.28-0.33	0.4-0.6	0.15-0.3	0.8-1.1	0.15-0.25	/	0-0.04	0-0.0035		
	4140	0.38-0.43	0.75-1.0	0.15-0.3	0.8-1.1	0.15-0.25	/	0-0.04	0-0.0035	2.51-6.38	0.54-0.91
	4142	0.4-0.45	0.75-1.1	0.15-0.3	0.8-1.1	0.15-0.25	/	0-0.04	0-0.0035		
Product		0.29	0.64	0.05	0.87	0.16	0.14	0.03	0.02	2.94	0.58
Part 3 Target composition	1010-1025	0.08-0.28	0.3-0.6	/	/	/	/	0-0.05	0-0.04	0.086-0.45	0.13-0.38
Product		0.176	0.575	0.488	0.127	0.012	0.108	0.03	0.023	0.28	0.27

Part 2 was designed to be made of 4130-4142 chromium-molybdenum alloy steel. As shown in Table 7, the chemical composition of the final product, except for silicon, fell within the specified range. Silicon is usually added to alloy steels during melting to act as a deoxidizer [58]. The lack of silicon could result in fine air bubbles in the final product. In our casting process, pure aluminum was also added as a final deoxidizer. Additionally, carbon and manganese in the alloy act as deoxidizers as well [58]. As shown in the representative microstructure image in Figure 34, final product contains austenite and tempered martensite, no air bubbles or porosity were observed in the final product.

The inclusion of silicon in the steel alloy is expected to increase the hardenability and strength of the steel product [58]. However, other alloying elements can serve a similar function, such as carbon, manganese, chromium, and molybdenum. Therefore, the Ideal Critical Diameter (DI) and Carbon Equivalent (CE) were calculated and used to reliably gauge the properties and performance of the steel alloy with multiple alloying elements. As shown in Table 7, the Ideal Critical Diameter (DI) and Carbon Equivalent (CE) values of the final product were calculated, and they were within the expected ranges [28]. This result confirms that the effect of the slightly lower than expected silicon content on hardenability has been compensated for by other alloying elements. Additionally, the mechanical properties of the final product can be adjusted by heat treatment to reach the target value. Therefore, the lower silicon content in the final product was not considered to be a major issue.

Different microstructures are observed in the as-cast steel when following the arrows from the surface to the center, as shown in Figure 32(a). A dense microstructure is formed in the chill layer (Figure 32(b)) due to a large overcooling rate. Well-formed dendrites are observed in the outer layer (Figure 32(c)), pointing in the same direction toward the center. As shown in Figure 32(d), the oriented dendrites transition to more randomly arranged dendrites. This is due to reduced overcooling and growth speed.

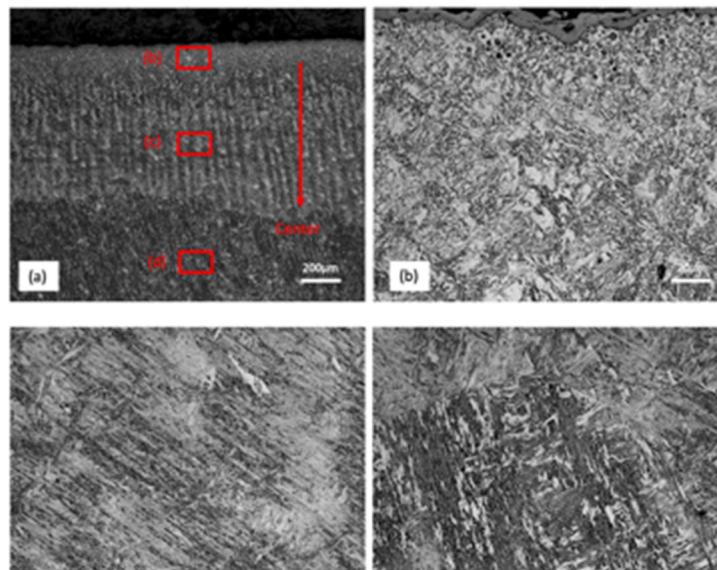


Figure 32(a) As-cast 4140 steel microstructure image, (b) chill layer (c) outer region, (d) transition region.

Dendrites are a common microstructure observed in cast steel [58]. In a casting process, liquid steel is poured into a casting mold and rapidly solidified. Due to the large deviation of the chemical equilibrium state at the solidification front, this tree-like structure is formed. The size of dendrites and the secondary dendrite arm spacing strongly depend on the solidification rate of a given material. In addition, the chemical composition of the alloy also has an influence on this structural characteristic [59].

As demonstrated in Figure 32, the as-cast steel exhibits inconsistent microstructures in different regions, resulting in suboptimal overall performance. To enhance quality, alleviate internal stress, and achieve preferred mechanical properties, heat treatment is necessary. Quenching and tempering experiments were conducted at various temperatures to optimize the mechanical properties. As mentioned, three demonstrating parts were fabricated in three different alloy grades and heat treated to achieve the target mechanical properties as specified in the drawings. Figure 33-35 depict the microstructure images of 1025, 4140 and 8640 steel after quenching and tempering, demonstrating a uniform distributing tempered austenite and fine microstructure in the final parts.

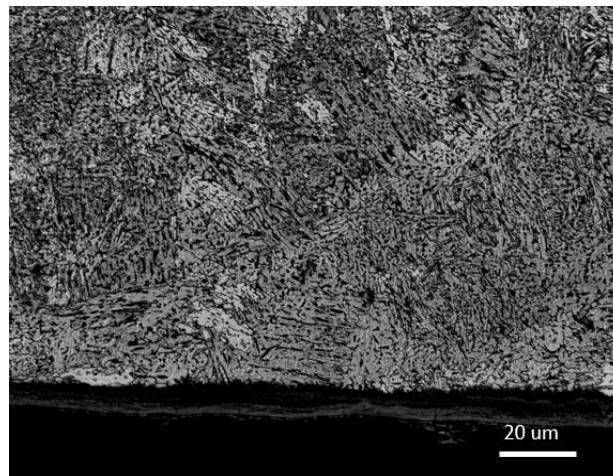


Figure 33 Microstructure of quench-tempered 1025 carbon steel.

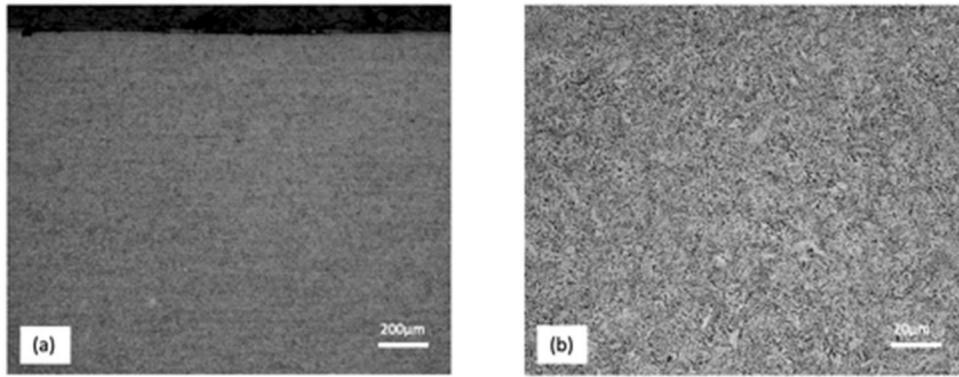


Figure 34 Microstructure of quench-tempered 4140 steel at different magnifications.

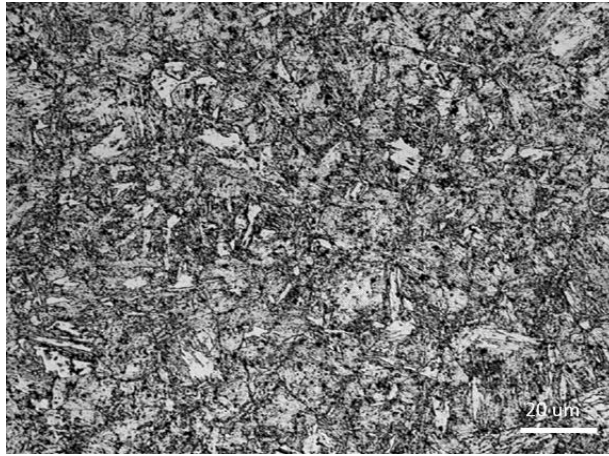


Figure 35 Microstructure of quench-tempered 8640 alloy steel.

3.4.2 Dimension Inspection

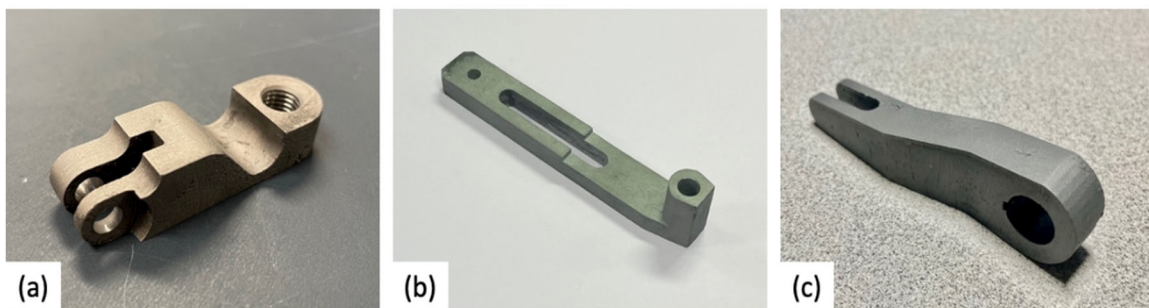


Figure 36 Final parts (a) Part 1; (b) Part 2; (c) Part 3.

After heat treatment, the parts were sandblasted for final surface finishing. The final products are shown in Figure 36. The key dimensions of the printed patterns and cast parts were measured

and summarized in the table insets in Figures 37, 38, and 39, correspondingly. The results show that all key dimensions of the final product were within the required tolerance.

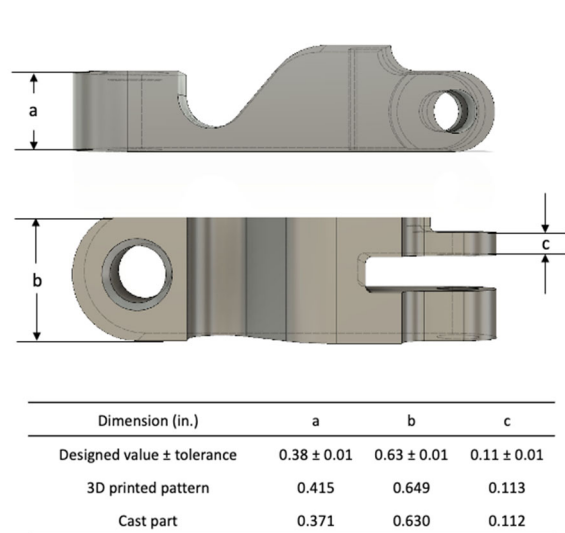


Figure 277 Part 1 final product dimension inspection.

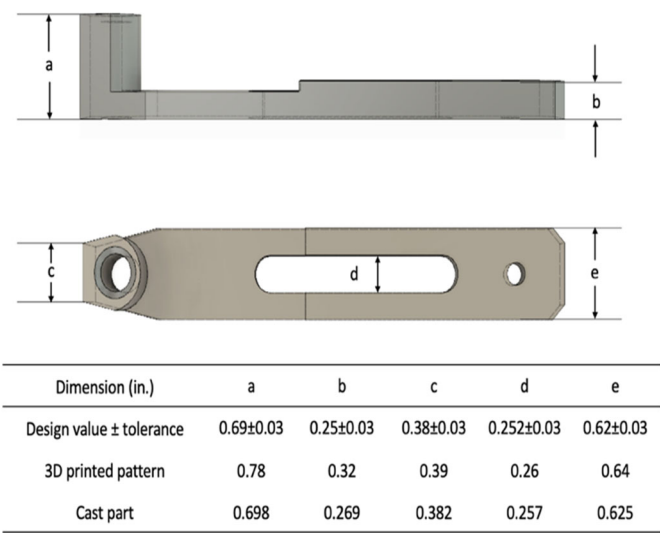


Figure 38 Part 2 final product dimension inspection.

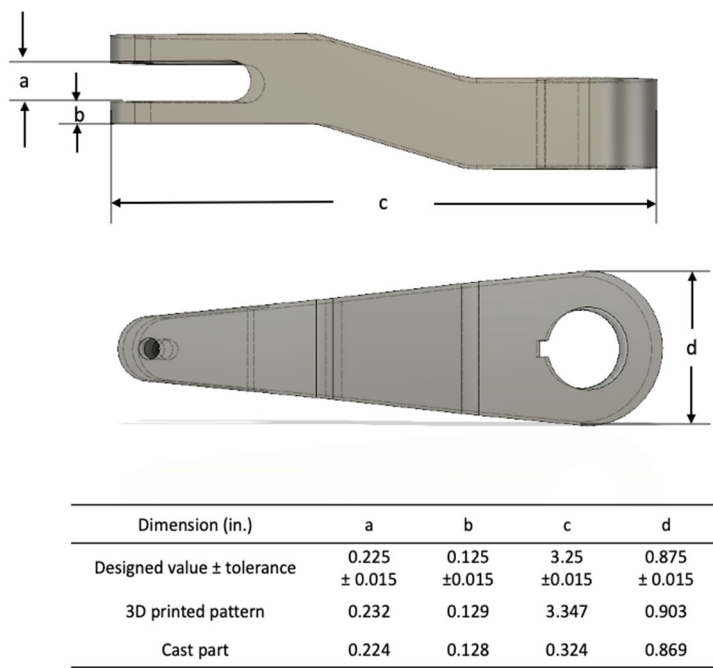


Figure 39 Part 3 final product dimension inspection.

Chapter 4: Compact Casting System and Mobile Foundry

4.1 Compact Steel Casting System Setup

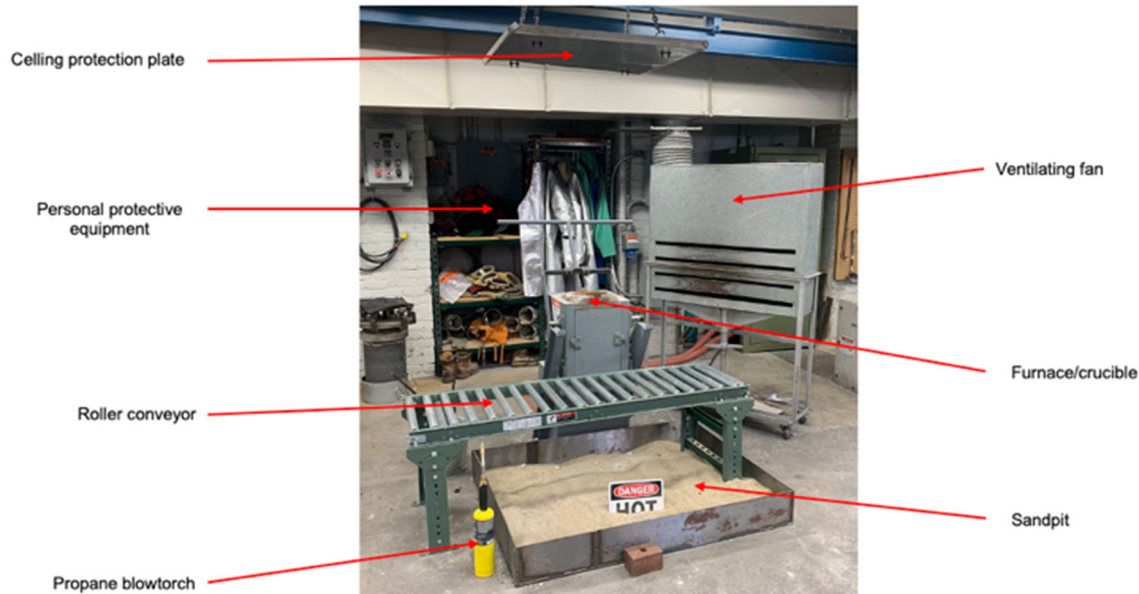


Figure 40 Compact foundry system in WPI Washburn Shop.

The steel casting system commonly used in commercial foundries requires a large space and is not feasible for the Expeditionary Laboratory (ExLab). To ensure an efficient and safe casting process in a smaller area, a compact mini-casting system has been designed, which can be housed in a trailer and operated within a 20-ft. x 20-ft. area. The foundry's arrangement is shown in Figure 40, where a conveyor (H-5012, Uline) is used to support and transport the casting mold. A 4-ft. x 3-ft. x 0.5-ft. sandpit is used to prevent molten metal from splashing onto the ground. To remove the gas generated during melting, a ventilating fan is installed next to the furnace. A steel plate is constructed to hang above the furnace, preventing heat radiation from damaging the ceiling or pipes in the lab.

The furnace (Double Trunnion 50# Minimelt Furnace), control unit (Power-Trak 35-96r), and crucible (Alumina Crucible Refractory Kit) used in this project were purchased from Inductotherm. The crucible protects the furnace, as shown in Figure 41 [64]. The gap between the crucible and the furnace is filled with refractory furnace finings (MAGNAVIBE 700) from Vesuvius. The top cap and spout are made of refractory clay (90-RAM PC HW plastic) from Vesuvius. The top cap

and spout are sintered to 300°C with a seven-day lead time after they are set in place. The cooling system (WX-250) used in the project is from WELL-X-TROL.

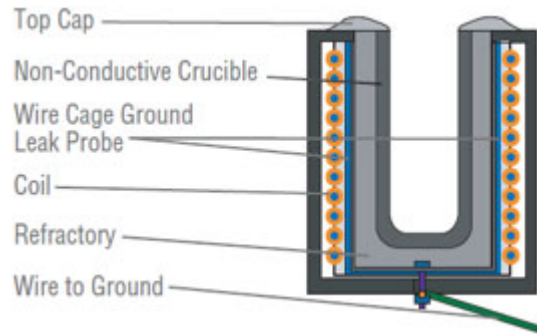


Figure 41 Schematic of the induction furnace [64].

4.2 Three-container Mobile Foundry Design

The mobile casting foundry system consists of three standard-size, 20-ft x 8-ft. x 8.5-ft. ISO shipping containers, each equipped with climate controls and ventilation units. The use of standard-size containers instead of longer or taller ones allows for easier transportation, improved ventilation, and casting system efficiency. The equipment required for the entire fabrication process is split among the three containers, with each container designated for a specific sub-process.

The first container is used for preparatory and storage materials, including a significant workspace for preparing samples and storing recovered scrap material. An SLA 3D printer is installed for investment casting pattern printing, along with a jar mill and sand mixer for ceramic making. A drying box with temperature and moisture control is also included to maintain the ceramic shell quality.

The second container is designed for melting and pouring and houses the Mini-Melt induction furnace, box furnace, PPE closet, sand pit, and conveyor system. Since molten metal and high-temperature box furnaces pose serious hazards, the second container is classified as a hazardous area, and extreme caution must be taken.

During the metal casting process, waste gas is produced while preheating and pouring, making it necessary to have ventilation systems in mobile foundry containers. In the first container, a ventilation system was designed to maintain a tolerable maximum temperature within the containers and circulate air sufficiently to displace metal-fume radiation produced by the crucible. The ventilation system for the exothermic container includes a Friedrich Kuhl L-Series Commercial Grade A/C unit capable of displacing 725 CFM, a Vent-A-Kiln overhead ventilation fan capable of displacing 500 CFM, and three roof vents for additional passive ventilation. The study targeted a minimum of twenty air changes per hour in the mobile foundry, equivalent to a minimum circulation of 453.33 CFM. The designed ventilation system not only satisfies the minimum recommended air changes per hour but can also circulate 725 CFM per hour and maintain a tolerable environment during worst-case scenarios that could occur during the casting process.

The third container is used for characterization and final inspection, with an OES machine for chemical composition characterization, a CT machine, and a microhardness indenter for non-destructive testing methods to detect whether the final product meets the mechanical property targets and whether there are internal defects or porosities.

A 3D model of the mobile foundry containers was created using Fusion 360. This modeling allowed for accurate evaluation of the design and quantification of the degree of safety. The use of SolidWorks assemblies provided a helpful visualization of the equipment arrangement in the containers and allowed for a timely alternative for assessing the design and safety efficacy of the mobile foundry.

4.3 Thermal Simulation

To ensure a safe and comfortable operating environment, thermal simulations have been conducted using ANSYS in collaboration with an MQP research team at WPI. In the mobile foundry system, the main heat sources are the box furnace for ceramic shell preheating and the induction furnace for remelting. Temperatures at different locations during operation have been measured and documented in Table 8. It is evident that the temperature at the outer surface of the closed box furnace is almost at room temperature. Additionally, the door of the box furnace

generally only needs to be opened for less than fifteen seconds to remove the preheated molds during actual operation. Therefore, the box furnace has little effect on the temperature of the entire system. Based on the measurements, the temperature of the side of the induction furnace is also close to room temperature. As a result, thermal simulation has been conducted using the induction furnace at its highest operating temperature as the only heat source. During most of the melting and casting process, the top of the induction furnace is covered with a ceramic fiber insulating blanket, which is removed only for active operations such as casting, temperature measurement, or composition adjustment. Hence, two scenarios have been simulated separately by ANSYS, with or without the insulating blanket covering the top of the operating induction furnace.

Table 8 Temperature measured at heat resources during operation.

Locations	Senior	Temperature (°C)
Box Furnace		27.6
Induction furnace (exposure surface)	Covered	456.45
	Uncovered	1682.22
Induction furnace (side surface)		36.6

In the scenario where the induction furnace is covered, the A/C is intaking 500 CFM of 160°C air while the exhaust fan is exhausting 500 CFM of air as well. Using these parameters for ventilation and 456.45°C as the surface temperature of the ceramic fiber insulating blanket, the temperature distribution within the mobile foundry has been simulated.

In this simulation, the maximum temperature reached in all operating areas is roughly 25°C, which is our maximum allowable temperature for a safe environment. The temperature above 26°C only appeared directly above the induction furnace and some areas close to the floor and will not affect normal operation. Therefore, the mobile foundry environment is safe for operators when the ceramic fiber insulation blanket is covering the top of the induction furnace, which represents the majority of the production process.

Secondly, the simulation has been conducted with the induction furnace open and operating at 1682.22°C, which is the maximum temperature of molten steel before pouring. In this scenario,

the induction furnace is open to the air without an insulating cover. The A/C is intaking 700 CFM of 13.9°C air while the exhaust fan is exhausting 700 CFM of air. The ventilation system is operating at increased capacity to accommodate the large increase in temperature of the main heat source. The temperature distribution diagram outputs from ANSYS validated a tolerable mobile foundry environment. The temperature in operating areas at head height in the container only reaches about 26°C, and the temperature at the two most frequently occupied locations around the induction furnace only reaches about 25°C.

The maximum temperature in typical operating areas within the container is 26°C for both simulated scenarios, which is reasonable for an indoor foundry working environment. Overall, thermal simulations were conducted to understand the indoor working environment under two scenarios. The first scenario, where the induction furnace is operating with the ceramic fiber insulating blanket covering the top, is the most likely scenario that operators will encounter throughout the casting process. In this scenario, the maximum temperature in the operating area is easily limited to 25°C by the ventilation system operating at medium capacity. The second scenario, where the induction furnace is open and operating at maximum temperature without the insulating cover on top, is usually not sustained for an extended period of time. In this more severe scenario, the A/C unit and exhaust fan assembly can maintain a maximum temperature in the operating area at or below 26°C. Therefore, the designed ventilation system is capable of maintaining a safe interior environment of the foundry at all stages of the casting process.

4.4 A List of Commercially Available Equipment and Corresponding Suppliers for the Mobile Foundry

The three-container system consists of the investment preparation area, casting area, and product characterization area. To equip each container with appropriate instruments and supplies, the team conducted extensive research on currently available equipment in the market and selected suitable options based on safety, size, power and cooling demand, ease of operation, and technology maturity. The possible options for required equipment in the mobile foundry system have been summarized with links to the websites of the suppliers whenever possible.

4.5 A Microgrid System Compatible with The Mobile Foundry

Many instruments in the mobile foundry design require electricity to function, and according to our calculation, the total power consumption of the mobile foundry system at its highest load is 45kW. The VIP-I® Power Supply Unit produced by Inductotherm is compatible with the mini-melt induction furnace, which consumes the most power in the system. Compared to other rectifier units with the same power range, these units are smaller and more compact. A standard VIP-I® Power Supply Unit comes equipped with an intelligent digital control board featuring fiber-optic connectors for clear signal processing, a digital display, and an integral keypad for control and data entry. To ensure the mobile foundry system functions properly, a microgrid or mobile power supply system is essential due to its compact size and portability.



Figure 42 The Boxpower solar container microgrid [65].

Microgrids have been identified as a key component of the Smart Grid for improving power reliability and quality, increasing system energy efficiency, and providing the possibility of grid-independence to individual end-user sites. The DOE defines the microgrid as "a group of interconnected loads and distributed energy resources within clearly defined electrical boundaries that act as a single controllable entity with respect to the grid. A microgrid can connect and disconnect from the grid to enable it to operate in both grid-connected and island mode."

One example of a compatible microgrid system for our mobile foundry system is the solar container microgrid produced by the BoxPower company [65]. This solar power system can be used both immediately after disasters and to make power supplies more portable and resilient to harsh environments. The system is easy to install quickly. Assembling its solar array on top of the microgrid container is feasible and doesn't require any heavy equipment or machinery. This means that installation can be done quickly and efficiently [66].

The microgrid offered by this company can easily fit inside a standard 20-foot shipping container, making it easy to transport, as shown in Figure 42. The container is equipped with solar panels, racks, a prewired battery, an inverter, and a backup generator that runs on fossil fuels. This is a great feature because if there are ever a series of cloudy days and the battery runs low, the backup generator can be used to ensure a consistent and reliable power supply. Furthermore, this generator operates at 80 or 90% fuel efficiency, which translates to a significant reduction in operating costs. This microgrid system provides a reliable power source that is both cost-effective and environmentally friendly. The system can provide around 50 kilowatt-hours of electricity, which can cover the power needs of the entire casting system.

Another advantage of the microgrid system is its scalable and replicable design, allowing for easy expansion as needed. The system is also versatile, with both off-grid and grid-tied functionality, giving users the flexibility to choose their power source. Installation is quick and easy, with minimal foundation requirements, and the pre-wired outlets make it a plug-and-play system. It has also been tested in extreme weather conditions, ensuring it can withstand harsh environments. Finally, the microgrid is fully automated with remote monitoring and control, making it easy to use and manage. All these features make it a reliable and efficient choice. The detailed parameters of all the microgrids produced by this company are listed below (Table 9):

Table 9 Boxpower microgrid key parameters

	Minimum	Maximum
Container-Mounted solar	4 kW	25.2 kW
Batteries (LiFePO4)	7.4 kWh	148kWh
Inverter capacity	6.8 kW	27.2 kW
Voltage	120/240 V	120/208 V
Phase Type	Single-phase	Three-phase
Generator (optional)	8.5 kW	50 kW

Chapter 5: Developing A Data-driven Tool for Mechanical Properties Prediction and Heat Treatment Design in Metallurgy Manufacturing

5.1 SFSA Data Pre-processing

To ensure the quality of the data used in machine learning, it is crucial to pre-process the data. The SFSA database utilized in this study was obtained from various foundries across the United States over several decades. The database was divided into three categories based on steel alloy components: 86xx steel, 43xx steel, and carbon steel. Each category was then further classified into six groups based on two primary heat treatments: normalized and quenched and tempered. During the pre-processing stage, any outliers and incorrect data caused by input errors were removed. After the pre-processing, the chemical composition and mechanical properties data showed a normal distribution, ensuring the quality of the data used in the machine learning models.

5.2 ANN Model for Mechanical Properties Prediction

An artificial neural network (ANN) model was optimized and utilized to predict multiple mechanical properties, including Yield Strength (YS), Ultimate Tensile Strength (UTS), Brinell hardness number (BHN), and Elongation (EL), for a wide range of steel chemical compositions.

Firstly, the TensorFlow package was imported as the framework of the model, and an all-built-in activation function was used to pass the string identifier. Then, RMSprop was imported as the optimizer with a learning rate of 0.001. The training dataset and testing dataset were imported as arrays, where the mechanical property of both arrays was used as the dependent variable. The independent variables in the machine learning model were the steel alloy composition information and heat treatments contained in the rest of the training and testing dataset arrays.

The number of epochs in the training process was optimized by testing between 50 to 2000. The average percentage errors of mechanical property predictions in the testing results with different epochs were compared in the Epoch Test. The number of epochs with the lowest average percentage errors was selected as the most efficient and appropriate number of epochs.

All steel grades were predicted for the four key mechanical properties. However, in this report, predictions for 43XX steel were used as an example to demonstrate the final results.

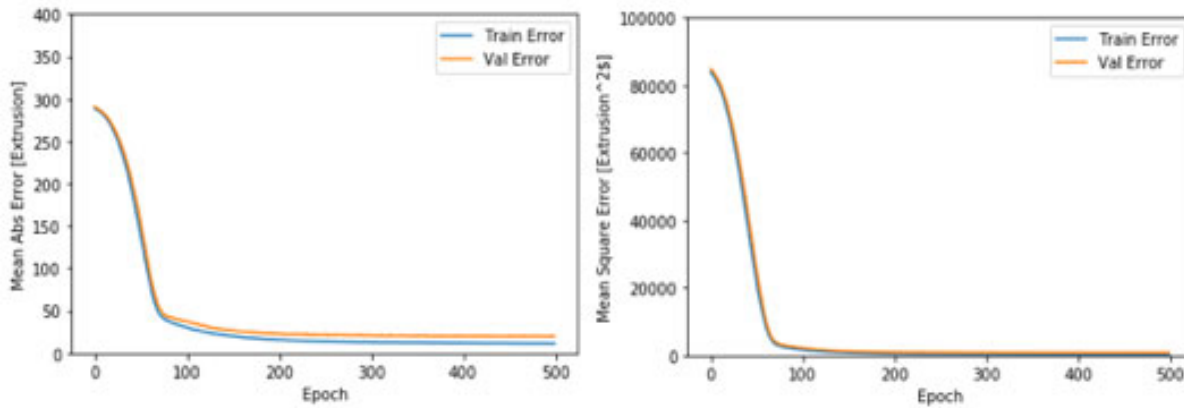


Figure 43 Normalized 43XX UTS training epoch vs. errors.

Figure 43 shows that the blue line represents the trend of training prediction error, and the orange line represents the trend of testing prediction error. The parallel and gradual leveling off of both lines indicate that the model training was successful, and the prediction reached its maximum accuracy. Based on the Epoch test, the model with 500 epochs had the lowest percent absolute error of 7.88% for the testing dataset, making it the most efficient and accurate model for the 43XX steel alloy database.

For 43XX steel, the ANN model was trained with 181 sets of normalized data and 522 sets of quenched and tempered data, while 45 sets of normalized data and 130 sets of quenched and tempered data were randomly selected as testing sets to verify the predictions. The accuracy of the UTS prediction for normalized 43XX steel was 91.23%, while the accuracy of YS prediction was 86.93%. The accuracy of BHN prediction was 94.30%, and the accuracy of %EL prediction was 94.11%. The distributions of prediction errors were shown in Figures 44 (a), (c), (e), (g), while the scatter diagrams for prediction testing results are shown in Figures 44 (b), (d), (f), (h). The dots on both diagrams are tightly clustered around the true value lines.

Overall, the prediction results for quenched and tempered 43XX steel were more accurate than those for normalized data. This could be attributed to the fact that quenching and tempering conditions result in more uniform mechanical properties compared to normalizing. The accuracy of UTS prediction for quenched and tempered 43XX steel was 92.83%, while the accuracy of YS

prediction was 92.15%. The accuracy of BHN prediction was 95.24%, and the accuracy of %EL prediction was 86.44%. The distributions of s prediction errors were shown in Figures 45 (a), (c), (e), (g), while the scatter diagrams for prediction testing results are shown in Figures 45 (b), (d), (f), (h).

The prediction accuracies of all six groups of data are high, ranging from 91.23% to 96.95%, and the mean errors of predictions are well within the acceptable range. These results confirm that the established model can be a useful tool for predicting mechanical properties of steel, and it will be especially beneficial for workers who have little in-depth knowledge of metallurgy. Additionally, the established tool will also be useful in the development of new steel alloys. The original code of the developed ANN program is provided in Appendix 1. Table 10 summarizes the prediction results for all six groups of data.

Table 10 ANN model prediction results

Steel grade	Prediction accuracy (%)				Mean error of prediction			
	UTS	YS	BHN	EL	UTS (ksi)	YS(ksi)	BHN	EL(%)
86XX normalized	93.3	86.73	95.23	88.64	6.02	10.33	11.09	2.1
86XX quenched	96.78	95.57	96.3	91.81	4.11	5.38	9.55	1.36
43XX normalized	91.23	86.93	94.3	94.11	10.43	11.52	13.98	0.88
43XX quenched	92.83	92.15	95.24	86.44	9.85	8.4	10.72	1.71
Carbon steel normalized	96.95	94.36	95	93.4	2.25	4.25	8.43	2.1
Carbon steel quenched	94.28	88.91	95.37	91.55	4.6	5.65	7.43	2.38

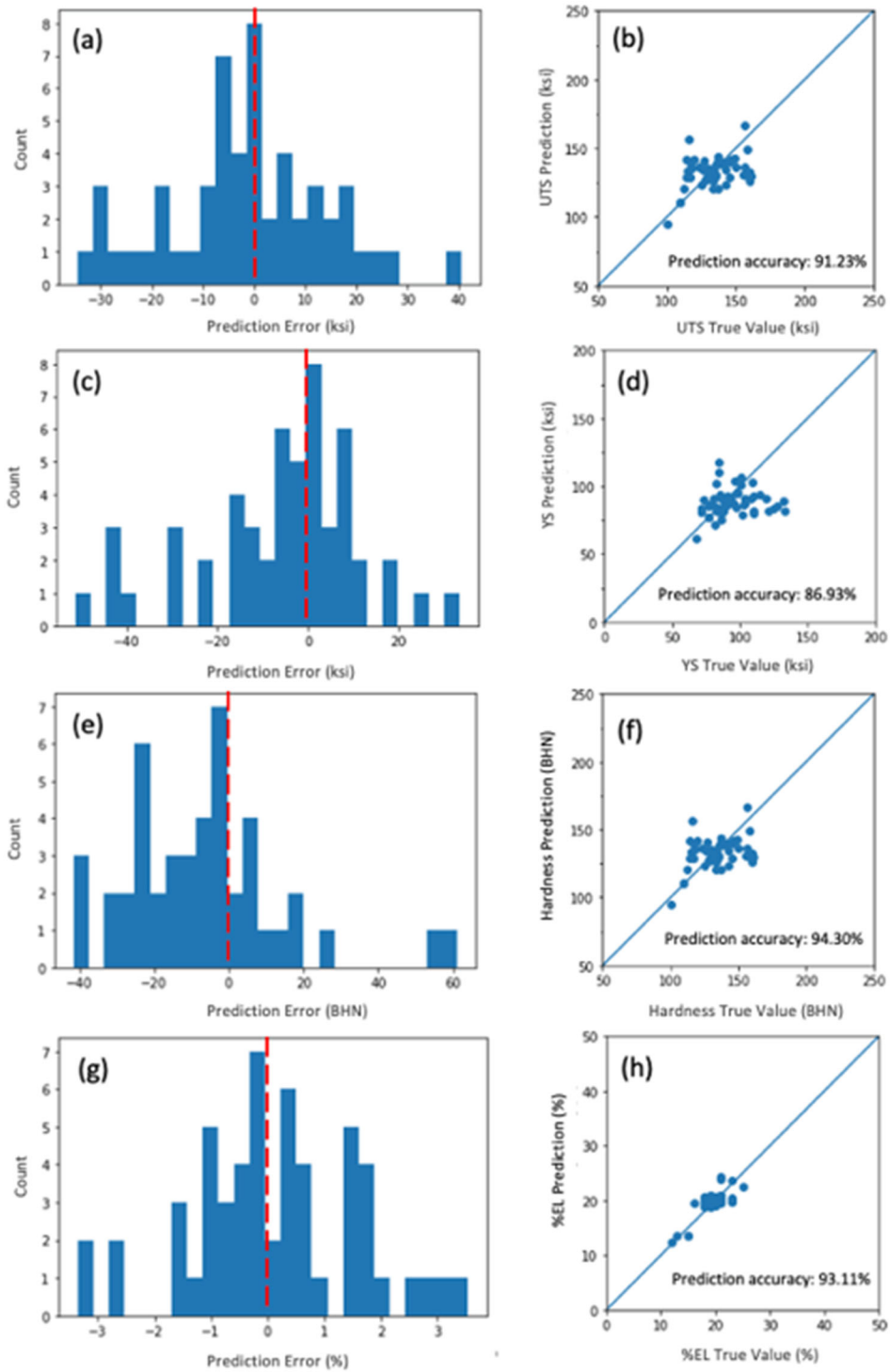


Figure 44 Mechanical properties of normalized 43XX steel: (a) UTS prediction error distribution; (b) UTS true value vs. prediction value; (c) YS prediction error distribution; (d) YS true value vs. prediction value (e) BHN prediction error distribution; (f) BHN t

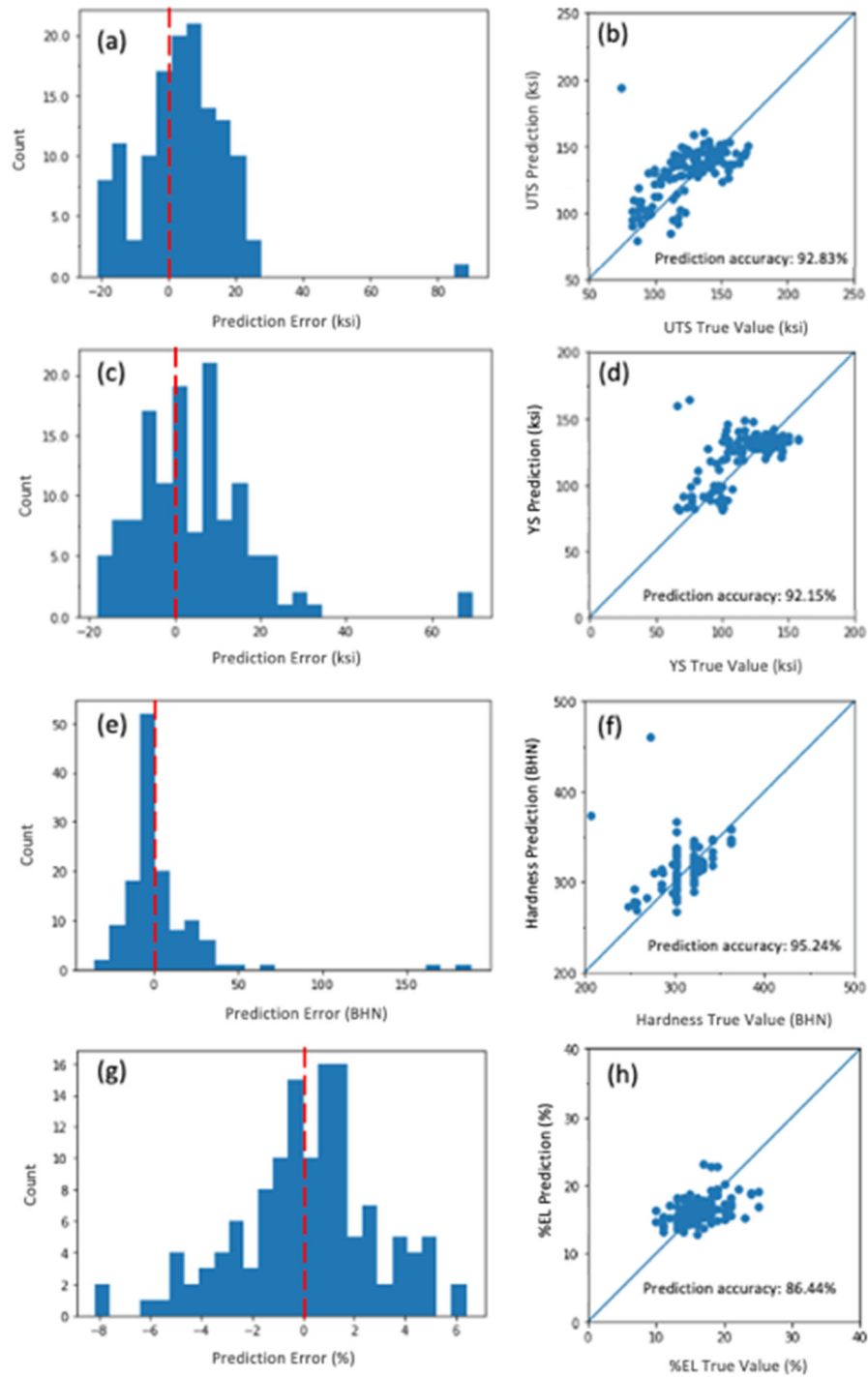


Figure 45 Mechanical properties of quenched and tempered 43XX steel: (a) UTS prediction error distribution; (b) UTS true value vs. prediction value; (c) YS prediction error distribution; (d) YS true value vs. prediction value (e) BHN prediction error distribution

Chapter 6 Conclusions

This project has successfully addressed multiple challenges in the field of material recycling, additive manufacturing, investment casting, and data-driven tools. A waste material database and blending model have been created to recycle ferrous scrap generated in forward operating bases, which reduces waste and increases the possibility of manufacturing urgently needed parts on battlefields. The investment casting process has been improved by using SLA patterns, which increases flexibility and reduces costs and lead times. The ceramic shell-making process has also been optimized with the establishment of a zirconium silicate-based slurry and a six-layer coating process.

Furthermore, data-driven tools have been developed and studied for post-treatment after casting. An ANN model has been created to study the relationship between steel chemical composition and multiple mechanical properties, while a CNN model has been developed to study the effects of heat treatment on steel alloy microstructure.

Finally, a mobile foundry system has been designed to enable the manufacturing of metal parts in remote locations. While there are still some tasks to be completed, this system has the potential to greatly increase the capability to manufacture urgently needed parts on the battlefield.

Overall, this project demonstrates that through the use of innovative techniques and tools, it is possible to improve the recycling of waste materials, optimize manufacturing processes, and develop novel systems for metal part production. These advancements have the potential to greatly benefit both military and civilian industries.

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Appendix 1: ANN code for mechanical properties prediction.

```
from __future__ import absolute_import, division, print_function, unicode_literals

import pathlib

import matplotlib.pyplot as plt
import pandas as pd
import seaborn as sns

import tensorflow as tf

from tensorflow import keras
from tensorflow.keras import layers

print(tf.__version__)

column_names = ['C', 'Mn', 'Si', 'P', 'S', 'Cr', 'Ni', 'Mo', 'YS']
raw_dataset = pd.read_csv('86xxNT noTEMP YS.csv', names=column_names,
                          na_values = "?", comment='\t',
                          sep=";", skipinitialspace=True)

dataset = raw_dataset.copy()
dataset.head(11)

import sys
print(sys.argv[60])
sys.path

dataset.isna().sum()

dataset.dropna()
dataset.head(5)

train_dataset = dataset.sample(frac=0.8, random_state=0)
test_dataset = dataset.drop(train_dataset.index)
```

```

train_dataset = train_dataset.dropna()
test_dataset = test_dataset.dropna()

train_dataset
dataset.head(5)

test_dataset
dataset.head(5)

ax=sns.histplot(data=train_dataset ['C'])
ax.set(xlabel="c")

train_dataset.describe()

sns.pairplot(train_dataset[['C', 'Mn', 'Si','P','S','Cr','Ni','Mo']], diag_kind="kde")
train_dataset=train_dataset[['C', 'Mn', 'Si','P','S','Cr','Ni','Mo','YS']]
train_dataset

train_stats = train_dataset.describe()
train_stats.pop('YS')
train_stats = train_stats.transpose()
train_stats

train_labels = train_dataset.pop('YS')
test_labels = test_dataset.pop('YS')

def norm(x):
    return (x - train_stats['mean']) / train_stats['std']
normed_train_data = norm(train_dataset)
normed_test_data = norm(test_dataset)
normed_train_data.head(20)

def build_model():
    model = keras.Sequential([
        layers.Dense(64, activation='relu', input_shape=[len(train_dataset.keys())]),

```

```

        layers.Dense(64, activation='relu'),
        layers.Dense(1)
    ])

    optimizer = tf.keras.optimizers.RMSprop(0.001)

    model.compile(loss='mse',
                  optimizer=optimizer,
                  metrics=['mae', 'mse'])
    return model

model = build_model()

model.summary()

example_batch = normed_train_data[:10]
example_result = model.predict(example_batch)
example_result

class PrintDot(keras.callbacks.Callback):
    def on_epoch_end(self, epoch, logs):
        if epoch % 100 == 0: print("")
        print('.', end="")

EPOCHS = 500

history = model.fit(
    normed_train_data, train_labels,
    epochs=EPOCHS, validation_split = 0.2, verbose=0,
    callbacks=[PrintDot()])

def plot_history(history):
    hist = pd.DataFrame(history.history)
    hist['epoch'] = history.epoch

    plt.figure()

```

```

plt.xlabel('Epoch')
plt.ylabel('Mean Abs Error [Extrusion]')
plt.plot(hist['epoch'], hist['mae'],
         label='Train Error')
plt.plot(hist['epoch'], hist['val_mae'],
         label='Val Error')
plt.ylim([0,150])
plt.legend()

plt.figure()
plt.xlabel('Epoch')
plt.ylabel('Mean Square Error [Extrusion^2$]')
plt.plot(hist['epoch'], hist['mse'],
         label='Train Error')
plt.plot(hist['epoch'], hist['val_mse'],
         label='Val Error')
plt.ylim([0,22500])
plt.legend()
plt.show()

plot_history(history)

test_predictions = model.predict(normed_test_data).flatten()

a = plt.axes(aspect='equal')
plt.scatter(test_labels, test_predictions)
plt.xlabel('True Values [YS]')
plt.ylabel('Predictions [YS]')
lims = [20, 150]
plt.xlim(lims)
plt.ylim(lims)
_ = plt.plot(lims, lims)

train_predictions = model.predict(normed_train_data).flatten()

```

```

a = plt.axes(aspect='equal')
plt.scatter(train_labels, train_predictions)
plt.xlabel('True Values [P2]')
plt.ylabel('Predictions [p2]')
lims = [20, 150]
plt.xlim(lims)
plt.ylim(lims)
_ = plt.plot(lims, lims)

error = test_predictions - test_labels
plt.hist(error, bins = 25)
plt.xlabel("Prediction Error [YS]")

_ = plt.ylabel("Count")

error = train_predictions - train_labels
plt.hist(error, bins = 25)
plt.xlabel("Prediction Error [YS]")

_ = plt.ylabel("Count")

train_error = train_predictions - train_labels
error

train_error=pd.DataFrame(train_error)
train_error

train_error=train_error.rename(columns={'YS': 'YS Error'})

train_error

train_result = train_dataset.join(train_error)
train_result

train_result1=train_result.join(train_labels)
train_result1

```

```
train_result1.to_csv('train-result.csv',index = False, header=True)

test_error = test_predictions - test_labels

test_error=pd.DataFrame(test_error)
test_error

test_error=test_error.rename(columns={'YS': 'YS Error'})
test_error

test_result=test_dataset.join(test_error)
test_result

test_result1=test_result.join(test_labels)
test_result1

test_result1.to_csv('test-result_86NT noTEMP YS.csv',index = False, header=True)
```

Appendix 2: Equations evaluated with SFSA dataset.

Author	Date	Formula	Steels
Carbon Equivalent (CE) developed to predict highest hardness in a weld and cracking.²²			
Dearden and O'Neill [1]	1940	$CE_{01} = C + Si/6 + P/0.8 + Mn/5$	Early steels C-Mn
Dearden and O'Neill [1]	1940	$CE_{02} = C + Si/6 + Mn/8 + Cr/7 + Ni/16 + Mo/4 + Co/16 + P/0.8$	Added alloys Cr, Ni, Mo, Co
Dearden and O'Neill [1],[4]	1940	$CE_{03} = C + (Mn+Cr)/5.5 + Ni/15 + V/5 + Mo/4 + Co/150 + P/2$	For predicting HV ₀₁
Wever, et al. [22]	1954	$CE_{MP} = C + Si/71.5 + Mn/5.2 + Cu/4.6 + Ni/128 + Cr/4.6 + Mo/6.3$	Max Planck early CE
BS2642[2] British Standard	1958	$CE_{BS} = C + Si/24 + Mn/6 + Cr/5 + Ni/13 + V/5 + Mo/4 + Cu/15$	BS standard for welding medium YS steel BS 968 a
Winterton [2],[4]	1961	$CE_{Winterton} = C + Mn/6 + Cr/10 + Ni/20 - V/10 - Mo/50 + Cu/40$	Analysis of 12 CE formulas
Interrante & Stout [29]	1964	$CE_{IS} = C + Mn/4 + Cr/10 + Ni/20 + Cu/40 - Mo/50 - V/10$	Included in WES 135
JWES [2] [5] [27] [30]	1973	$CE_{Wes} = C + Si/24 + Mn/6 + Ni/40 + Cr/5 + Mo/4 + V/14$	C-Mn with high CE
IIW [2] [5] [27] [30]	1967	$CE_{IIW} = C + Mn/6 + (Cu+Ni)/15 + (Cr+Mo+V)/5$	C-Mn with high CE
Ito and Bessyo [2],[5],[27],[30]	1968	$P_{cm} = C + Si/30 + Mn/20 + Cu/20 + Ni/60 + Cr/20 + Mo/15 + V/10 + 5*B$	C ≤ 0.12 pipeline steels
Bastien [31]	1970	$CE_{Bastien} = C + Mn/4.4 + Ni/10.3 + Cr/15.4 + Mo/7.7$	CE calculating CR _{mBastien}
Beckert [3] [4]	1973	$CE_{Beckert} = C + Si/11 + Mn/2.9 + Ni/17 + Cr/3.2 + Mo/3.4 + Cu/3.9$	CE calculating HV _{mBeckert}
Stout [3] [27]	1976	$CE_{Stout} = C + Mn/6 + Ni/20 + (Cr+Mo)/10 + Cu/40$	C ≤ 0.12 pipeline steels
Stout [27]	1976	$CE_{StoutII} = 1000 * C * (Mn/6 + (Cr+Mo)/10 + Ni/20 + Cu/40)$	Adds C- alloy interaction
Graville [3] [27]	1976	$CE_{Graville} = C + Mn/16 - Ni/50 + Cr/23 + Mo/7 + Nb/8 + V/9$	C-Mn with high CE
Hannerz [31]	1980	$CE_{Hannerz} = C + Si/24 + Mn/10 + (Ni+Cu)/40 + Cr/5 + Mo/4 + V/10$	
Lorenz & Duren [3] [30]	1981	$CE_{psl} = C + Si/25 + Mn/16 + Cu/16 + Ni/60 + Cr/20 + Mo/40 + V/15$	Low carbon pipeline steels
Lorenz & Duren [3] [30]	1981	$CE_{eq} = C + Si/11 + Mn/8 + Cu/9 + Ni/17 + Mo/6 + V/3$	For estimating HV _b
PMPSA [32]	2009	$CE_{GE} = C + Mn/6 + Ni/20 + Cr/10 + Cu/40 + Mo/50 + V/10$	CE from GE
Proprietary [32]		$CE_{x2} = C + (Mn+Cr)/3 + (Si+Ni)/6 + Mo/2$	C-Mn with higher C
Yurioka et al. [3]	1981	$CE_{Yurioka} = C + (A_c) * (Si/24 + Mn/6 + (Cu+Ni)/15 + (Cr+Mo+Nb+V)/5 + 5*B)$	CE to cover the wide range of C content
Yurioka et al. [3]	1981	$A_c = 0.25 * (3 + ((1 - \exp(-40 * (C - 0.12))) / (1 + \exp(-40 * (C - 0.12)))))$	Factor for CE _{Yurioka}
Yurioka et al. [3]	1981	$CE_I = C + Si/24 + Mn/6 + Cu/15 + Ni/40 + Cr/6 + Mo/4 + (Nb+V)/5 + 10*B$	Calculate the H _{v-10}
Yurioka et al.[3]	1981	$CE_{II} = C - Si/30 + Mn/5 + Cu/5 + Ni/20 + Cr/4 + Mo/6 + 10*B$	Calculate the H _{v-10}

Yurioka et al. [3]	1983	$CEN = C + (0.75 + 0.25 * \arctan(20 * (C - 0.12))) * (Si/24 + Mn/6 + Cu/15 + Ni/20 + (Cr + Mo + Nb + V)/5 + 5 * B)$	Modified to have interaction of alloys with C
Yurioka et al. [33]	1987	$CE_{my} = C + Si/24 + Mn/6 + Cu/15 + Ni/12 + Mo/4 + Cr/8 + \Delta H$	For martensite
Yurioka et al. [33]	1987	$\Delta H = 0$ if $B \leq 1$ ppm, 0.03 if $B = 2$ ppm, 0.06 if $B = 3$ ppm, 0.09 if $B \geq 4$ ppm	CE_m factor for Boron
Yurioka et al. [33]	1987	$CE_{by} = C + Mn/3.6 + Cu/20 + Ni/9 + Cr/5 + Mo/4$	For $t_{8/5by}$ time for bainite
Yurioka et al. [33]	1987	$CE_{llby} = C + Si/24 + Mn/5 + Cu/10 + Ni/18 + Cr/5 + Mo/2.5 + V/5 + Nb/3$	For HV_{by} and HV_{fpy}
Yurioka et al. [33]	1987	$CE_{fpy} = C + 0.28 * Mn + 0.053 * Ni + 0.36 * Cr + 0.42 * Mo$	For ferrite-pearlite
Yurioka et al. [33]	1987	$CE_{fp100y} = C + 1.14 * Mn + 1.06 * Ni + 2.02 * Cr + 2.33 * Mo$	For 100% ferrite - pearlite
Uwer & Hohne [31]	1991	$CE_{UW} = C + Mn/10 + Cu/20 + Ni/40 + Cr/20 + Mo/10$	Lower effect of Mn
AWS D1.1 [5]	2010	$CE_{d1.1} = C + (Mn + Si)/6 + (Cr + Mo + V)/5 + (Ni + Cu)/15$	Used in steels for AWS D1.1
JWES [5]	2010	$CE_{wes136} = C + Mn/6 + Si/24 + Mo/29 + V/14$	C-Mn with higher C
Koch & Bersch [5]	2010	$CE_{KB} = C + (Mn + Mo + Ni + Cr + V + Cu + Si)/20$	$C \leq 0.12$ pipeline steels
Breadstreet [5]	2010	$CE_{Br} = C + Mn/20 + Ni/15 + (Cr + Mo + V)/10$	C-Mn with higher C
Cottrell [5]	2010	$CE_{Co} = C + Mn/6 + (Cr + Mo)/5 + V/3 + Nb/(4 * C) + 0.0001/S$	C-Mn with higher C
CET [5]	2010	$CET = C + (Mn + Mo)/10 + (Cu + Cr)/20 + Ni/40$	Lower carbon content
AWS [5]	2010	$CE_{aws} = C + Mn/4 + Ni/20 + (Cr + V)/10 + Cu/40 + Mo/50$	C-Mn with higher C
C_{HSLA} [5]	2010	$CE_{HSLA} = C + Mn/16 + Cr/23 + Mo/7 + Nb/5 + V/9 - Ni/50$	$C \leq 0.12$ pipeline steels
Talaş [5]	2010	$CE_{WM} = C + (Mn + Cr + V + Si)/6 + Mo/4 + Nb/9 + Ti/3 + Cu/20 + Ni/25 + 5 * B$	Analysis of CE formulations
Ideal critical diameter (DI)		DI to calculate the largest diameter that is fully martensitic with an infinite quench	
Grossman [7] [9]	1942	$DI_g = f(N_A) * f_C * f_{Si} * f_{Mn} * f_P * f_S * f_{Cu} * f_{Ni} * f_{Cr} * f_{Mo}$	Calculate hardenability
Holloman & Jaffe [22]	1945	$DI_{HJ} = f(N_A) * C^{1/2} * (1 + 0.64 * Si) * (1 + 4.10 * Mn) * (1 + 2.83 * P) * (1 - 0.62 * S) * (1 + 0.27 * Cu) * (1 + 0.52 * Ni) * (1 + 3.33 * Cr) * (1 + 3.14 * Mo) * f_B$	
ASTM A255 [15]		$DI_{A255} = 0.54 * C * (1 + 3.333 * Mn) * (1 + 0.7 * Si) * (1 + 0.33 * Ni + 0.066 Ni^2 - 0.55 Ni^3 + 0.18 Ni^4) * (1 + 2.16 * Cr) * (1 + 3 * Mo) * (1 + 0.365 * Cu) * (1 + 1.73 * V)$	
Proprietary		$DI_P = (0.56C + 0.0795) * (3.3331 * Mn + 1.0008) * (0.6993 * Si + 1.0006) * (0.3626 * Ni + 1.001) * (2.1605 * Cr + 0.999) * (3 * Mo + 1)$	
Ho [23]	1976	$DI_{C7}^2 = 0.9551 * C$	DI base N=7
Ho [23]	1976	$DI_{C8}^2 = 0.8240 * C$	DI base N=8

Ho [23]	1976	$DI_H = (0.8240 \cdot C)^{1/2} \cdot (1 + 0.2211 \cdot Si + 0.1280 \cdot Si^2) \cdot (1 + 0.2353 \cdot Mn + 0.5698 \cdot Mn^2) \cdot (1 + 1.634 \cdot Cr + 0.0270 \cdot Cr^2) \cdot (1 + 0.7671 \cdot Ni + 0.1229 \cdot Ni^2) \cdot (1 + 1.572 \cdot Mo + 0.5893 \cdot Mo^2) \cdot (1 + 1.176 \cdot Cu + 0.3339 \cdot Cu^2)$	
Dobrzanski & Sitek [20] [24]	1999	$DI_{BDS} = 0.6 \cdot (C)^{0.5} \cdot \exp(-0.816 \cdot N_A)$	Base DI
Moser & Legat [20]	1969	$DI_{M\&L} = DI_{BDS} \cdot 3.28^{Mo} \cdot 2.21^{Mn} \cdot 2.13^{Cr} \cdot 1.4^{Si} \cdot 1.47^{Ni}$	Modified version of Grossman
Mostert & Rooyen [20]	1991	$DI_{M\&R} = 46.5 \cdot C^{0.61} \cdot (2.0)^{Mn} \cdot (3.7 \cdot C^{0.43} \cdot (1 + Mo)^{-0.89})^{Cr} \cdot (C^{-0.74})^{Mo} \cdot (1.6 \cdot C^{0.07})^{Ni} \cdot (1.26)^{Si} \cdot 0.95^{NA}$	For carburizing grades
Hardness			
Dearden and O'Neill [1]	1940	$HV_{01} = 120 \cdot CE_{03} + 200$	Estimate HV max from CE_{03}
Beckert & Holz [4]	1973	$HV_{mBH} = 939 \cdot C + 284$	
Beckert [3]	1973	$HV_{mBeckert} = (A_B - B_B) \cdot \exp(-b_B \cdot t_{8/5}^2) + B_B$ where $A_B = 939 \cdot C + 284$, $B_B = 167 \cdot CE_{Beckert}^{2.42} + 137$, $b_B = \exp(-0.013 B_B + 0.8)$	
Seyffart [3]	1977	$H_{v-30} = 323.6 - 114.6 \cdot \ln \Delta t_{8/5} + 11.33 \cdot \ln \Delta t_{8/5}^2 + 123.7 \cdot \ln \Delta t_{8/5} \cdot CE_{Wes} - 15.88 \cdot \ln \Delta t_{8/5}^2 \cdot CE_{Wes} - 1299 \cdot C - 79.11 \cdot Si - 120.7 \cdot Mn + 79.22 \cdot Ni - 539 \cdot Cr + 2830 \cdot C \cdot Cr + 620.8 \cdot CE_{Wes} + 875.4 \cdot P_{cm}$	
Brisson et al. [50]	1972	$HV_{mBr} = 133 + 1066 \cdot C + 29 \cdot Si + 37.5 \cdot Mn + 15.5 \cdot Ni + 21.5 \cdot Cr + 23 \cdot \log(CR_V)$	Hardness martensite
Brisson et al. [50]	1972	$HV_{bBr} = 72 + 337 \cdot C + 68 \cdot Si + 63 \cdot Mn + 27 \cdot Ni + 62 \cdot Cr + 60 \cdot Mo + 64 \cdot V + 18 \cdot \log(CR_V)$	Hardness bainite
Maynier et.al. [46] [51]	1978	$HV_{mm} = 127 + 949 \cdot C + 27 \cdot Si + 11 \cdot Mn + 8 \cdot Ni + 16 \cdot Cr + 21 \cdot \log CR$	
Maynier et.al. [46] [51]	1978	$HV_{bm} = -323 + 185 \cdot C + 330 \cdot Si + 153 \cdot Mn + 65 \cdot Ni + 144 \cdot Cr + 191 \cdot Mo + \log CR \cdot (89 + 53 \cdot C - 55 \cdot Si - 22 \cdot Mn - 10 \cdot Ni - 20 \cdot Cr - 33 \cdot Mo)$	
Maynier et.al. [46] [51]	1978	$HV_{fpm} = 42 + 223 \cdot C + 53 \cdot Si + 30 \cdot Mn + 12.6 \cdot Ni + 7 \cdot Cr + 19 \cdot Mo + \log CR \cdot (10 - 19 \cdot Si + 4 \cdot Ni + 8 \cdot Cr + 130 \cdot V)$	
Maynier et.al. [46] [51]	1978	$HV_{mTm} = -74 - 434 \cdot C - 368 \cdot Si + 15 \cdot Mn + 37 \cdot Ni + 17 \cdot Cr - 335 \cdot Mo - 2235 \cdot V + 10^3 / Pa \cdot (260 + 616 \cdot C + 321 \cdot Si - 21 \cdot Mn - 35 \cdot Ni - 11 \cdot Cr + 352 \cdot Mo + 2345 \cdot V)$	
Maynier et.al. [46] [51]	1978	$HV_{bTm} = 262 + 163 \cdot C - 349 \cdot Si - 64 \cdot Mn - 6 \cdot Ni - 186 \cdot Cr - 458 \cdot Mo - 857 \cdot V + 10^3 / Pa \cdot (-149 + 43 \cdot C + 336 \cdot Si + 79 \cdot Mn + 16 \cdot Ni + 196 \cdot Cr + 498 \cdot Mo + 1094 \cdot V)$	
Satoh & Terasaki [22]	1979	$HV_{mST} = 812 \cdot C + 293$	Hardness martensite
Arata et al. [52]	1979	$HV_{mYK} = 835 \cdot C + 287$	Hardness martensite
Arata et al. [52]	1979	$HV_{bYK} = 500 \cdot (C - Mn/19 - Si/68 - Ni/45 + Cr/9 + Mo/9.9 + V/2.1 + B/0.48) + 153$	Hardness bainite
Lorenz & Duren [3] [30]	1981	$HV_{mpsl} = 802 \cdot C + 305$	CE_{psl} HV_m for martensite
Lorenz & Duren [3] [30]	1981	$HV_{bpsl} = 350 \cdot CE_{eq} + 101$	CE_{eq} HV_b for bainite
Lorenz & Duren [3] [30]	1981	$HV_{mbpsl} = 2019 \cdot (C \cdot (1 - 0.5 \cdot \log \Delta t_{8/5}) + 0.3 \cdot (CE_{eq} - C)) + 66 \cdot (1 - 0.8 \cdot \log \Delta t_{8/5})$	CE_{eq} HV_{mb} for m+b
Lorenz & Duren [3] [30]	1981	$HV_{cpsl} = 802 \cdot C - 452 \cdot C \cdot A_1 + 350 \cdot A_1 \cdot (CE_{eq} \cdot C) + 305 \cdot (1 - 0.67 \cdot A_1)$	HV for composition and cooling rate

Lorenz & Duren [3] [30]	1981	$A_I = (HV_{mpsl} - HV_{bpsl}) / (HV_{mpsl} - HV_{mbpsl})$	
Yurioka et al. [3] [22]	1981	$H_{v-10} = 406 \cdot C + 164 \cdot CE_I + 183 - (368 \cdot C - 149 \cdot CE_I + 100) \cdot \arctan((\log \Delta t_{8/5} - 2.822 CE_{II} + 0.262) / (0.526 - 0.195 \cdot CE_{II}))$	HV for composition and cooling rate
Leshie [4]	1982	$HV_{mL} = 1667 \cdot C - 926 \cdot C^2 + 150$	Hardness martensite
Suzuki [53]	1985	$HV_{maxs} = (884 \cdot C + 287 - (237 + 1633 \cdot C - 1157 \cdot P_{cm}) + (237 + 1633 \cdot C - 1157 \cdot P_{cm}) / (1 + \exp((566 + 5532 \cdot C - 2280 \cdot P_{cm}) \cdot (\log(t_{8/5}) + 0.03) \cdot 6 \cdot C - 7.77 \cdot P_{cm})))$	Maximum hardness
Yurioka et al. [33]	1987	$HV_{cy} = HV_m \cdot V_m + HV_b \cdot V_b + HV_{fp} \cdot V_{fp}$	HV from volume and HV_m , HV_b , HV_{fp}
Yurioka et al. [33]	1987	$HV_{my} = 884 \cdot C \cdot (1 - 0.3 \cdot C^2) + 294$	Hardness martensite
Okumura et al. [33]	1987	$HV_{by} = 197 \cdot CE_{IIby} + 117$	Hardness bainite
Yurioka et al. [33]	1987	$HV_{fpy} = 90.9 \cdot CE_{IIby} + 115$	Hardness ferrite-pearlite
Yurioka et al. [4]	1987	$HV_{byII} = 145 + 130 \cdot \tanh(2.65 \cdot CE_{IIby} - 0.69)$	Hardness bainite
Zaczek & Cwiek [53]	1987	$HV_{maxzc} = 442 \cdot C + 99 \cdot CE_{IIby} + 206 + (402 \cdot C - 90 \cdot CE_{IIby} + 80) \cdot \arctan(x_{zc})$	Maximum hardness
Zaczek & Cwiek [53]	1987	$x_{zc} = (\log(t_{8/5}) - 2.3 \cdot CE_{my} - 1.35 \cdot CE_{by} + 0.882) / (1.15 \cdot CE_{my} - 0.673 \cdot CE_{by} - 0.601)$	Factor for HV_{maxzc}
Nicholas & Abson [54]	2008	$HV_{mNA} = \frac{1}{2} \cdot (802 \cdot CE_{eq} + 305 + 406 \cdot C + 164 \cdot CE_I + 183 - (369 \cdot C - 149 \cdot CE_I + 100) \cdot \arctan((\log t_m - 2.822 \cdot CE_{II} + 0.262) / (0.526 + 0.195 \cdot CE_{II})))$	Lorenz & Duren ^{24-26,51} Martensite hardness
Nicholas & Abson [54]	2008	$HV_{bNA} = \frac{1}{2} \cdot (305 \cdot 406 \cdot CE_{eq} + 101 + C + 164 \cdot CE_I + 183 - (369 \cdot C - 149 \cdot CE_I + 100) \cdot \arctan((\log t_{8/5} - 2.822 \cdot CE_{II} + 0.262) / (0.526 + 0.195 \cdot CE_{II})))$	Lorenz & Duren ^{24-26,51} Bainite hardness
Mukherjee et al. [55]	2012	$\ln(HV_{c1}) = 7.1768 + 0.5719 \cdot C + 0.1516 \cdot Si + 0.0765 \cdot Mn + 0.1387 \cdot Cr - 0.0316 \cdot Mo - 0.4459 \cdot V + 0.3517 \cdot W + 0.6006 \cdot N + 0.0266 \cdot Ni + 0.2350 \cdot P + 0.9319 \cdot S - 6.6813 \cdot Ti + 0.1209 \cdot Cu - 1.1849 \cdot Nb - 0.0423 \cdot \ln(t(s)) - 0.0018 \cdot T(K)$	Regression for tempered HV
Mukherjee et al. [55]	2012	$\ln(HV_{c2}) = 8.4592 + 0.2417 \cdot C + 0.0092 \cdot Si - 0.0094 \cdot Mn + 0.0063 \cdot Cr + 0.0113 \cdot Mo - 0.0049 \cdot V + 0.0184 \cdot W - 0.0076 \cdot N + 0.0006 \cdot Ni - 0.0027 \cdot P - 0.0020 \cdot S - 0.0350 \cdot Ti + 0.0087 \cdot Cu + 0.0666 \cdot Nb - 0.0438 \cdot \ln(t(s)) - 0.0018 \cdot T(K)$	Regression for tempered HV
Trzaska [56]	2013	$HV_T = -86 + 492 \cdot C + 92 \cdot Mn + 69 \cdot Cr + 25 \cdot Ni + 102 \cdot Mo + 267 \cdot V + 0.064 \cdot T_A + 27.7 \cdot v_R^{0.25} - 38 \cdot F - 70 \cdot P - 32 \cdot B + 72 \cdot M$	
Trzaska [56]	2013	$P_F = \exp(K_F) / (1 + \exp(K_F))$, $F=0$ $P_F < 0.5$, $F=1$ $P_F > 0.5$	ferrite
Trzaska [56]	2013	$K_F = 17 - 20.9 \cdot C - 0.01 \cdot Mn - 2.3 \cdot Cr - 1.2 \cdot Ni - 7.4 \cdot Mo - 6.5 \cdot V - 1.5 \cdot v_R^{0.25}$	
Trzaska [56]	2013	$P_P = \exp(K_P) / (1 + \exp(K_P))$, $P=0$ $P_P < 0.5$, $P=1$ $P_P > 0.5$	pearlite
Trzaska [56]	2013	$K_P = 16 - 3.5 \cdot C - 4 \cdot Mn - 3.5 \cdot Cr - 1.5 \cdot Ni - 11.8 \cdot Mo - 1.7 \cdot V - 1.9 \cdot v_R^{0.25}$	
Trzaska [56]	2013	$P_B = \exp(K_B) / (1 + \exp(K_B))$, $B=0$ $P_B < 0.5$, $B=1$ $P_B > 0.5$	bainite
Trzaska [56]	2013	$K_B = 0.0015 - 2.54 \cdot C - 0.74 \cdot Mn - 0.3 \cdot Cr - 0.2 \cdot Ni - 2.3 \cdot Mo - 1.85 \cdot V - 0.018 \cdot v_R^{0.25}$	
Trzaska [56]	2013	$P_M = \exp(K_M) / (1 + \exp(K_M))$, $M=0$ $P_M < 0.5$, $M=1$ $P_M > 0.5$	martensite
Trzaska [56]	2013	$K_M = 10.9 - 1.7 \cdot C - 2.9 \cdot Mn - 3.7 \cdot Cr - 0.9 \cdot Ni - 3.7 \cdot Mo - 2.5 \cdot V - 1 \cdot v_R^{0.25}$	
Kurkin et al. [57]	2017	$HV_{fpk} = 105 + 310 \cdot C + 16 \cdot Mn - 140 \cdot Mo$	
Kurkin et al. [57]	2017	$HV_{bk} = 195 + 136 \cdot C + 29 \cdot Si + 35 \cdot Cr + 29 \cdot Ni + 132 \cdot V + 10 \cdot W + 173 \cdot Al$	

Kurkin et al. [57]	2017	$HV_{mk} = 289 + 792 \cdot C + 37 \cdot Si + 15 \cdot W$	
Kang & Lee [58]	2014	$P_{kl} = \log(t_{8/5}) + 17.396 - 6.661 \cdot C - 3.412 \cdot Si - 1.604 \cdot Mn - 0.248 \cdot Ni - 1.112 \cdot Cr - 4.355 \cdot Mo$	Parameter for tempered hardness
Kang & Lee [58]	2014	$HV_{TKL} = (1542.97 - 25.31/C) \cdot \exp(-1.23 \cdot 10^{-4} \cdot P_{kl})$	Tempered hardness
Hodge & Orehoski [23]	1946	$HRC_{99m} = 28.61 + 85.30 \cdot C - 39.15 \cdot C^2 - 14.49 \cdot C^3$	Hardness for 99% martensite
Hodge & Orehoski [23]	1946	$HRC_{95m} = 27.37 + 65.25 \cdot C + 13.47 \cdot C^2 - 49.38 \cdot C^3$	Hardness for 95% martensite
Hodge & Orehoski [23]	1946	$HRC_{90m} = 26.43 + 54.55 \cdot C + 37.03 \cdot C^2 - 65.24 \cdot C^3$	Hardness for 90% martensite
Hodge & Orehoski [23]	1946	$HRC_{80m} = 21.42 + 71.71 \cdot C - 12.17 \cdot C^2 - 27.45 \cdot C^3$	Hardness for 80% martensite
Hodge & Orehoski [23]	1946	$HRC_{50m} = 11.22 + 128.66 \cdot C - 169.5 \cdot C^2 + 94.96 \cdot C^3$	Hardness for 50% martensite
Hodge & Orehoski [20] [24] [25]	1946	$HRC_{mH\&O} = 35.4 + 7 \cdot C + 312.3 \cdot C^2 - 821.7 \cdot C^3 - 1015.5 \cdot C^4 - 538.4 \cdot C^5$	Hardness for martensite
Just [20] [29]	1969	$HRC_{JE} = 88 \cdot C^{0.5} - 0.0135 \cdot (E/1.5875)^2 \cdot C^{0.5} + 19 \cdot Cr + 6.3 \cdot Ni + 16 \cdot Mn + 35 \cdot Mo + 5 \cdot Si - 0.82 \cdot N - 20 \cdot (E/1.5875)^{0.5} + 2.11 \cdot E/1.5875 - 2$	HRC at Jominy position E (mm)
Just [20] [29]	1969	$HRC_{JE2} = 22 + 87 \cdot C + 16 \cdot Mn + 5.3 \cdot Ni + 14 \cdot Cr + 20 \cdot Mo - 21.2 \cdot E^{0.5} + 2.21 \cdot E$	$C < 0.28$
Just [20] [29]	1969	$HRC_{JE3} = 18 + 78 \cdot C + 21 \cdot Mn + 6.9 \cdot Ni + 22 \cdot Cr + 33 \cdot Mo - 30.3 \cdot E^{0.5} + 1.86 \cdot E$	$C > 0.29$
Just [20] [29]	1969	$HRC_{JE4} = -2 + 88 \cdot C^{0.5} + 16 \cdot Mn + 5 \cdot Si + 6.3 \cdot Ni + 19 \cdot Cr + 35 \cdot Mo - 0.0135 \cdot E^2 \cdot C^{0.5} - 20 \cdot E^{0.5} + 2.11 \cdot E - 0.82 \cdot N$	$E (1/16")$
Just [20] [29]	1969	$HRC_{JE5} = 33 + 52 \cdot C + 1.9 \cdot Mn + 1.4 \cdot Cr$	$E=1$
Just [20] [29]	1969	$HRC_{JE6} = -30 + 89 \cdot C + 24 \cdot Mn + 4.5 \cdot Si + 7.4 \cdot Ni + 23 \cdot Cr + 34 \cdot Mo$	$E=6$
Just [20] [29]	1969	$HRC_{JE7} = -29 + 74 \cdot C + 15 \cdot Mn + 5.2 \cdot Ni + 18 \cdot Cr + 21 \cdot V + 33 \cdot Mo$	$E=22$
Just [20] [29]	1969	$HRC_{JE8} = -7 + 98 \cdot C^{0.5} + 19 \cdot Mn + 6.4 \cdot Ni + 20 \cdot Cr + 28 \cdot V + 34 \cdot Mo - 0.025 \cdot E^2 \cdot C^{0.5} - 24 \cdot E^{0.5} + 2.86 \cdot E$	$E(1/16")$
Ho [23]	1976	$HRC_{J1} = 35.55 + 22.26 \cdot C + 177.5 \cdot C^2 - 305.1 \cdot C^3 + 132.6 \cdot C^4$	Hardness J1
Ho [23]	1976	$HRC_{J8} = HRC_{J1} / (1 + \exp(1.534 - 0.8597 \cdot DI_H))$	Hardness J8
Ho [23]	1976	$HRC_{J12} = HRC_{J1} / (1 + \exp(1.516 - 0.6507 \cdot DI_H))$	Hardness J12
Ho [23]	1976	$HRC_{J16} = HRC_{J1} / (1 + \exp(1.471 - 0.5444 \cdot DI_H))$	Hardness J16
Ho [23]	1976	$HRC_{J20} = HRC_{J1} / (1 + \exp(1.462 - 0.4814 \cdot DI_H))$	Hardness J20
Ho [23]	1976	$HRC_{J24} = HRC_{J1} / (1 + \exp(1.411 - 0.4192 \cdot DI_H))$	Hardness J24
Ho [23]	1976	$HRC_{J28} = HRC_{J1} / (1 + \exp(1.393 - 0.3798 \cdot DI_H))$	Hardness J28
Ho [23]	1976	$HRC_{J32} = HRC_{J1} / (1 + \exp(1.373 - 0.3578 \cdot DI_H))$	Hardness J32
Liscic & Filetin [66]	1988	$E_S = D^{0.718} / (5.11 \cdot H^{1.28})$	
Liscic & Filetin [66]	1988	$E_{3/4r} = D^{1.05} / (8.62 \cdot H^{0.668})$	
Liscic & Filetin [66]	1988	$E_{1/2r} = D^{1.16} / (9.45 \cdot H^{0.51})$	
Liscic & Filetin [66]	1988	$E_{1/4r} = D^{1.14} / (7.7 \cdot H^{0.44})$	
Liscic & Filetin [66]	1988	$E_C = D^{1.18} / (8.29 \cdot H^{0.44})$	
Canale, et.al. [65]	2008	$T_{TC} = 917 \cdot ((\ln((HRC_{qc}-8)/(HRC_t-8))/S_{rc})^{1/6} - 273$	
Canale, et.al. [65]	2008	$HRC_{qc} = S_{rc} \cdot (20 + 60 \cdot C^{0.5})$	
Canale, et.al. [65]	2008	$S_{rc} = HRC_q(\text{measured}) / HRC_q(\text{max calculated})$	
Smoljan et.al. [42] [43]	2011	$HRC_{q1} = (T_T/167 - 1.2) \cdot HRC_t - 17$	
Smoljan et.al. [42] [43]	2011	$HRC_{q2} = 8 + (HRC_t - 8) \cdot \exp(C \cdot (T_T/917)^6)$	

Strength Equations			
Suikkanen [62]	2009	$YS = S_{Fe} + S_{ss} + S_{ppt} + S_{gs} + S_{dis} + S_{text}$	strength factors
Suikkanen [62]	2009	$SS_{bSu} = 0*Cr + 84*Si + 33*Ni + 30*Al + 32*Mn + 38$	solid solution strengthening bainite
Baker [63]	2016	$SS_{MA} = 678*P + 83*Si + 32*Mn + 38*Cu + 11*Mn$	solid solution strengthening microalloyed
Shah, et al. [60]	2019	$SS_{bSh} = 1722.5*C^{0.5} + 85*Si + 32*Mn + 30*Mo - 30*Cr + 9*V$	solid solution strengthening bainite
McWilliam [1]	1918	$UTS_{o1} = 38,000 + 800*C + 100*Mn + 100*P$	Earliest for C-Mn-P steels
McWilliam [1]	1918	$UTS_{o2} = 38000 + (800 + 4*(C - 20)) + 120*Si + (100 + 2*(C - 20)) * Mn + 100*P$	Added Si and C-Mn interaction
Dearden and O'Neill [1]	1940	$UTS_{o3} = 16 + 40*CE_{o1} (\pm 2)$	UTS from CE
Walters [59]	1942	$UTS_{walters} = 3800 * (1 + 0.024*C) * (1 + 0.0009Mn + 0.00001*Mn^2) * (1 + 0.015*P) * (1 + 0.004*Si) * (1.07 - 0.22*PT + 0.01*PT^2)$	UTS for normalized steels
Soboslay & Dukelow [29]	1965	$UTS_{sd} = 476.1 + 581.9*C + 83.4*Mn + 535.2*P + 129.5*Si - 0.117*T_f$	Strength from composition (MPa)
Soboslay & Dukelow [29]	1965	$YS_{sd} = 533.1 + 249.1*C + 56.8*Mn + 268.7*P + 72.45*Si - 0.186*T_f$	Strength from composition (MPa)
Soboslay & Dukelow [29]	1965	$El(\% 8in.)_{sd} = -0.138 - 31.8*C - 3.10*Mn - 78.09*P - 13.3*Si + 0.020*T_f$	El from composition
Cahoon [37]	1971	$UTS_{ca} = (HV_t/2.9) * (n/0.217)^n$	
Cahoon [37]	1971	$YS_{ca} = (HV_t/3) * (0.1)^n$	
Defries [39]	1975	$YS_D = 4.226*HRC$	For YS 130-190 ksi
Callister [40]	2007	$UTS_{Ca} = 3.45*HBW$	
Custer [29]	1978	$UTS_{cu} = 142 + 774.9*C + 170*Mn + 370.9*P - 226.4*S + 216.5*Si + 50.97*Cu + 71.5*Ni + 204*Cr + 1776*V + 48.2*Mo$	Strength from composition (MPa)
Custer [29]	1978	$YS_{cu} = 120 + 319.2*C + 127.7*Mn + 131.7*P + 34.5*S + 196.9*Si + 37.6*Cu + 92.0*Ni + 174.3*Cr + 2426*V + 5.24*Mo$	Strength from composition (MPa)
Custer [29]	1978	$El_{cu} = 33.35 - 31.75*C - 3.6*Mn - 0.79*P + 6.11*S - 2.36*Si - 2.90*Cu - 0.10*Ni - 7.42*Cr + 14.22*V + 4.68*Mo$	El from composition
Seyffart & Kasatkin [64]	1979	$YS_{fp} = 187 + 92*C + 47*Mn + 90*V$	
Seyffart & Kasatkin [64]	1979	$YS_m = 602 * 2150*C + 500*Mo$	
Seyffart & Kasatkin [64]	1979	$YS_b = 500 + 460*C - 120*C^2 + 150*V + 360*Mo$	
Seyffart & Kasatkin [64]	1979	$UTS_{fp} = 297 + 1360*C + 60*Mn + 140*V$	
Seyffart & Kasatkin [64]	1979	$UTS_m = 798 * 3215*C$	
Seyffart & Kasatkin [64]	1979	$UTS_b = 590 + 960*C + 39.7*Mn + 200*V$	
Seyffart & Kasatkin [64]	1979	$El_{fp} = 36.5 - 127*C + 135*C^2 - 1.16*Mn + 8.0*V + 0.66* \ln(t_{8/5})$	
Seyffart & Kasatkin [64]	1979	$El_m = 12.267*C^2 - 1.5*Mn + 0.76* \ln(t_{8/5})$	
Seyffart & Kasatki [64]	1979	$El_b = 21.3 - 35.6*C - 4.0*Mn - 5.0*V + 1.84* \ln(t_{8/5})$	
Seyffart & Kasatkin [64]	1979	$RA_{fp} = 65.4 - 88*C - 82*C^2 - 6.7*Mn + 18*V + 0.6* \ln(t_{8/5})$	
Seyffart & Kasatkin [64]	1979	$RA_m = 48.5 - 158*C + 116*C^2 - 0.98* \ln(t_{8/5})$	

Seyffart & Kasatkin [64]	1979	$RA_b = 53.3 - 132 \cdot C + 103 \cdot C^2 - 5.1 \cdot Mn - 10 \cdot V + 3.4 \cdot \ln(t_{8/5})$	
Svensson [41]	1994	$YS_{Sv} = 3.3 \cdot HV \cdot (0.1)^n$	
Svensson [41]	1994	$YS_{Svw} = 3.1 \cdot HV \cdot (0.1)^n - 80$	
Svensson [41]	1994	$n_s = 0.065 \cdot (t_{8/5})^{0.17}$	
Smoljan et.al. [42] [43]	2018	$UTS_{smoljan} = 3.3 \cdot HV$	
Smoljan et.al. [42] [43]	2018	$YS_{smoljan1} = (0.8 + 0.1 \cdot (HRC_t/HRC_q)) \cdot UTS + 170 \cdot (HRC_t/HRC_q) - 200$	
Smoljan et.al. [42] [43]	2006	$YS_{smoljan2} = (0.24 + 0.03 \cdot HV_q/HV_m) \cdot HV_a + 170 \cdot HV_q/HV_m - 200$	
Smoljan et.al. [42] [43]	2011	$El_{smoljan} = 46 - (0.04 - 0.012 \cdot C) \cdot YS$	
Smoljan et.al. [42] [43]	2011	$RA_{smoljan} = 96 - (0.062 - 0.029 \cdot C) \cdot YS$	
Pavlina&Vantyne [37]	2008	$YS_{PVa} = -90.7 + 2.876 \cdot HV$	All steels
Pavlina&Vantyne [37]	2008	$UTS_{PVa} = -99.8 + 3.734 \cdot HV$	All steels
Pavlina&Vantyne [37]	2008	$YS_{Pvm} = 110.9 + 2.507 \cdot HV$	martensitic
Pavlina&Vantyne [37]	2008	$UTS_{Pvm} = -273.6 + 4.279 \cdot HV$	martensitic
Pavlina&Vantyne [37]	2008	$YS_{PVnm} = -84.8 + 2.646 \cdot HV$	Not martensitic
Pavlina&Vantyne [37]	2008	$UTS_{PVnm} = 2.5 + 3.339 \cdot HV$	Not martensitic
Pavlina&Vantyne [37]	2008	$YS_{PVls} = 15.3 + 2.860 \cdot HV$	Low UTS&YS
Pavlina&Vantyne [37]	2008	$UTS_{PVls} = 10.9 + 3.150 \cdot HV$	Low UTS&YS
Pavlina&Vantyne [37]	2008	$YS_{PVms} = -70.5 + 2.736 \cdot HV$	Mid UTS&YS
Pavlina&Vantyne [37]	2008	$UTS_{PVms} = -99.8 + 3.800 \cdot HV$	Mid UTS&YS
Pavlina&Vantyne [37]	2008	$YS_{PVhs} = -94.8 + 2.466 \cdot HV$	High UTS&YS
Pavlina&Vantyne [37]	2008	$UTS_{PVhs} = -205.7 + 4.410 \cdot HV$	High UTS&YS
Cao et al. [44]	2012	$UTS_{Cao} = 3.3 \cdot HV$	
Cao et al. [44]	2012	$YS_{Cao} = 0.8 \cdot UTS + 170 \cdot HV_a/HV_m - 200$	
Heat Treat Equations			
Holloman & Jaffe [65]	1945	$P_h = T_T \cdot (C_c + \log t_T) / 1000$	Tempering parameter
Fullman [65]	1954	$F_p = \log t_T - (14030/T_T)$	Tempering parameter
Totten et. al. [67]	2004	$C_{ct} = 21 - (5.8 \cdot C)$	Tempering constant
Gulvin et. al. [65]	1972	$t_{Teq} = T_T / (2.3 \cdot R_{c-h} \cdot (20 - \log R_{c-h}))$	Added time in tempering for heating- cooling
Wever et al.	1954	$t_{MP} = \exp(7.54 \cdot CE_{MP} - 4.19)$	Time to form martensite
Bastien [31]	1970	$\ln(CR_{mBastien}) = 13.9 - 10.6 \cdot CE_{Bastien}$	cooling rate martensite
Brisson et al. [50]	1972	$\log(CR_{V1}) = 3 - (4.62 \cdot C + 1.05 \cdot Mn + 0.54 \cdot Ni + 0.50 \cdot Cr + 0.66 \cdot Mo)$	Cooling rate for martensite
Brisson et al. [50]	1972	$\log(CR_{V1(50)}) = 2.4 - (4.13 \cdot C + 0.8 \cdot Mn + 0.57 \cdot Ni + 0.41 \cdot Cr + 0.94 \cdot Mo)$	Cooling rate for 50/50 martensite/bainite
Brisson et al. [50]	1972	$\log(CR_{V2}) = 1.9 - (3.8 \cdot C + 1.07 \cdot Mn + 0.7 \cdot Ni + 0.57 \cdot Cr + 1.58 \cdot Mo)$	Cooling rate for bainite
Maynier et.al. [46] [51]	1978	$Pa = (1/T(^{\circ}K) - nR/H \cdot \log(t_{hr}))^{-1}$ Where n is naperian log of 10 ≈ 2.3 , R universal gas constant, 2, H is activation energy, 110 kcal/mole	Austenitizing parameter
Maynier et.al. [46] [51]	1978	$\log CR_{m100} = 9.81 - (4.62 \cdot C + 1.05 \cdot Mn + 0.54 \cdot Ni + 0.50 \cdot Cr + 0.66 \cdot Mo + 0.00183 \cdot Pa)$	cooling rate 100% martensite
Maynier et.al. [46] [51]	1978	$\log CR_{m90} = 8.76 - (4.04 \cdot C + 0.97 \cdot Mn + 0.49 \cdot Ni + 0.58 \cdot Cr + 0.97 \cdot Mo + 0.0010 \cdot Pa)$	cooling rate 90% martensite

Maynier et.al. [46] [51]	1978	$\text{Log CR}_{m50} = 8.50 - (4.12 \cdot C + 0.86 \cdot \text{Mn} + 0.57 \cdot \text{Ni} + 0.41 \cdot \text{Cr} + 0.94 \cdot \text{Mo} + 0.0012 \cdot \text{Pa})$	cooling rate 50% martensite
Maynier et.al. [46] [51]	1978	$\text{Log CR}_{b100} = 10.17 - (3.80 \cdot C + 1.07 \cdot \text{Mn} + 0.70 \cdot \text{Ni} + 0.57 \cdot \text{Cr} + 1.58 \cdot \text{Mo} + 0.0032 \cdot \text{Pa})$	cooling rate 100% bainite
Maynier et.al. [46] [51]	1978	$\text{Log CR}_{b90} = 10.55 - (3.65 \cdot C + 1.08 \cdot \text{Mn} + 0.77 \cdot \text{Ni} + 0.61 \cdot \text{Cr} + 1.60 \cdot \text{Mo} + 0.0032 \cdot \text{Pa})$	cooling rate 90% bainite
Maynier et.al. [46] [51]	1978	$\text{Log CR}_{b50} = 8.74 - (2.23 \cdot C + 0.86 \cdot \text{Mn} + 0.56 \cdot \text{Ni} + 0.59 \cdot \text{Cr} + 1.60 \cdot \text{Mo} + 0.0032 \cdot \text{Pa})$	cooling rate 50% bainite
Maynier et.al. [46] [51]	1978	$\text{Log CR}_{fp100} = 6.36 - (0.43 \cdot C + 0.49 \cdot \text{Mn} + 0.78 \cdot \text{Ni} + 0.27 \cdot \text{Cr} + 0.38 \cdot \text{Mo} + 2 \cdot \text{Mo}^{0.5} + 0.0019 \cdot \text{Pa})$	cooling rate 100% ferrite-pearlite
Maynier et.al. [46] [51]	1978	$\text{Log CR}_{fp90} = 7.51 - (1.38 \cdot C + 0.35 \cdot \text{Mn} + 0.93 \cdot \text{Ni} + 0.11 \cdot \text{Cr} + 2.31 \cdot \text{Mo} + 0.0033 \cdot \text{Pa})$	cooling rate 90% ferrite-pearlite
Arata et al. [52]	1979	$\text{Log} (t_{8/5mYK}) = 5.9 \cdot (C + \text{Mn}/19 + \text{Si}/14 + \text{Ni}/37 + \text{Cr}/19 + \text{Mo}/9.1 + \text{V}/49 + \text{B}/0.31) - 1.13$	Yurioka et al. ⁵⁴ martensite
Arata et al. [52]	1979	$\text{Log} (t_{8/5bYK}) = -0.2 \cdot (C - \text{Mn}/4.3 - \text{Si}/0.4 - \text{Ni}/0.58 + \text{Cr}/0.45 - \text{Mo}/0.4 - \text{V}/240 - \text{B}/0.0020) + 1.60$	Yurioka et al. ⁵⁴ bainite
Kasatkin & Seyffart [64]	1984	$\text{Log}(t_{8/5bks}) = -1.8 + 28.3 \cdot C + 17.1 \cdot \text{Mn} - 59.6 \cdot \text{Si} - 20 \cdot \text{Cr} + 13.2 \cdot \text{Ni} + 0.1 \cdot \text{Mo} - 5.3 \cdot \text{V} + 47.0 \cdot \text{Nb} - 289.6 \cdot C^2 - 3.7 \cdot \text{Mn}^2 + 65.4 \cdot \text{Si}^2 + 38.6 \cdot \text{Cr}^2 - 7.0 \cdot \text{Ni}^2 - 21.0 \cdot \text{Mo}^2 - 9.8 \cdot C \cdot \text{Mn} - 19.5 \cdot \text{Mn} \cdot \text{Si} + 232.1 \cdot C \cdot \text{Si}$	bainite
Kasatkin & Seyffart [64]	1984	$\log (t_{8/5fks}) = 5.8 \cdot (C + \text{Si}/291 + \text{Mn}/14 + \text{Ni}/67 + \text{Cr}/16 + \text{Mo}/6 + \text{V}/425) - 0.83$	ferrite
Kasatkin & Seyffart [64]	1984	$\log (t_{8/5pks}) = 5.14 \cdot (C + \text{Si}/17 + \text{Mn}/19 + \text{Ni}/25 + \text{Cr}/16 + \text{Mo}/4 + \text{V}/3) + 0.06$	pearlite
Yurioka et al. [33]	1987	$\ln (t_{8/5my}) = 10.6 \cdot \text{CE}_{my} - 4.8$	time 800-500°C for martensite
Yurioka et al. [33]	1987	$\ln (t_{8/5by}) = 6.2 \cdot \text{CE}_{by} + 0.87$	time 800-500°C for bainite
Yurioka et al. [33]	1987	$\ln (t_{8/5fpy}) = 8.74 \cdot \text{CE}_{fpy} - 0.19$	time 800-500°C for ferrite-pearlite
Yurioka et al. [33]	1987	$\ln (t_{8/5fp100y}) = 0.99 \cdot \text{CE}_{fp100y} + 4.5$	time 800-500°C for 100% ferrite-pearlite
Yurioka et al. [33]	1987	$V_m = 0.5 - 0.455 \cdot \arctan(4 \cdot ((\log(t_{8/5}/t_{8/5my})/(\log(t_{8/5by}/t_{8/5my}))^{-2}))$	Volume of martensite
Yurioka et al. [33]	1987	$V_{fp} = 0.5 - 0.455 \cdot \arctan(4 \cdot ((\log(t_{8/5}/t_{8/5fpy})/(\log(t_{8/5fp100y}/t_{8/5fpy}))^{-2}))$	Volume of ferrite- pearlite
Yurioka et al. [33]	1987	$V_b = 1 - V_m - V_{fp}$	Volume of bainite
Nicholas & Abson [54]	2008	$\log (t_{8/5mNA}) = (611.3 \cdot C + 605.7 \cdot \text{CE}_{eq} - 239)/(1009.5 \cdot C + 52.8)$	Lorenz & Duren ^{24-26,51} time 800-500°C for martensite
Nicholas & Abson [54]	2008	$\log (t_{8/5bNA}) = (1413.3 \cdot C + 300.7 \cdot \text{CE}_{eq} - 35)/(1009.5 \cdot C + 52.8)$	Lorenz & Duren ^{24-26,51} time 800-500°C for bainite
Miettinen et al. [68]	2019	$\log (t_{8/5F}) = 6.253 - 5.471 \cdot C - 0.149 \cdot \text{Si} - 0.380 \cdot \text{Mn} - 1.222 \cdot \text{Cr} - 2.647 \cdot \text{Mo} - 0.271 \cdot \text{Ni} + 4.122 \cdot C^2 - 0.717 \cdot C \cdot \text{Si} + 0.059 \cdot C \cdot \text{Mn} - 0.664 \cdot C \cdot \text{Cr} + 0.082 \cdot C \cdot \text{Mo} - 0.582 \cdot C \cdot \text{Ni} + 0.040 \cdot \text{Si}^2 + 0.306 \cdot \text{Si} \cdot \text{Mn} + 0.819 \cdot \text{Si} \cdot \text{Cr} + 1.212 \cdot \text{Si} \cdot \text{Mo} + 0.042 \cdot \text{Si} \cdot \text{Ni} - 0.179 \cdot \text{Mn}^2 + 0.237 \cdot \text{Mn} \cdot \text{Cr} - 0.412 \cdot \text{Mn} \cdot \text{Mo} - 0.069 \cdot \text{Mn} \cdot \text{Ni} + 0.079 \cdot \text{Cr}^2 + 0.491 \cdot \text{Cr} \cdot \text{Mo} - 0.025 \cdot \text{Cr} \cdot \text{Ni} + 0.355 \cdot \text{Mo}^2 - 0.110 \cdot \text{Mo} \cdot \text{Ni} - 0.013 \cdot \text{Ni}^2 - 0.00200 \cdot P_A$	
Miettinen et al. [68]	2019	$\log (t_{8/5P}) = 6.031 - 1.843 \cdot C - 0.857 \cdot \text{Si} - 1.310 \cdot \text{Mn} - 1.398 \cdot \text{Cr} - 4.430 \cdot \text{Mo} - 0.689 \cdot \text{Ni} + 0.949 \cdot C^2 + 0.562 \cdot C \cdot \text{Si} - 0.148 \cdot C \cdot \text{Mn} + 1.105 \cdot C \cdot \text{Cr}$	

		$+1.517 \cdot C \cdot \text{Mo} - 0.067 \cdot C \cdot \text{Ni} + 0.026 \cdot \text{Si}^2$ $+ 0.453 \cdot \text{Si} \cdot \text{Mn} - 0.104 \cdot \text{Si} \cdot \text{Cr} + 1.052 \cdot \text{Si} \cdot \text{Mo} -$ $0.775 \cdot \text{Si} \cdot \text{Ni} + 0.186 \cdot \text{Mn}^2 + 0.097 \cdot \text{Mn} \cdot \text{Cr} -$ $0.270 \cdot \text{Mn} \cdot \text{Mo} + 0.306 \cdot \text{Mn} \cdot \text{Ni} + 0.094 \cdot \text{Cr}^2 -$ $0.717 \cdot \text{Cr} \cdot \text{Mo} + 0.183 \cdot \text{Cr} \cdot \text{Ni} + 0.809 \cdot \text{Mo}^2 -$ $0.339 \cdot \text{Mo} \cdot \text{Ni} - 0.003 \cdot \text{Ni}^2 - 0.00227 \cdot P_A$	
Hume-Rothery Alloy Formulation rules			
Wang, et al. [61]	2015	$\gamma_{\text{mix}} = (1 - ((r_s + r_{\text{avg}})^2 - r_{\text{avg}}^2) / (r_s + r_{\text{avg}})^2) / (1 - ((r_L + r_{\text{avg}})^2 - r_{\text{avg}}^2) / (r_L + r_{\text{avg}})^2)$	Measure of atomic radius difference
Fang, et al. [61]	2003	$\Delta\chi_{\text{mix}} = (C_{\text{at}\%} \cdot (\chi_C - \chi_{\text{avg}})^2 + (Mn_{\text{at}\%} \cdot (\chi_{\text{Mn}} - \chi_{\text{avg}})^2 + (Si_{\text{at}\%} \cdot (\chi_{\text{Si}} - \chi_{\text{avg}})^2 + (Cr_{\text{at}\%} \cdot (\chi_{\text{Cr}} - \chi_{\text{avg}})^2 \dots)^{0.5}$	Measure of atomic radius difference
Zhang, et al. [61]	2008	$\delta_{\text{mix}} = (C_{\text{at}\%} \cdot (1 - r_C / (r_{\text{avg}})^2 + (Mn_{\text{at}\%} \cdot (1 - r_{\text{Mn}} / (r_{\text{avg}})^2 + (Si_{\text{at}\%} \cdot (1 - r_{\text{Si}} / (r_{\text{avg}})^2 + (Cr_{\text{at}\%} \cdot (1 - r_{\text{Cr}} / (r_{\text{avg}})^2 \dots)^{0.5}$	Measure of atomic radius difference
Swalin [61]	1991	$\Delta S_{\text{mix}} = -R (C_{\text{at}\%} \cdot \ln C_{\text{at}\%} + Mn_{\text{at}\%} \cdot \ln Mn_{\text{at}\%} + Si_{\text{at}\%} \cdot \ln Si_{\text{at}\%} + Cr_{\text{at}\%} \cdot \ln Cr_{\text{at}\%} \dots)$	Entropy of mixing
Zhang, et al. [61]	2008	$\Delta H_{\text{mix}} = 4 \cdot \Delta H_{\text{AB}} \cdot A_{\text{at}\%} \cdot B_{\text{at}\%} \quad \text{note } (\Delta H_{\text{AB}} \text{ of AB equiatomic mixes})$	Energy of mixing
Guo, et al. [61]	2011	$\text{VEC}_{\text{mix}} = C_{\text{at}\%} \cdot \text{VEC}(C) + Mn_{\text{at}\%} \cdot \text{VEC}(Mn) + Si_{\text{at}\%} \cdot \text{VEC}(Si) + Cr_{\text{at}\%} \cdot \text{VEC}(Cr) \dots$	

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