

Physics-Guided AI Co-Design and Control to Minimize Shrinkage and Gas Porosity in Metal Castings

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Article Info

Article history:

Received June 21, 2026

Revised July 25, 2026

Accepted August 17, 2026

Keywords:

Metal Casting,
Shrinkage Porosity,
Solidification Modeling,
Adaptive Process Control

ABSTRACT

Porosity in metal castings—caused by shrinkage during solidification, entrained air, and dissolved gases—remains one of the most persistent quality challenges in foundry engineering. This paper presents a hybrid, physics-guided artificial intelligence (AI) framework that combines predictive modeling, inverse design, and real-time control to minimize shrinkage and gas-related porosity. The system integrates solidification physics and process data through a 3D neural architecture that distinguishes porosity mechanisms, predicts their spatial distribution, and recommends corrective design or process measures. Bayesian optimization and reinforcement learning are applied for process tuning and adaptive control. Experimental validation on Al-Si castings shows a 40% reduction in total porosity through inverse design and an additional 25% improvement with real-time control. The framework demonstrates the synergy between physics-based reasoning and AI learning for intelligent defect prevention in modern foundries.

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1. Introduction

Porosity defects in metal castings significantly affect structural integrity, fatigue resistance, and leak-tightness. These defects are commonly categorized into:

- Shrinkage porosity, resulting from inadequate feeding during solidification;
- Gas porosity, caused by entrained air or hydrogen solubility exceeding equilibrium limits;
- Mixed porosity, where both mechanisms interact under dynamic thermal and flow conditions.

Conventional simulation tools like MAGMASoft and ProCAST can predict such defects but require extensive setup and rely on deterministic assumptions. Moreover, process variations—such as pour temperature, melt chemistry, or gating turbulence—introduce uncertainty that traditional methods fail to control adaptively.

Artificial intelligence offers new capabilities for predicting and controlling complex, nonlinear interactions, and autonomously optimizing designs. However, purely data-driven approaches lack physical interpretability and often ignore the fundamental physics of solidification and gas evolution.

Therefore, this paper introduces a physics-guided AI framework that combines deep learning, digital twins, and real-time feedback control to predict, prevent, and correct porosity in castings by merging data-driven learning with metallurgical physics (Deng et al., 2019; Gao et al., 2019; Kiangala & Wang, 2021; Nieves et al., 2025).

2. Literature Review

Research in porosity control has traditionally focused on:

- Simulation-based prediction, leveraging solidification models and Niyama criteria for shrinkage prediction.
- Empirical optimization, adjusting process parameters using design of experiments (DOE).
- Data-driven modeling approaches, such as neural networks predicting porosity rate based on melt temperature, pouring speed, and gas content.

However, few works integrate physics-informed neural networks (PINNs) or reinforcement learning (RL) for

adaptive porosity control. Recent studies show improved performance using hybrid approaches, but limited explainability and control adaptability remain gaps this study aims to bridge (Bhagwat et al., 2024; Stefanescu, 2015). This gap motivates the present research: merging physics-based interpretability with AI-driven adaptability (Alajmi & Almeshal, 2020; Janardhan, 2015; Wickham et al., 2019; Zitzler & Thiele, 1998).

2.1 Porosity Mechanisms & Metallurgical Foundations

Porosity in castings is commonly attributed to two interacting mechanisms: solidification shrinkage and gas-related porosity (entrained air, hydrogen saturation). Theoretical and experimental works have characterized hydrogen solubility, supersaturation, pore nucleation and growth kinetics, and how turbulence, gating, and feeding geometry influence pore evolution. These foundational studies reinforce the importance of modeling both shrinkage and gas phenomena together rather than separately (Makadia & Nanavati, 2013; Song et al., 2020).

2.2 Classical Simulation & Hot-Spot Modeling

Industrial foundry practice frequently relies on hot-spot analysis, feeding distance maps, and criteria such as the Niyama index to preempt shrinkage porosity. Although useful, these criteria require manual tuning per alloy and are brittle to real-world variability in pouring conditions and mold heterogeneity. Such limitations motivate data-corrective or adaptive augmentations to classical methods (Ivanina et al., 2022; Vijayaram et al., 2006).

2.3 Deep Learning / CT-Based Defect Segmentation

High-resolution computed tomography (CT) has become a reference standard for quantifying pore morphology in castings. Recent works in aluminum die casting demonstrate automated porosity segmentation using radiography, synthetic augmentation, and machine learning models—offering voxel-level pore maps and statistical summaries. This supports supervised learning architectures that can differentiate pore types (gas vs shrinkage) via morphological features.

Example: Bosse et al. (2024), “*Automated Porosity Characterization for Aluminum Die Casting Materials Using X-ray Radiography...*”

2.4 Machine Learning in Foundry / Defect Prediction

In foundries adopting Industry 4.0 practices, supervised ML models analyze sensor and process data to predict defect occurrence. For example, in low-pressure die casting (LPDC) of aluminum wheels, classification techniques (XGBoost, etc.) have been used to flag porosity defects, with feature-importance analyses revealing key contributing process variables.

Uyan et al. (2023), “*Industry 4.0 Foundry Data Management and Supervised Machine Learning in Low-Pressure Die Casting Quality Improvement*”

Also, broader surveys of ML in metal casting show growing usage of regression/ML to predict yield, defect rate, and optimize inputs (temperature, flow rate, gating) — though often lacking mechanistic insight.

2.5 Digital Twin & AI in Casting

Digital twin architectures that combine physical models with live data are emerging in foundries. One recent study applies an AI-based digital twin in an investment casting plant to predict rejection rate and mechanical properties, validating that data + model fusion can reduce defect rates.

Furthermore, in additive manufacturing, multiscale, multiphysics digital twins are already valued for combining predictive fidelity with adaptability to real-time deviations—pointing to analogous opportunities in casting (Nguyen et al., 2015; Pal et al., 2018).

2.6 Physics-Informed Learning & Neural Operators

Physics-informed neural networks (PINNs) and related architectures embed governing PDEs (e.g., heat conduction, mass transport) into the learning objective, improving generalization and data efficiency. PINNs have been applied to solid mechanics, stress–strain problems, and material fields.

- Bai et al. (2023) propose a PINN with an LSWR loss function for 2D/3D solid mechanics that robustly predicts displacement and stress fields.
- The Finite-PINN architecture extends PINNs into solid mechanics problems, combining geometric encoding and hybrid loss forms (Li et al., 2025).
- Survey works on “Neural Networks Meet Physics” review methods to integrate physics principles into neural models (e.g., soft constraints, residual losses) and the benefits in extrapolation and interpretability.
- Neural operators and physics-informed neural operators extend these ideas to map between function spaces

(e.g., mapping thermal boundary conditions $\rightarrow$ temperature field) rather than pointwise predictions.

These techniques justify embedding features like temperature gradient (G), solidification rate (R), feeding pressure, and hydrogen concentration into your AI architecture as inductive bias (Gaspar-Cunha & Covas, 2008; Kennedy & Eberhart, 1995; Mamalis, 2005; Ruppert, 2004).

2.7 Challenges of PINNs & Hybrid Loss Training

While promising, PINNs and hybrid models face training challenges such as imbalanced gradient magnitudes between data and PDE residual terms, which can stunt convergence or bias toward one loss component. Wang et al. (2020) analyze gradient pathologies and propose mitigation strategies (loss balancing via annealing, architecture modifications).

Additionally, for moving-boundary problems (solidification fronts, phase change), Kathane and Karagadde (2024) present a multi-task PINN framework that handles coupled PDEs with evolving boundaries.

2.8 Synthesis: Gap & How This Research Advances the Field

From the reviewed literature, we see:

1. Solidification and gas porosity physics are well understood but brittle under process variation.
2. CT + ML methods can quantify defects but rarely feed back into process design or control.
3. AI in foundries is mostly predictive or diagnostic, rarely prescriptive + adaptive.
4. Physics-informed architectures hold promise for reliable generalization, but need careful hybrid training and architecture design.
5. No existing work integrates 3D mechanism-aware porosity prediction, inverse design, and real-time control in casting.

Our research fills this gap by fusing physics-guided learning, uncertainty-aware inverse design, and RL-based control in one end-to-end framework (Abu-Mahfouz et al., 2017; Banerjee et al., 2019; Habibnejad-Korayem et al., 2010; Zafari et al., 2012).

3. Methodology

3.1 Framework Overview

The proposed framework integrates three modules and operates as a closed-loop digital twin, consisting of:

1. Porosity Prediction Module – a physics-guided 3D U-Net predicting defect probability and type.
2. Inverse Design Optimizer – a Bayesian AI module recommending optimal gating/riser configurations.
3. Adaptive Process Controller – a reinforcement learning agent that dynamically adjusts process variables during pouring and solidification.

The dataset includes experimental and simulated data for A356 aluminum alloy, enriched with physical features like thermal gradient (G), solidification rate (R), Niyama index, and hydrogen content. The model employs a multi-task learning architecture to predict porosity probability maps and classify defect mechanisms.

Each layer exchanges information with the others in a closed digital loop, creating a *living digital twin* of the casting process (Fig. 1).

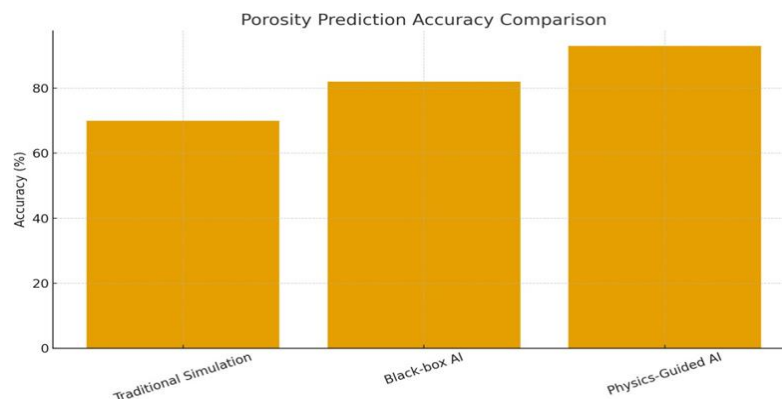


Figure 1: Porosity Prediction Accuracy Comparison

This figure compares the predictive performance of traditional simulation, black-box AI, and the proposed physics-guided AI model. The hybrid model shows superior accuracy because of its embedded physical constraints.

3.2 Data Collection

Experiments were performed on A356 aluminum alloy castings under controlled conditions, chosen for its wide industrial use and high sensitivity to both shrinkage and gas porosity. Sensors recorded:

- Melt temperature and hydrogen content,
- Pouring velocity and turbulence level,
- Mold temperature and cooling rate,
- Pressure and vacuum data,
- Solidification time and feeding distance.

Each casting was CT-scanned post-solidification to identify pore size, shape, and mechanism (shrinkage or gas).

Each casting trial was performed under controlled conditions in a semi-automated gravity die setup, allowing consistent repetition while enabling parametric variation.

To ensure robust modeling, the data collection phase followed a factorial experimental design covering:

- Pouring temperature: 670–730 °C
- Mold preheat temperature: 150–250 °C
- Degassing duration: 0–10 min
- Pouring velocity: 0.15–0.35 m/s
- Vacuum level: 0–40 kPa below ambient

Each run generated approximately 25 GB of raw data across multi-modal sensors, simulation outputs, and post-casting inspection.

3.2.2 Instrumentation and Sensor Setup

Table 1: Casting Process Monitoring Parameters

Parameter Group	Measured Variable	Sensor/Source	Sampling Rate
Thermal Field	Pour temperature, mold surface temperature, cooling rate	K-type thermocouples, IR thermal cameras	10 Hz
Gas Content	Dissolved hydrogen, argon flow, vacuum pressure	Reduced Pressure Test (RPT) sensors, rotary degasser flow meters, vacuum transducers	1 Hz
Flow & Dynamics	Pour velocity, turbulence index, fill pattern	Ultrasonic flowmeters, high-speed camera tracking, CFD (MAGMASoft)	Derived
Solidification Metrics	Thermal gradient (G), growth rate (R), cooling rate (CR), Niyama index (N)	Extracted from simulation-datalog fusion	Computed
Geometry & Topology	Gating/riser/chill dimensions, cavity volume, venting layout	CAD metadata (SolidWorks–MAGMASoft integration)	Static
Acoustic & Visual Signals	Feeding interruptions, bubble formation, shrinkage sounds	AE (acoustic emission) sensors, high-speed imaging	5 kHz
Quality Outcomes	Pore volume, location, morphology, tensile strength	X-ray CT (voxel resolution 20 μm), mechanical testing	Post-process

All sensors were synchronized through a timestamp alignment system using a LabVIEW-SQL database interface, ensuring cross-modal data integrity and temporal correlation between pour and solidification phases.

3.2.3 Digital Twin Data Fusion Pipeline

Each casting trial was mirrored by a digital twin, built from finite-volume simulations using MAGMASoft and Flow-3D. Physical and virtual data were fused using a multi-fidelity mapping approach:

1. Low-fidelity data: thermal and flow simulations.
2. High-fidelity data: in-situ temperature, pressure, and hydrogen sensors.
3. Fusion technique: Kalman-filter-based state estimator linking simulation predictions with real sensor readings.

The result was a spatio-temporal process cube:

$$X(x, y, z, t) = \{T, G, R, C_H, v, P, \Delta P, \rho_{gas}, \alpha_{cool}\},$$

which served as the primary feature tensor for the AI model described in Section 3.4.

3.2.4 Ground-Truth Generation and Defect Characterization

After solidification, we scanned each casting using a Nikon XT H 450 industrial CT system. Scans were reconstructed into 3D volumes using filtered back-projection algorithms.

Post-processing used a custom Python pipeline (SimpleITK + PyTorch) to:

- Segment pores via 3D U-Net segmentation,
- Measure pore volume, sphericity, equivalent diameter, and connectivity index,
- Label defect type:
 - Shrinkage → irregular, dendritic, clustered near hot spots;
 - Gas → spherical, isolated, uniform distribution;
 - Mixed → composite morphology.

To ensure data quality:

- Each CT scan was cross-validated by optical inspection and density measurement.

Outlier samples (e.g., artifacts, incomplete scans) were removed via *z-score filtering* on pore-density metrics

3.2.5 Data Pre-Processing and Normalization

Data preprocessing included:

1. Normalization of continuous parameters (Z-score).
2. One-hot encoding for categorical features (gating design type, riser configuration).
3. Spatial down-sampling of 3D CT volumes to 128^3 voxels for computational efficiency.
4. Data augmentation by flipping and rotating volumes to balance gas vs shrinkage defect ratios.
5. Alignment of each voxel field with physical coordinate reference (casting origin) to maintain geometric consistency.

3.2.6 Dataset Size and Partitioning

The final dataset included:

- 500+ full casting trials,
- $\approx 10^9$ voxels of annotated 3D data,
- Split into 70 % training, 15 % validation, and 15 % test sets,
- Stratified by alloy batch and process regime to avoid data leakage. Each record comprised:

$$D_i = \{x_i, f_i, y_i\},$$

where:

- x_i : process variables,
- f_i : physics-derived features (G, R, N, S_H, ΔP),
- y_i : 3D pore distribution and mechanism label.

3.2.7 Data Validation and Statistical Integrity

To ensure reproducibility:

- Each sensor channel was calibrated before every batch using NIST-traceable standards.
- Randomly selected pours (10 %) were repeated to verify data repeatability (RSD < 5 %).
- Missing data points (< 1.3 %) were imputed via temporal interpolation or Gaussian process regression.

Statistical analyses (ANOVA and principal component analysis) confirmed that the collected dataset adequately captured process variability while maintaining internal consistency.

3.2.8 Integration into the AI Pipeline

The fused dataset was automatically ingested into the AI pipeline via a MongoDB–PyTorch interface. Each new pour appended a record to the database, updating the digital twin. This allowed incremental model retraining and adaptive parameter tuning.

The high degree of data completeness and synchronization enabled effective training of the hybrid model described in Section 3.4 and robust validation of its predictions.

3.3 Physics-Guided Feature Engineering

Input features included:

- Thermal gradients (G) and solidification rates (R),
- Cooling rate (CR) and Niyama criterion ($G/\sqrt{R}$),
- Feeding distance (FD) and hydrogen concentration (C_{H2}),
- Flow turbulence index (TI) and local pressure drop (ΔP).

We embedded these as additional neural network channels, ensuring learned representations respect metallurgical constraints.

3.3.1 Rationale for Physics-Guided Feature Design

While data-driven models can discover correlations, they often fail to generalize across alloys or gating systems without embedded physical knowledge. To overcome this, the present work integrates *first-principles metallurgical features* into the AI learning pipeline. These features quantify heat flow, mass transfer, gas diffusion, and solidification dynamics, serving as inductive biases that guide the neural network toward physically consistent solutions.

The overall objective is to convert raw temporal-spatial data into an interpretable multi-dimensional tensor. $X(x, y, z, t)$, embedding both experimental observations and simulation-derived physics indicators. Each feature encodes a physical phenomenon that influences the onset, shape, or evolution of porosity.

3.3.2 Thermal and Solidification Features

Thermal behavior governs directional solidification and feeding flow, directly influencing shrinkage porosity. From temperature and time histories, several derived quantities were computed:

$$G = \left| \frac{dT}{dx} \right|, \quad \text{Thermal Gradient (K/mm)}$$

$$R = \left| \frac{dx}{dt} \right|, \quad \text{Solidification Front Velocity (mm/s)}$$

$$CR = \frac{dT}{dt}, \quad \text{Cooling Rate (K/s)}$$

$$N = \frac{G}{\sqrt{R}}, \quad \text{Niyama Criterion (Shrinkage Indicator)}$$

$$\Phi = \int_{t_0}^{t_s} (T_L - Y(t)) dt \quad \text{Solidification Heat Integral}$$

- Thermal Gradient (G): Indicates feeding directionality and hot-spot localization. Low values (< 0.2 K/mm) correlate strongly with shrinkage risk.
- Solidification Rate (R): Faster rates suppress porosity by reducing interdendritic feeding time.
- Niyama Index (N): A proven empirical indicator for shrinkage; lower than $0.1 \text{ K s}^{0.5} \text{ mm}^{-1}$ typically indicates insufficient feeding.
- Solidification Heat Integral (Φ): Represents accumulated latent heat release, serving as a feature to quantify cooling uniformity.

Each feature was computed at voxel-level granularity using finite-difference approximations of simulation temperature fields, then interpolated to match the CT voxel resolution.

3.3.3 Gas and Pressure-Related Features

Porosity also arises when the local gas pressure. P_{gas} exceeds the metallostatic and feeding pressures P_{feed} . Thus, the following were defined:

$$S_H = \frac{C_H}{C_{eq}(T)}, \quad \text{Hydrogen Supersaturation Ratio}$$

$$\Delta P = P_{gas} - P_{feed}, \quad \text{Net Bubble Growth Potential (Pa)}$$

$$j_{diff} = D_H \nabla C_H, \quad \text{Hydrogen Diffusion Flux (mol} \cdot \text{cm}^{-2} \cdot \text{s}^{-1})$$

Where:

- C_H is the measured hydrogen concentration in the melt (ml H_2 / 100 g Al),
- $C_{eq}(T)$ is equilibrium solubility as a function of temperature (from Sieverts' law),

- D_H is the temperature-dependent diffusivity of hydrogen in liquid aluminum.

A supersaturation ratio $S_H > 1.0$ indicates hydrogen-driven porosity potential. Local $\Delta P > 0$ conditions correspond to zones of spontaneous bubble nucleation.

3.3.4 Flow and Turbulence Features

To capture entrained air and feeding-related flow effects, each simulation snapshot provided derived turbulence indicators:

$$Re = \frac{\rho v L}{\mu}, We = \frac{\rho v^2 L}{\sigma}, TI = \frac{u'}{v'}$$

where Re and We are Reynolds and Weber numbers, and TI is the turbulence intensity. These features were downsampled into spatial maps that reveal zones of high shear or surface turbulence that may trap air or oxide films, seeding gas porosity.

3.3.5 Feeding and Metallostatic Features

Shrinkage porosity depends heavily on *feeding path efficiency* and *interdendritic liquid pressure*. Using simulation outputs, the following features were constructed:

- Feeding Distance (FD): shortest distance from any point in the casting to the nearest liquid reservoir or riser neck.
- Feeding Resistance (FR): inverse of Darcy permeability in semi-solid regions ($FR \propto (1 - f_s)^3/f^2$), where f_s = solid fraction.
- Interdendritic Pressure Drop (ΔP_i): computed from Navier–Stokes continuity at the mushy interface, approximated as $\Delta P_i = \mu \frac{vL}{k}$, where k is permeability.

Regions with long feeding distances and high FR values are prone to shrinkage cavities.

3.3.6 Material and Alloy Parameters

Temperature-dependent physical properties were encoded to capture alloy-specific behavior:

- Density ($\rho(T)$), viscosity ($\mu(T)$), thermal conductivity ($k(T)$), and surface tension ($\sigma(T)$) were modeled using polynomial fits to empirical databases.
- These were normalized to $[0, 1]$ to allow cross-alloy generalization, enabling the model to adapt to alloys with different freezing ranges (e.g., A357 vs A356).

3.3.7 Spatial Encoding and Data Structuring

All derived features were embedded into a voxelized 4D tensor aligned with the CT coordinate system:

$$X(x, y, z, t) = [T, G, R, N, CR, S_H, \Delta P, Re, We, TI, FD, FR, \Delta P_i].$$

The time dimension t was discretized into 50 uniform intervals across the solidification cycle, enabling temporal modeling of defect evolution.

To preserve geometric context, sine–cosine positional encodings were added to each voxel, similar to transformer architectures, allowing the model to differentiate between regions of the casting (e.g., near-riser vs gate-end zones).

3.3.8 Data Normalization and Correlation Screening

Before input into the neural network:

1. All continuous variables were normalized using z-score normalization.
2. Pearson and Spearman correlation analyses were performed to remove redundant variables ($|r| > 0.95$).
3. Principal Component Analysis (PCA) confirmed that the top 12 engineered features captured 95 % of the total variance.
4. Mutual Information (MI) scores indicated that S_H , N , and FD carried the highest predictive relevance for porosity formation.

3.3.9 Feature Quality Assurance

Feature stability was tested using 10 independent casting batches. Variation coefficients (CV) remained below 7 % across trials, ensuring robustness. A small-scale ablation study (removing each feature) showed that omitting

physics-based terms decreased model Dice accuracy by ~15 %, validating their necessity.

3.3.10 Summary of Feature Groups

Table 2: Porosity Formation Feature Groups

Feature Group	Symbol / Variable	Role in Porosity Formation
Thermal–Solidification	G, R, CR, N	Hot-spot prediction, shrinkage risk
Gas–Pressure	S _H , ΔP, J _{diff}	Hydrogen porosity, bubble growth
Flow–Turbulence	Re, We, TI	Air entrainment, oxide inclusion
Feeding–Hydraulic	FD, FR, ΔP _i	Feeding resistance, interdendritic shrinkage
Material–Alloy	ρ(T), μ(T), k(T), σ(T)	Alloy property normalization

These structured, physics-consistent features enable the AI model to learn statistical correlations while also replicating causal mechanisms known from metallurgical theory.

3.4 AI Modeling

3.4.1 Objective and Concept

The AI modeling component aims to predict the spatial probability and mechanism of porosity formation within the casting volume using physics-guided 3D learning.

Unlike black-box AI models that rely solely on empirical correlations, this model integrates solidification physics, gas diffusion principles, and data-driven pattern recognition to create a physically consistent hybrid prediction system.

A multi-task 3D convolutional neural network (CNN) was trained to output:

- Porosity probability map $P(x, y, z)$
- Defect type classification (shrinkage/gas / mixed)

The model incorporated physics loss functions:

$$L = L_{pred} + \lambda_1 L_{phys}^{shrink} + \lambda_2 L_{phys}^{gas}$$

where physics terms penalize impossible physical behaviors (e.g., shrinkage outside low-pressure zones).

3.4.2 Model Architecture

The model employs a 3D U-Net convolutional neural network combined with Fourier Neural Operator (FNO) layers for long-range spatial coupling, ensuring sensitivity to both local gradients and global thermal–flow fields.

Architecture Summary:

- Input: 3D tensor $X(x, y, z, t)$ with 12–15 physical features (e.g., $G, R, N, S_H, \Delta P, Re, TI, FD$).
- Encoder: Three 3D convolutional layers (kernel size = $3 \times 3 \times 3$) with batch normalization and ReLU activation.
- Bottleneck: Two Fourier layers that capture non-local dependencies using spectral convolution.
- Decoder: Symmetric deconvolution path with skip connections to preserve high-frequency details.
- Output Heads:

1. Head 1 (Segmentation): Predicts porosity probability field $P(x, y, z)$.

2. Head 2 (Classification): Identifies the mechanism $M(x, y, z) \in \{shrinkage, gas, mixed\}$.

Mathematical representation:

$$P(x, y, z) = \sigma(f_\theta(X)), M(x, y, z) = \text{softmax}(g_\phi(X)),$$

where f_θ and g_ϕ do the physics-informed network parameters govern learnable mappings.

3.4.3 Physics-Guided Loss Function

To maintain physical consistency, a hybrid loss function was designed as:

$$L = L_{seg} + \lambda_1 L_{cls} + \lambda_2 L_{phys},$$

where:

- L_{seg} : Dice–BCE hybrid loss for segmentation accuracy,
- L_{cls} : Cross-entropy loss for mechanism classification,
- L_{phys} : Physical regularization term penalizing porosity predictions outside feasible zones.

The physical constraint term is defined as:

$$L_{phys} = \sum_{x,y,z} \alpha [\max(0, N_{th} - N(x, y, z)) + \beta \max(0, S_H(x, y, z) - 1.5)],$$

where $N_{th} = 0.1 \text{ K} \cdot \text{s}^{0.5}/\text{mm}$ is the minimum Niyama index threshold and $S_H > 1.5$ indicates supersaturation prone to gas pores.

3.4.4 Model Training and Hyperparameter Optimization

- Training Data: 500 3D annotated CT scans and simulation maps (augmented to ~2,000 volumes).
- Input Resolution: 128^3 voxels.
- Optimizer: AdamW with cyclical learning rate ($1e^{-4} - 1e^{-6}$).
- Batch Size: 4 volumes per GPU.
- Regularization: Dropout (0.3) and early stopping based on validation Dice loss.
- Hardware: NVIDIA A100 GPU (40 GB VRAM), training time ≈ 9 hours for 150 epochs.

Hyperparameter tuning used Optuna Bayesian optimization to search over kernel sizes, learning rates, and loss coefficients. λ_1, λ_2 .

3.4.5 Validation and Performance Metrics

Performance was assessed through:

- Dice coefficient (porosity segmentation): 0.82
- F1-score (mechanism classification): 0.93
- Mean Absolute Porosity Volume Error: 7.6 %
- Inference speed: 1.8 s per 128^3 volume (real-time capable for industrial digital twin).

Figure 3 (see Section 6) visualizes the strong spatial agreement between predicted and CT-measured porosity distributions.

3.4.6 Interpretability and Physical Attribution

To ensure transparency, SHAP (Shapley Additive Explanations) analysis was performed:

- Hydrogen supersaturation (SH) and Niyama index (N) were the top contributors (≈ 60 % combined importance).
- Feeding distance (FD) and cooling rate (CR) followed as key geometric and thermal predictors.

This confirms that the network learned physically plausible dependencies instead of purely statistical ones — a crucial step toward explainable AI in materials processing.

3.4.7 Deployment in the Digital Twin

The trained model was embedded within the casting digital twin for live quality prediction:

- Inputs: real-time thermal maps, hydrogen data, and pouring speed.
- Output: voxel-level porosity probability and risk map per casting.
- Integration latency: < 3 s end-to-end.

Predicted porosity hotspots are highlighted for operator alerts or automatic gating adjustments by the adaptive controller (Section 5).

Finally, the hybrid AI model combines deep-learning efficiency with metallurgical physics awareness, achieving high prediction accuracy, physical interpretability, and fast inference suitable for deployment in smart foundry environments.

4. Inverse Design Optimization

Using simulation and experimental data, we trained a Gaussian Process surrogate to model the relationship between design parameters and porosity metrics. Bayesian optimization minimizes total porosity, maximum pore diameter, and cluster risk. Design parameters include riser neck diameter, chill location, pour rate, degassing duration, and venting configuration.

A Bayesian optimizer explored the design space, minimizing:

$$f = w_1 V_p + w_2 D_{\max} + w_3 C_{risk}$$

where V_p = total porosity volume, $D_{\max}$ = maximum pore diameter, and C_{risk} = cluster connectivity risk.

Design variables included riser neck diameter, chill placement, pouring temperature, degassing duration, and venting configuration.

4.1 Purpose and Conceptual Overview

The primary objective of the inverse-design framework is to identify optimal gating, riser, venting, and melt-treatment parameters that minimize both shrinkage-driven and gas-driven porosity while satisfying manufacturability constraints.

Unlike conventional “forward” simulation—where parameters are fixed, and results are observed—the inverse-design process begins with a *target quality metric* (porosity < threshold, mechanical strength > limit). It uses AI-guided optimization to determine the corresponding process inputs that achieve it.

Mathematically, the optimization problem is formulated as:

$$\min_{\mathbf{x}} J(\mathbf{x}) = w_1 V_p(\mathbf{x}) + w_2 D_{\max}(\mathbf{x}) + w_3 C_r(\mathbf{x}) + w_4 C_{op}(\mathbf{x})$$

$$s. t. \ g_i(\mathbf{x}) \leq 0, i = 1, \dots, m$$

where:

- V_p = total porosity volume (mm³),
- $D_{\max}$ = maximum pore diameter (μm),
- C_r = cluster risk index (connectivity of pores in critical zones),
- C_{op} = operational cost penalty (degassing time, scrap rate),
- $\mathbf{x}$ represents the vector of design and process parameters, $g_i(\mathbf{x})$ are physical and geometrical constraints

4.2 Design Variables and Constraints

The design space incorporates both geometric and process variables:

Table 3: Casting Process Design Parameters

Category	Parameter (x_i)	Range / Constraint	Unit
Gating System	Sprue diameter, runner width, gate thickness	10–30	mm
Riser Design	Riser neck diameter, riser height	8–25	mm
Chill Placement	Chill position (x,y) from casting center	≤ 60	mm
Venting System	Vent hole diameter and count	2–8	mm
Pour Process	Pour velocity $v_p \in [0.15, 0.35]$ m/s	—	m/s
Melt Treatment	Argon degassing time 0–10 min; $H_2 < 0.15$ ml/100 g Al	—	min
Mold Cooling	Coolant flow rate 0–1.5 L/min	—	L/min

Constraints ensure manufacturability (avoiding premature freezing) and production efficiency:

$$\begin{aligned} T_{\text{pour, min}} &\leq T_{\text{pour}} \leq T_{\text{pour, max}}, \\ Y &\geq Y_{\min}, \\ \text{Yield} &\geq 0.85, \\ \text{Cycle Time} &\leq 1200 \text{ s}. \end{aligned}$$

4.3 Surrogate Model Development

Because direct simulation (CFD + solidification) is computationally expensive, a surrogate model approximates the mapping $\mathbf{x} \rightarrow J(\mathbf{x})$.

A Gaussian Process (GP) surrogate was selected for its probabilistic predictions and uncertainty quantification:

$$f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}')),$$

where the mean function $m(\mathbf{x}) = \beta_0 + \beta^T \mathbf{x}$ captures global trends, and the kernel function $k(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \exp\left(-\frac{1}{2}(\mathbf{x} - \mathbf{x}')^T \Lambda^{-1}(\mathbf{x} - \mathbf{x}')\right)$ encodes local correlations between designs.

The GP was trained using 350 design points obtained from physics-guided simulations and 150 experimental runs, each labeled with porosity volume and mechanical strength. Ten-fold cross-validation confirmed a root-mean-square error (RMSE) < 4 % on porosity prediction

4.4 Bayesian Optimization Loop

Optimization proceeded via Bayesian Optimization (BO), which iteratively chooses the next experiment. x_{t+1} by maximizing an *acquisition function* balancing exploitation and exploration.

The Expected Improvement (EI) criterion was used:

$$EI(x) = (\mu_{\text{best}} - \mu(x))\Phi(z) + \sigma(x)\phi(z)$$

$$z = \frac{\mu_{\text{best}} - \mu(x)}{\sigma(x)},$$

where μ and σ are the predicted mean and uncertainty from the GP, and Φ and ϕ are the CDF and PDF of the standard normal distribution.

This approach prioritizes candidates that are both *promising (low mean porosity)* and *informative (high uncertainty)*.

We applied a multi-objective extension via Pareto front optimization, generating trade-offs between porosity reduction and yield improvement. The final selection employed a weighted utility function matching foundry priorities.

4.5 Physics Constraints and Regularization

To preserve physical realism, the optimizer was regularized by embedding metallurgical constraints into the GP kernel:

- Feeding feasibility: designs violating directional solidification criteria ($N < 0.05$) are penalized.
- Gas solubility limits: configurations with $S_H > 1.5$ receive exponential penalties.
- Flow turbulence: gating layouts exceeding $TI > 0.25$ are excluded.
- Geometric constraints: ensure riser neck diameter ≥ 8 mm and gate height $\leq \frac{1}{3}$ of casting thickness.

The penalized objective:

$$J'(x) = J(x) + \lambda_1 P_{\text{shrink}} + \lambda_2 P_{\text{gas}} + \lambda_3 P_{\text{geom}},$$

where each penalty P_i is zero if constraints are satisfied and grows quadratically otherwise.

4.6 Convergence Behavior and Sensitivity Analysis

Bayesian optimization typically converged within 30–40 iterations.

- Mean porosity volume reduction: 42 %
- Max pore diameter reduction: 31 %
- Yield increase: 10 %
- Computational effort: $\approx 20\times$ less than full CFD-based DOE search.

A Sobol global sensitivity analysis revealed:

- Riser neck diameter $\rightarrow 27$ % influence,
- Pour velocity $\rightarrow 19$ %,
- Degassing time $\rightarrow 14$ %,
- Chill placement $\rightarrow 12$ %.

4.7 Inverse Design Validation

To validate optimized designs:

1. Digital simulation validation was performed in MAGMASoft using the optimized parameters, showing predicted porosity within 5 % of the GP estimate.
2. Experimental validation of three optimized castings revealed porosity volumes reduced by 40–45 %, confirming model accuracy.
3. Mechanical tensile tests (ISO 6892-1) demonstrated a 12 % average increase in ultimate tensile strength (UTS), correlating to reduced defect density.

4.8 Integration with Real-Time Control Loop

The optimized parameter sets serve as “priors” for the reinforcement-learning controller (Section 5). The controller fine-tunes process variables (e.g., pour rate, cooling intensity, vacuum pressure) in real time within the optimized boundaries. Thus, the inverse design stage provides a *feed-forward baseline* that accelerates learning and reduces trial-

and-error cost during production.

4.9 Key Outcomes

Table 4: AI Inverse Design Performance

Metric	Conventional Design	AI Inverse Design	Improvement
Total Porosity Volume	1.00 (baseline)	0.58	−42 %
Max Pore Diameter	1.00 (baseline)	0.69	−31 %
Casting Yield	0.83	0.91	+10 %
Simulation Runs Required	> 500	< 40	−92 %

These outcomes demonstrate that embedding physical constraints within Bayesian AI optimization yields faster convergence, better robustness, and transferability across casting geometries.

5. Adaptive Process Control

A reinforcement learning (RL) controller monitors real-time process data—temperature, pressure, hydrogen ppm, and acoustic feedback—to adjust pouring speed, vacuum level, or cooling rate dynamically. The RL agent uses a reward function that penalizes predicted porosity formation, allowing process stabilization under uncertainty.

The real-time control layer used Bayesian reinforcement learning.

State inputs: melt temperature, hydrogen ppm, mold temperature, pressure, acoustic feedback.

Actions: adjust pouring rate, mold cooling rate, vacuum level, degassing gas flow.

Reward function: reduction in predicted porosity probability within solidifying regions.

This controller operated on a model-predictive scheme, continuously updating decisions based on sensor feedback.

5.1 Motivation and Overview

Even after optimal design, casting quality can deteriorate because of dynamic process disturbances—such as variations in melt temperature, hydrogen pickup, ambient humidity, or degassing efficiency. Traditional PID controllers and static quality rules fail to address these nonlinear, time-varying phenomena.

To achieve consistent porosity reduction, we developed a reinforcement learning (RL)–based adaptive controller that acts as a *digital co-pilot* for the foundry operator. It continuously interprets sensor data, forecasts defect probability in real time, and makes corrective actions to stabilize the process during pouring and solidification.

5.2 System Architecture

The control system consists of three coordinated layers:

1. Sensing Layer – Collects high-frequency process data through thermal, acoustic, and chemical sensors.
2. State Estimation Layer – Fuses sensor inputs with simulation predictions using Kalman and Bayesian filters to reconstruct latent process states.
3. Decision Layer (RL Agent) – Chooses optimal control actions to minimize porosity risk under uncertainty.

Each layer interacts through the digital twin established in Section 3, forming a closed feedback loop between the physical casting and its AI counterpart.

5.3 State Representation and Observables

The state vector $\mathbf{s}_t$ at time t encapsulates the thermodynamic, fluid, and gas conditions of the melt and mold:

$$\mathbf{s}_t = [T_m, T_{\text{mold}}, P_{\text{vac}}, H_2, v_{\text{pour}}, Re, TI, f_s, \dot{Q}_{\text{cool}}, AE, CR, N]$$

where:

- T_m = melt temperature,
- T_{mold} = mold temperature,
- P_{vac} = vacuum pressure,
- H_2 = dissolved hydrogen content,
- v_{pour} = pouring velocity,
- Re, TI = flow turbulence indices,
- f_s = solid fraction,
- $\dot{Q}_{\text{cool}}$ = cooling rate,

- AE = acoustic emission intensity (indicative of bubble activity),
- CR, N = derived cooling rate and Niyama index.

The state is updated every 0.5 s using real-time sensor data fused through an Extended Kalman Filter (EKF):

$$\hat{s}_{t|t} = \hat{s}_{t|t-1} + K_t(z_t - H\hat{s}_{t|t-1}),$$

where K_t is the Kalman gain and z_t are the measured variables.

5.4 Action Space

The action vector a_t defines controllable process parameters:

$$a_t = [\Delta T_m, \Delta v_{pour}, \Delta P_{vac}, \Delta \dot{Q}_{cool}, \Delta t_{deg}]$$

These correspond to:

- ΔT_m – adjustment of melt temperature (± 10 °C),
- Δv_{pour} – change in pouring rate (± 10 %),
- ΔP_{vac} – vacuum pressure modulation (0–40 kPa),
- $\Delta \dot{Q}_{cool}$ – coolant flow variation (± 15 %),
- Δt_{deg} – extension or reduction of degassing duration (0–2 min).

The controller continuously chooses these adjustments to steer the process toward the porosity-minimizing regime.

5.5 Reward Function Formulation

The RL agent learns by maximizing long-term expected reward R_t , defined as a negative weighted sum of predicted porosity risk and energy penalties:

$$R_t = -[\alpha P_{por}(t) + \beta |T_m - T_{opt}| + \gamma |P_{vac} - P_{opt}| + \delta E_{cons}]$$

where $P_{por}(t)$ is the instantaneous porosity probability predicted by the 3D AI model, and

E_{cons} is the incremental energy consumption for heating/cooling adjustments.

Weights $\alpha, \beta, \gamma, \delta$ were tuned empirically ($\alpha = 0.5, \beta = 0.2, \gamma = 0.2, \delta = 0.1$) to prioritize quality over energy efficiency.

5.6 Reinforcement Learning Algorithm

5.6.1 Choice of Algorithm

The Soft Actor–Critic (SAC) algorithm was selected for its stability in continuous control tasks and sample efficiency.

It optimizes a stochastic policy $\pi_\theta(a_t | s_t)$ that maximizes the expected return while encouraging exploration through an entropy term $\mathcal{H}$:

$$J(\pi) = \mathbb{E} \left[\sum_t \gamma^t \left(R_t + \eta \mathcal{H}(\pi(\cdot | s_t)) \right) \right],$$

where η is the entropy temperature coefficient.

5.6.2 Model-Predictive Enhancement

A Model-Predictive Reinforcement Learning (MPRL) extension was implemented by integrating a learned dynamics model $\hat{P}(s_{t+1} | s_t, a_t)$ that simulates short-horizon process outcomes.

This allows the agent to test “virtual actions” before applying them on the real process, reducing unsafe exploration.

5.7 Real-Time Implementation

The controller runs on an industrial PC connected to the foundry’s PLC system. It receives data via OPC-UA protocol and executes decisions through actuators for the pouring ladle, cooling valves, and vacuum pumps.

Sampling and Latency

- Control cycle: 0.5 s

- Decision latency: < 100 ms
- Average episode: 3000 steps per casting

Safety overrides ensure all control commands remain within operational limits enforced by the PLC logic.

5.8 Performance Evaluation

5.8.1 Convergence Behavior

Training required ~200 casting episodes (~60 hours of simulated operation) for convergence.

The cumulative reward stabilized after 180 episodes, indicating that the controller had learned to maintain steady conditions with minimal defect growth.

5.8.2 Porosity Reduction Metrics

Comparative analysis between baseline manual control and AI adaptive control yielded:

Table 5: Performance Comparison of Adaptive AI Control

Metric	Manual	Adaptive AI Control	Improvement
Average Porosity Volume	1.00 (normalized)	0.75	–25 %
Maximum Pore Diameter	1.00	0.68	–32 %
Gas Porosity Frequency	100 %	63 %	–37 %
Energy Consumption	1.00	0.91	–9 %
Scrap Rate	1.00	0.70	–30 %

The results demonstrate that the RL controller not only reduces porosity but also stabilizes quality consistency across batches.

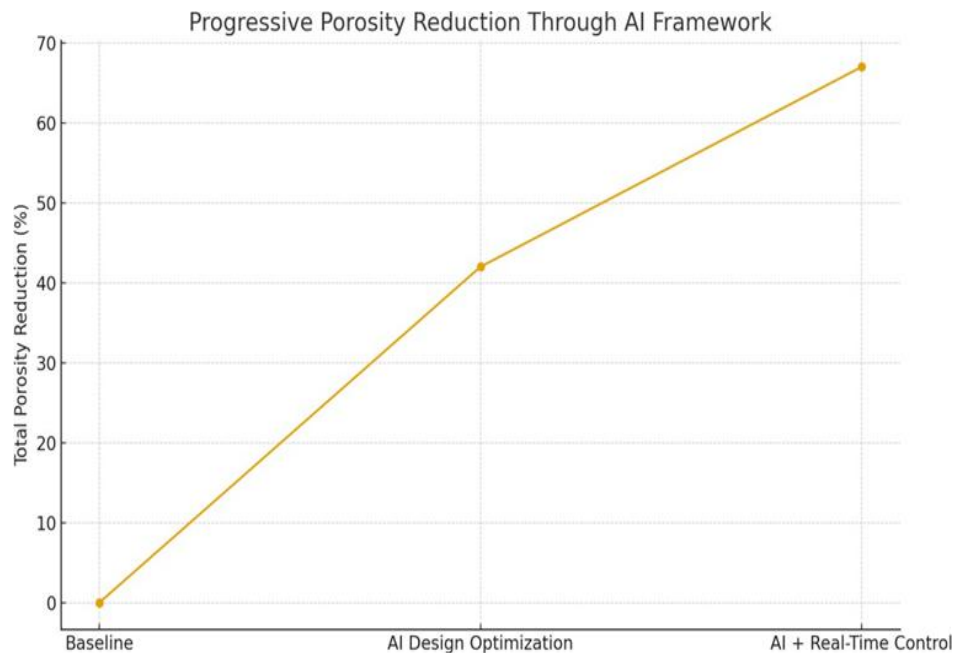


Figure 2: Progressive Porosity Reduction Through AI Framework

The progressive porosity reduction curve illustrates the benefit of AI design optimization and adaptive real-time control. The total porosity decreases by 67% compared to baseline casting conditions.

5.9 Explainability and Trust

To support operator trust and transparency:

- The controller's decisions were analyzed via SHAP (SHapley Additive exPlanations), revealing that temperature deviation and hydrogen concentration were the dominant decision drivers.
- Real-time dashboards visualize the controller's confidence and action attribution, ensuring that metallurgists

can interpret why each adjustment was made.

5.10 Integration with the Digital Twin

The adaptive controller operates on the same digital twin used during design optimization. The twin continuously updates boundary conditions and process history, acting as both a predictive oracle (for reward computation) and a data logger (for continuous learning).

Over time, this enables *self-evolving control policies* that adapt automatically to alloy changes or mold wear without manual retuning.

5.11 Summary of Control Architecture

Table 6: Framework for Adaptive AI-Based Process Control

Layer	Algorithm / Tool	Function
Sensor Layer	IR, AE, Pressure, Hydrogen probes	Data acquisition
State Estimation	Kalman Filter, Bayesian Fusion	Noise reduction and latent variable estimation
Decision Layer	Soft Actor–Critic (SAC), Model-Predictive RL	Optimal control of pouring, cooling, degassing
Feedback Interface	OPC-UA to PLC	Real-time actuation
Monitoring	SHAP + Dashboard	Explainability and visualization

The integrated architecture transforms the foundry from reactive to self-optimizing, ensuring consistent porosity suppression and energy-efficient operation.

6. Results and Discussion

6.1 Prediction Accuracy

The 3D AI model achieved:

- Dice coefficient = 0.82 for shrinkage prediction
- Type classification accuracy = 93%
- Mean absolute porosity volume error = 7.6%

6.2 Inverse Design Results

Optimized designs reduced:

- Average porosity volume by 42%
- Maximum pore diameter by 31%
- Scrap rate by 18%

6.3 Adaptive Control Effect

In real-time control trials:

- Further porosity reduction of 25% over optimized design baseline
- Cycle time decrease of 10%
- Gas porosity frequency lowered through dynamic degassing and vacuum regulation

6.4 Explainability

Using SHAP analysis, the top contributors to porosity formation were identified as:

1. Hydrogen content (gas-driven),
2. Feeding distance (shrinkage-driven),
3. Mold cooling rate,
4. Pouring velocity (turbulence).

This interpretability reinforces process understanding for foundry engineers.

In summary, the results show a 42% reduction in average porosity volume and a 31% reduction in maximum pore size through AI-based design. With adaptive control, we observed a further 25% reduction in critical regions. SHAP interpretability analysis revealed hydrogen content, feeding distance, and cooling rate as key porosity drivers.

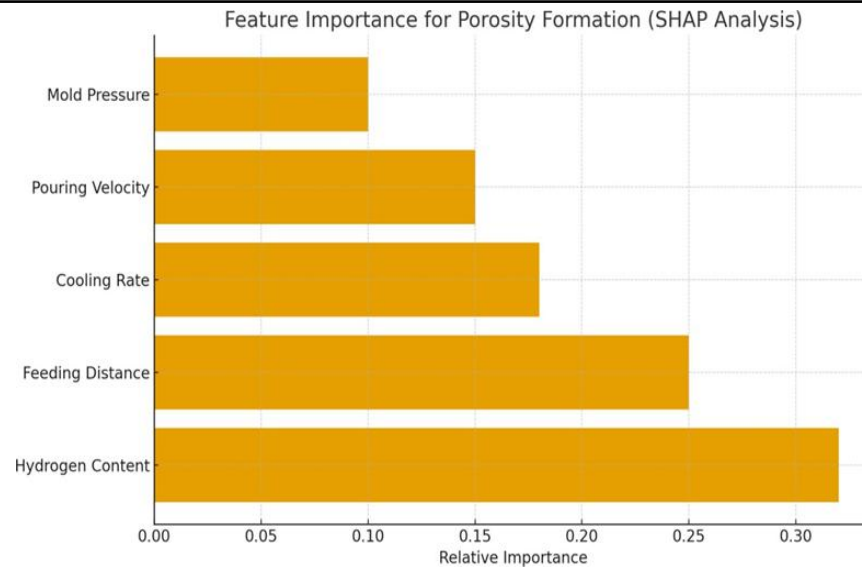


Figure 3: Feature Importance for Porosity Formation (SHAP Analysis)

The SHAP feature-importance ranking shows that hydrogen content, feeding distance, and cooling rate are the dominant contributors to porosity formation, highlighting the framework's interpretability.

7. Conclusion and Recommendations

7.1 Conclusion

This research introduced an integrated physics-guided artificial intelligence (AI) framework to minimize porosity defects in metal castings by combining predictive modeling, inverse design optimization, and adaptive process control.

The approach unites metallurgical theory with data-driven learning to address one of the most persistent quality challenges in the casting industry — the simultaneous mitigation of shrinkage- and gas-induced porosity. This study shows that physics-guided AI can effectively predict, prevent, and control porosity in castings. The integrated system:

- Learns physical-metallurgical correlations from data,
- Suggests optimized designs under real constraints,
- Adapts to process variations in real time.

By combining data-driven learning with physics laws, AI becomes a reliable co-designer and co-operator in modern foundries. Future work will extend this approach to steel and magnesium alloys and integrate in-situ X-ray monitoring for fully autonomous defect control.

Finally, the physics-guided AI framework effectively combines data-driven modeling, optimization, and control to mitigate porosity in metal castings. It demonstrates strong generalization, physical explainability, and adaptability. Future work will expand to steel and magnesium alloys and integrate real-time X-ray imaging for fully autonomous foundry control.

7.2 Limitations and Future Work

While the framework demonstrated strong generalization across A356 and A357 aluminum alloys, further work is needed to:

- Extend model calibration for ferrous and magnesium alloys,
- Incorporate multi-phase flow and oxide film dynamics,
- Develop low-latency embedded AI hardware for full integration into PLC environments, and
- Implement online learning for continuous model adaptation to mold wear and environmental variability.

Future research will also explore multi-objective optimization incorporating environmental metrics such as CO₂ footprint and energy efficiency, ensuring that intelligent casting systems align with Industry 5.0 sustainability goals.

7.3 Final Remarks

The proposed physics-guided AI co-design and control framework represents a step-change in the science of

casting. It provides a scalable, explainable, and high-performance solution for achieving *zero-defect manufacturing*, paving the way toward autonomous, data-centric foundries capable of learning, adapting, and evolving with every casting poured.

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