

# Integrated Computational Materials Engineering and Artificial Intelligence for Sustainable Casting Industry

**Alan A. Luo<sup>1, \*</sup>, Diran Apelian<sup>2</sup>**

1. Advanced Casting Research Center, The Ohio State University, Columbus, OH 43210, USA

2. Advanced Casting Research Center, University of California, Irvine, CA 92697, USA

\*Corresponding address: e-mail: luo.445@osu.edu

**Abstract:** The global metal casting industry is facing enormous sustainability and regulatory challenges related to carbon reduction and carbon neutrality. Digital design and manufacturing of metal castings, enabled by integrated computational materials engineering (ICME) technologies and the recent boom in artificial intelligence and machine learning (AI/ML), provide great opportunities for the industry to overcome these challenges. This presentation provides some examples of cast alloy design and process innovations using the ICME approach. The talk will also present application cases of AI/ML tools to support casting quality control and property prediction. We will also discuss future opportunities to combine ICME and AI/ML tools to revitalize and revolutionize the metal casting industry for sustainable growth.

**Keywords:** metal casting; sustainability; integrated computational materials engineering (ICME); artificial intelligence (AI); machine learning (ML)

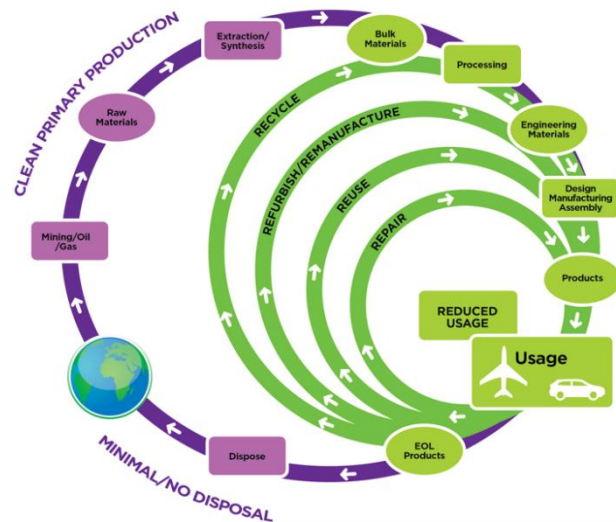
## 1 Introduction

Materials and manufacturing industries including metal casting are the backbone of global economies but also a climate liability, thus making their decarbonization a key priority for carbon mitigation strategies. To achieve the Paris Climate Agreement goal of reaching climate neutrality by 2050, major economies including the United States, China, and European Union have announced ambitious emission reduction commitments. Therefore, the global casting industry is facing enormous regulatory and sustainability challenges related to carbon emission reduction, as its customers in all sectors especially the automotive industry are transitioning to clean energy and sustainable production. Presently, a large portion of the industrial emissions comes from the production of iron and steel (24%) and aluminum (3%). However, the recycling rates for these metals are astonishingly low, 45% for steel and 30% for aluminum. Increasing the circularity of these nonrenewable metals and reducing energy consumption in manufacturing activities would significantly contribute to a carbon-neutral society and a circular economy. Figure 2 shows a vision of material circularity and sustainability which can be achieved by 1) reduced/prolonged usage via better material design and manufacturing/energy efficiency; 2) increased repair,

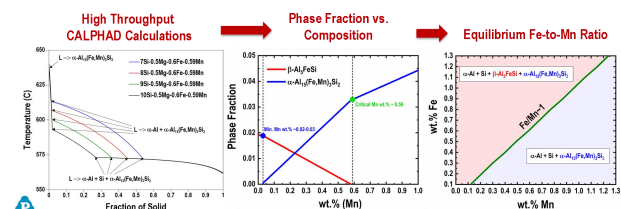
reuse, refurbish, remanufacturing and recycling; 3) limited but clean primary material production; and 4) minimal or no disposal of non-renewable materials.

## 2 Integrated computational materials engineering

Integrated computational materials engineering (ICME) is defined as the integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing-process simulation. Figure 2 shows a CALPHAD-based ICME approach for designing secondary (recycled) aluminum alloys for structural die casting applications.



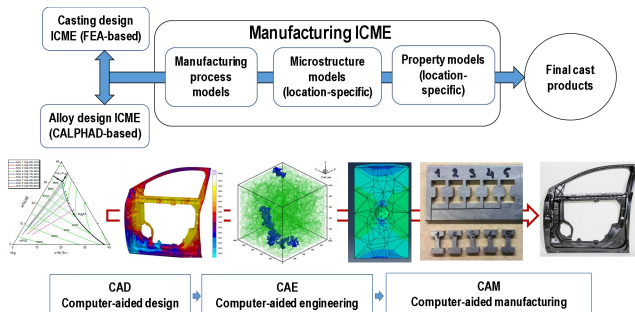
**Figure 1 Vision of material circularity and manufacturing sustainability (modified, based on [1])**



**Figure 2 CALPHAD-based approach for alloy design [2]**

In the last few decades, casting simulation and digital manufacturing tools have been increasingly used in the

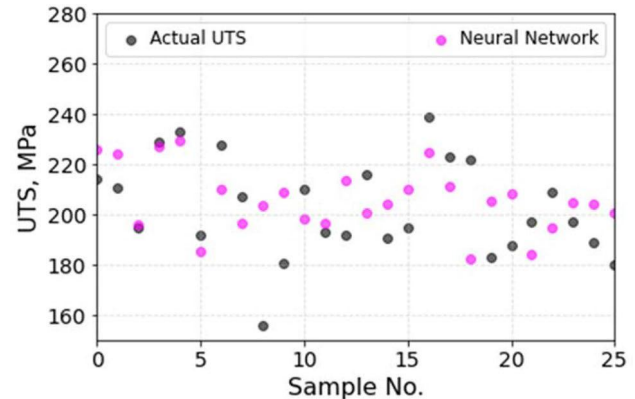
industry as part of product development process, based on computer-aided design (CAD), computer-aided engineering (CAE), and computer-aided manufacturing (CAM). As shown in Figure 3, ICME is a relatively new approach based on location-specific microstructure and property models predictions, as opposed to the current CAD/CAE/CAM approach largely using uniform material properties. These ICME models, based on computational thermodynamics, kinetics and process models, can provide further mass and cost savings as well as improved quality/efficiency. The recent development of large thin-wall die casting (giga-casting), using ICME tools, will enhance the sustainability of the metal casting industry.



**Figure 3 ICME framework for casting design and process development<sup>[3]</sup>**

### 3 Artificial intelligence and machine learning

Artificial intelligence (AI), including machine learning (ML), is a broad term defined as a “system that can, for a given set of objectives, generate outputs such as predictions, recommendations or decisions influencing real or virtual environments” <sup>[4]</sup>. These systems use data and human-built algorithms to simulate how humans perceive, learn and respond to questions and prompts. Metal casting processes such as high-pressure die casting can generate extensive datasets, which can be used to train deep ML algorithms to model the prediction of good parts and process scrap as determined by a die-casting machine. Additionally, neural network ML models can be used to predict the ultimate tensile strength (UTS) of die castings (Figure 4). Future applications of AI/ML in metal casting include defect control, predictive maintenance, and supply chain logistics. AI/ML and ICME tools can be combined to co-design of alloys, processes and topology for multi-objective optimization of sustainable castings.



**Figure 4 Actual UTS testing data vs. the values predicted by the Neural Network model of die castings<sup>[5]</sup>**

### 4 Conclusion

Metal casting has a long history but is presently facing technical and social challenges related to carbon footprint. It is imperative to use recycled alloys in the industry, embracing the circular material concept. To overcome these challenges, the casting industry needs to utilize new ICME and AI/ML tools to improve its efficiency and reduce energy consumption. Opportunities also exist in transportation industries as they migrate to clean energy technologies will require lightweight and high-performance castings.

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