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Neural Network-Based Machine Learning Model for Spatiotemporal Prediction of Temperature and Fraction Solid in Low-Pressure Sand Casting

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Abstract. This paper presents a development methodology for a metamodel-based machine learning approach for spatiotemporal prediction of temperature and solid fraction evolution of aluminum castings during cooling under low pressure sand casting (LPSC) conditions, for various pouring temperatures (T_P) ranging from 614°C to 720°C. High-fidelity finite element (FE) simulations were performed, based on a representative case study produced by the LPSC process to generate a comprehensive database, recording nodal temperatures across the casting symmetry plane at different cooling times, and for several T_P values within the studied domain. Three different machine learning (ML) algorithms were evaluated using comparative metrics (R^2, MAE and MSE). Among the evaluated algorithms, the artificial neural network (ANN)-based ML model was selected for its superior predictive accuracy and robustness. The accuracy of the selected ML-model was assessed by comparing predicted and FE-simulated temperature fields. The results indicate that the predicted temperature error within the cast symmetry plane remains below 1%. Furthermore, a graphical user interface (GUI) was developed to visualize the predicted casting temperature field for different T_P values not used during the learning stage, as well as the corresponding solid fraction, which is computed based on the solidification curve of the aluminum alloy $AlSi_7Mg_{0.3}$ given by the ProCAST® database. This methodology could provide a fast, robust, and scalable framework for extending predictive models to higher-dimensional cases and diverse LPSC casting process configurations.

Introduction

Despite its millennia-long history, the increasing complexity of components and stricter process performance requirements make integrating Industry 4.0 technologies essential for reducing defects, energy consumption, and material waste, thereby improving the resilience, efficiency, and sustainability of foundry operations [1]. To bridge the gap between traditional metal casting practices and the objectives of Casting 4.0, several advanced technologies have been integrated into casting processes to enhance their intelligence and connectivity. These technologies enable the emergence of digital twin (DT) frameworks, which are virtual representations of casting processes designed to support real-time monitoring, decision-making, and process optimization. A DT links the physical process to its virtual model through continuous data exchange, allowing the model to reflect actual conditions and predict system behavior. In this framework, machine learning (ML) based metamodels play a central role by providing fast, simplified approximations of complex and computationally intensive physics-based simulations, making real-time analysis and control possible. Metamodels improve process optimization and monitoring by identifying optimal parameter combinations that produce components with the desired properties. When embedded in a DT, they enable continuous tracking and adjustment of process conditions to meet predefined objectives, improving product quality, service life, and overall sustainability [2].

Developing a metamodel requires access to extensive datasets describing the metal casting process. These data can be obtained from experiments [3], numerical simulations [4,5], published literature [6], or hybrid approaches that combine multiple sources [7,8]. When time and financial resources allow, experimental data are generally preferred; however, they remain susceptible to human error and uncontrolled process variations. Physics-based simulations provide a safe alternative to physical experiments by reducing measurement variability and isolating the effects of individual input parameters. Because they are inherently deterministic, numerical simulations yield identical outputs for identical inputs, eliminating external disturbances but limiting the ability to replicate real-world variability. Building sufficiently large datasets for training metamodels can be costly. Therefore, sampling techniques such as stratified sampling, probabilistic sampling, and Taguchi-based approaches were widely used to provide a cost-effective way to explore the design space with a limited number of design points while maintaining good generalization performance [2,4].

The application of metamodels based ML is used in various metal casting processes such as gravity casting [2–4], precision casting [9], continuous casting [10] and low-pressure (LP) casting [7,8]. Deng et al. [3] analyzed aluminum–silicon gravity-cast components with different mold coating thicknesses using surface images and roughness measurements. Six convolutional neural network (CNN) metamodels were developed to predict surface roughness, with three achieving errors below 2 μm. Ktari and Elmansori [4] developed an artificial neural network (ANN)-based metamodel for predicting the ingate velocity of liquid metal in gravity sand casting for different filling system design parameters and to optimize the functional design parameters that keep the ingate velocity below critical values to avoid defects such as bubbles and oxide bi-films. Vosniakos et al. [9] developed ANN metamodels for precision investment casting to predict product quality based on different input parameters such as mold temperature, casting material, and the number and location of feeding points. Their performance was evaluated using training and generalization errors, and an expandable user interface was implemented for practical use. Diniz et al. [10] evaluated three deep neural network approaches to detect clogging in continuous steel casting using historical process data, with ANN as a baseline, and reported superior performance on imbalanced industrial data, with the spatiotemporal model achieving nearly 99% recall and 98% precision. Duan et al. 2023 [7] proposed a ML approach using a multimodal neural network including visual, textural and numerical features for designing an efficient gating system for large, thin-walled castings. Shahane et al. [7] conducted a sensitivity analysis to identify initial and wall temperatures that improve microstructure and yield strength of the cast in low-pressure die casting process by using an 3D finite-volume simulations, ANN predictions, and NSGA-II optimization algorithm.

The above studies shows that ML-based metamodels have been applied in the past five years to solve multiphysics and multiscale phenomena occurring in casting processes, particularly in LPC, which is widely used for producing high quality casting from light alloys such as aluminum and magnesium. These models are used to optimize process parameters such as the design of the gating system and temperature conditions. However, the application of ML metamodels has so far been limited to relatively small-scale trials and does not fully address real industrial cases. Further investigation is particularly needed for the low-pressure casting (LPC) process to better understand solidification behavior under applied pressure, which enables continuous feeding during solidification and helps reduce casting defects [11].

This paper aims to present a methodology for building a metamodel for the LPSC process that can predict the temperature and the resulting solid fraction throughout the casting at any time during its cooling within a sand mold under LPSC conditions.

Methodology

In this study, a high-fidelity finite element (FE) model was employed to perform simulations using ProCAST® software. Numerous simulations were conducted, each corresponding to a different pouring temperature (T_P) of the AlSi7Mg0.3 alloy ranging from 614°C and 720°C. **Fig.1** shows the initial casting and mold design as well as the associated FE model, which was validated through fully instrumented experiments. Further details of the FE model can be found in Ref. [12].

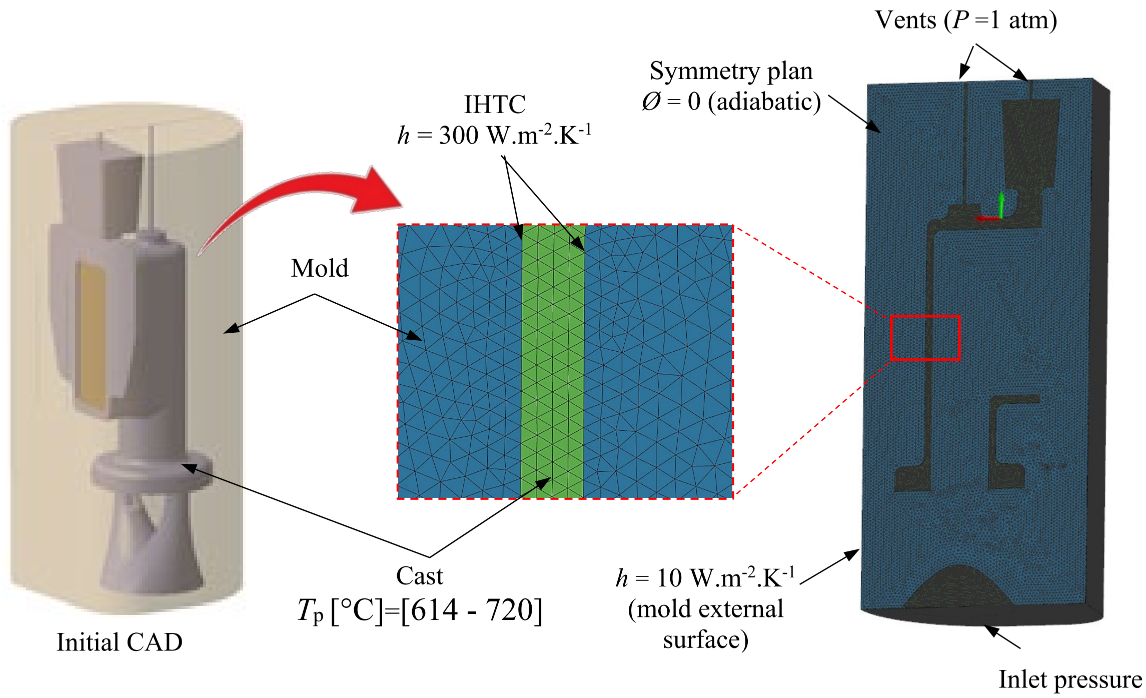

Fig. 1 FE modeling of the cooling problem in LPSC process

The temperature values computed at each node from the simulation result was extracted and collected in a database using Python®. The resulting dataset was postprocessed through normalization and subsequently divided into three subsets: learning, validation and test. Several ML algorithms including polynomial regression, XGBoost and artificial neural networks (ANN) were implemented and fine-tuned during the training phase to optimize their hyperparameters. Based on evaluation metrics such as mean squared error (MSE) and the coefficient of determination (R^2), the best algorithm was selected for the prediction of the casting temperature map (**Fig. 2**) and to calculate the corresponding solid fraction values.

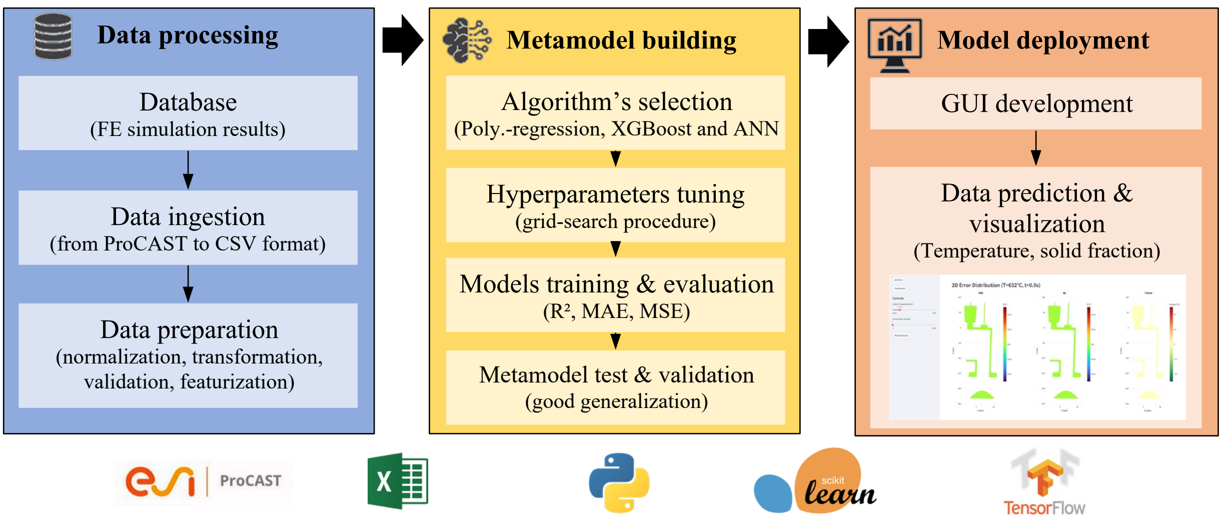

Fig. 2 Data processing workflow from FE simulation to ML results visualization

Although the metamodel uses a 2D symmetry plane, the training dataset was extracted from full ProCast® 3D computations. This ensures that the input data inherently capture out-of-plane thermal gradients and their effects on solidification, making the training dataset consistent for both learning and subsequent 2D predictions. The 2D plane is therefore not a simple geometric reduction but a projection that retains the influence of 3D thermal behavior. This approach aims to assess the feasibility of the neural network-based metamodel at a reduced computational cost while still considering the essential physics of the 3D process, allowing assessment of the validity of this method before its full scalability to 3D simulations.

Data Generation and Metamodel Building

As described below, thirteen FE-simulations were conducted using ProCast® software to simulate the temperature evolution in the case study casting geometry, made of Al-alloy (AlSi7Mg0.3) for different T_P ranging from 614 °C (liquidus + 1 °C) to 720 °C. The temperature evolution of the nodes located on the symmetry plane was extracted using ERFH5 files and imported into Phyton® for data preprocessing. **Fig 3** shows the structure of the extracted ERFH5 file. These data undergo a preprocessing step, transforming them into a tabular format of the type (X, Y, Z, T_P, T_{state_1}, T_{state_2}, …, T_{state_n}), from which the neural network input vector is generated. Each row represents a spatial node, treated as an independent input during training, allowing the network to learn the relationship between node features and temperature evolution. Using a multi-output regression model, the network simultaneously predicts all temperatures associated with a given node, implicitly capturing temporal evolution from the input-output pairs between consecutive states (i→ i+1). While sequence-based models such as Long Short-Term Memory (LSTM) can explicitly model temporal correlations, this approach is sufficient, as the problem is formulated as supervised regression at each node and the dataset inherently reflects the temporal dynamics.

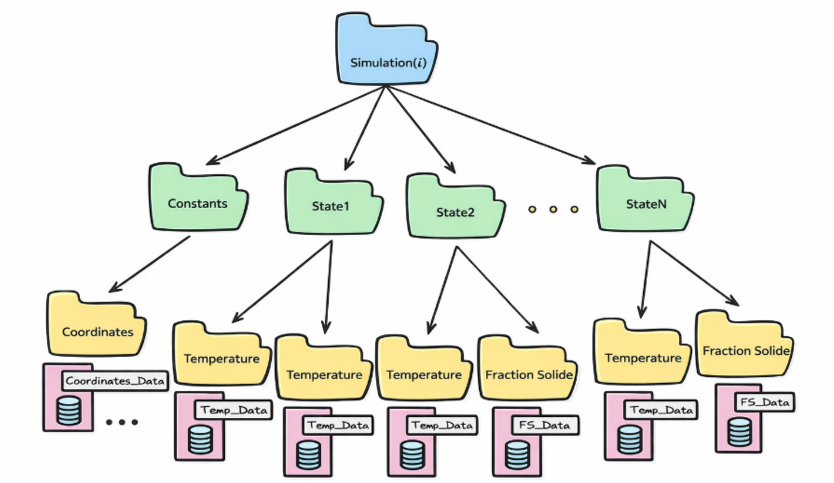

Fig. 3 Hierarchical view of the ERFH5 file highlighting the dataset structure

The dataset was divided into three subsets for training, validation, and testing, containing approximately 75%, 10%, and 15% of the simulation case, respectively (**Table 1**).

Table 1 Dataset partition for train, validation and test used for FE simulation

Dataset	T_p [°C]
Training	614; 622; 630; 647; 655; 677; 685; 690; 705; 720
Validation	710
Test	635; 664

Three ML algorithms - polynomial regression, XGBoost, and ANN - were used in the learning process because they are well-suited for solving regression problems. In this work, it is important to note that, each node at a given spatial coordinate and simulation time has only a single input variable (the nodal pouring temperature, Tp, which is identical for the initial condition) and a single output (the nodal temperature). Therefore, for this simplified 2D geometry, the number of simulations is considered sufficient, as the required number depends strongly on the quality of the dataset, the number of input parameters and the degree of nonlinearity in their variations over time and in their relationships [13]. In this work, the early stopping method was used during neural network training, with an epoch number of 1000 specified as an arbitrarily large value. The error on the validation dataset (the simulation result for Tp=710°C) was monitored during training. Both training and validation errors decrease during the initial learning phase, but when the neural network model begins to overfit, the validation error starts to increase. The network weights and biases were saved at the point of minimum validation set error, enabling the selection of an optimal neural network model that balances bias and variance [14]. In this model, the errors for the training, validation, and test datasets were found to be comparable, indicating that the model generalizes well and does not overfit the data. This shows that implementing a more sophisticated cross-validation strategy is unnecessary for the present study.

A grid-search procedure was conducted to fine-tune the hyperparameters of all three algorithms. This efficient exploration of predefined parameter spaces enabled the identification of optimal hyperparameter configurations that produced the best overall model performance (**Table 2**). The results show that among the tested algorithms, the ANN achieved the best metric values. The minimal MAE (1.5 °C) and MSE (4.76 °C²) values, along with the maximum R^2 (0.99) value, indicate the highest predictive accuracy; therefore, it was selected for performing the thermal prediction of the casting during the cooling phase.

Table 2. Optimal hyperparameter settings and performance metrics for ML algorithms

Algorithm	Optimal hyperparameters	MAE [°C]	MSE [°C²]	R^2
Polynomial	degree =7	5.922	93.933	0.984
XGBoost	n_estimators = 100; max_depth = 5 learning rate = 0.01	7.192	82.322	0.982
ANN	hidden layers (265, 64, 256, 1024); activation = Relu; learning rate = 0.001; batch size = 32	1.558	4.766	0.999

Results and Discussion

ML metamodel validation

The ML model is validated both qualitatively, through spatial temperature maps at different cooling times, and quantitatively, by comparing the simulated and predicted temperature evolution across several casting zones during cooling. **Fig. 4** illustrates the 2D temperature distribution on the symmetry plane of the case-study part during cooling under LPSC conditions at three different cooling times, for an initial filling temperature of 630 °C. The maps show the progressive heat dissipation throughout the part, with hotter regions persisting near thicker sections and faster cooling occurring in thinner areas. The comparison between FE simulation and ML prediction indicates excellent agreement, with the temperature error below 1% throughout the cooling phase. This small error highlights the high accuracy and effectiveness of the ML model in reproducing the thermal behavior of the casting.

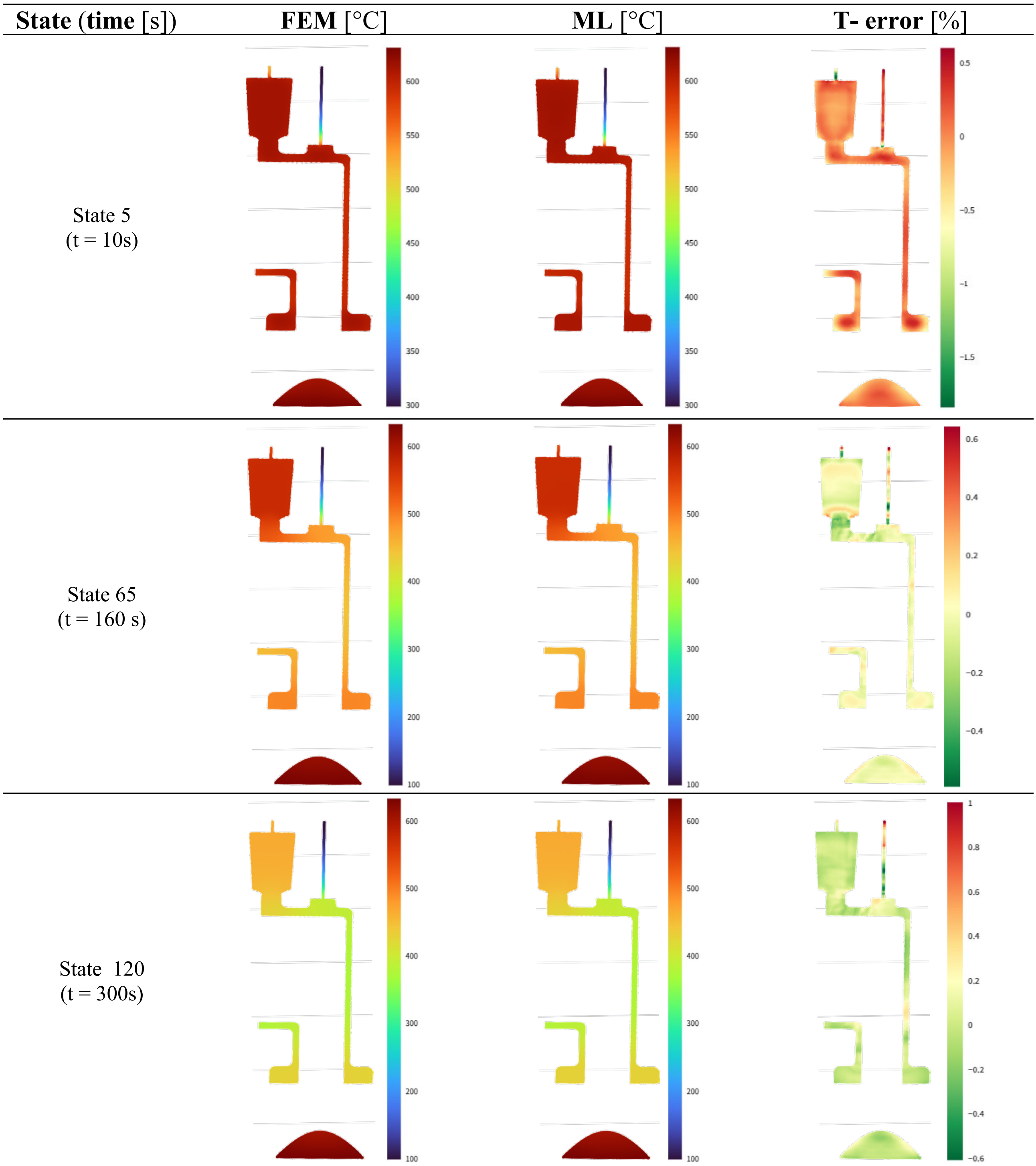

Fig. 4 FE simulation vs. ML prediction of the cast temperature and its deviation error (T_p = 630°C)

Fig. 5 shows a comparison between the FE simulation and ML predictions of temperature evolution in the casting during the cooling phase across five zones, each with distinct thermal behavior under LPSC cooling conditions.

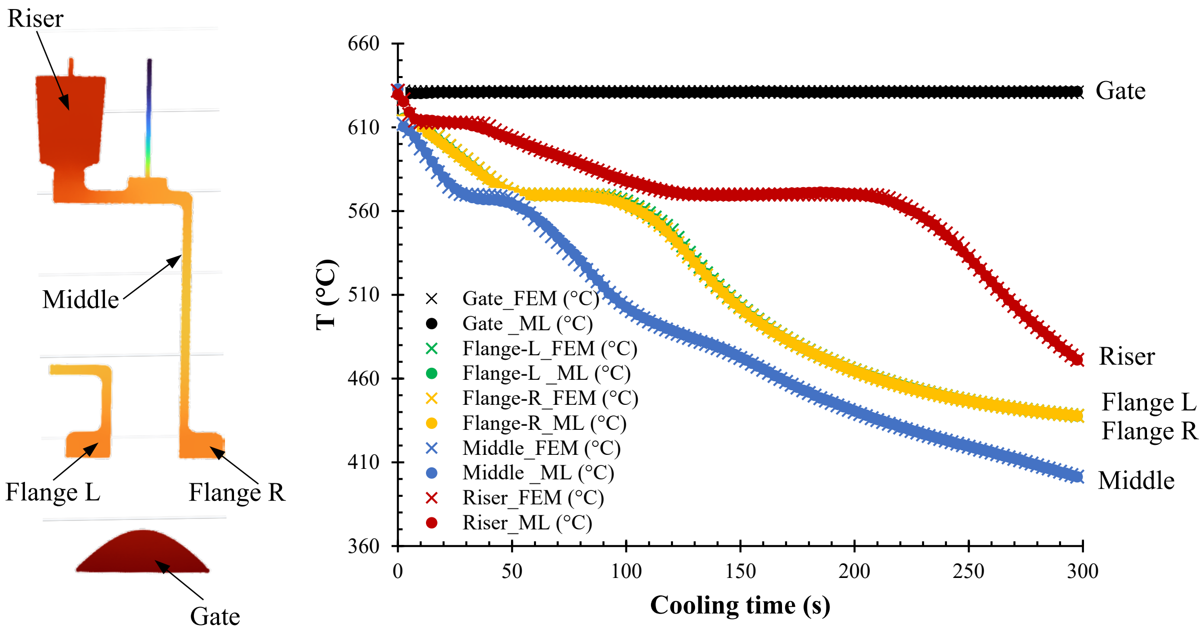

Fig. 5 Temperature evolution in various casting zones: FE simulation vs. ML prediction (T_P =630°C)

The temperature in the gate remains nearly constant due to its proximity to the riser tube, which serves as the fluid flow inlet. In contrast, the vent cools rapidly because it is the thinnest region, with a diameter of only 3 mm. The middle of the riser cools more slowly, as it is the thickest section and has the highest thermal modulus. Overall, the results show that the ML model accurately predicts 2D temperature map evolution across multiple spatially disconnected regions, capabilities that conventional FE simulations cannot achieve without performing 3D modeling. The curves illustrate how closely the ML model reproduces the thermal behavior captured by the FE simulation across different regions of the part, demonstrating its ability to provide rapid and reliable predictions suitable for real-time process monitoring and control required for the DT framework.

Temperature and solid fraction prediction

Once validated, the ANN-based model enables prediction of the casting temperature field during the cooling phase for T_P values not used in the learning phase. Using Python®, the solid fraction at each node was computed from the solidification curve (**Fig. 6**) to compute the progression of solidification.

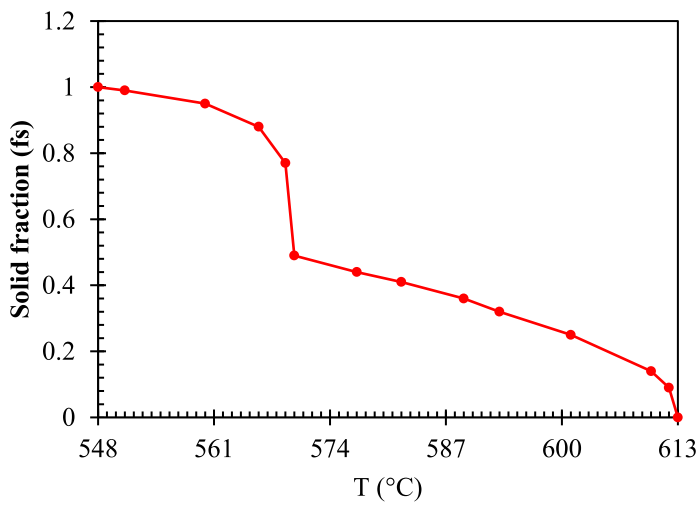

Fig. 6 Fraction solid vs. temperature ($AlSi_7Mg_{0.3}$, ProCAST® database)

A graphical user interface (GUI) was developed to visualize the predicted temperature and solid fraction enabling the examination of their evolution across the casting symmetry plane during cooling stage. **Fig. 7** illustrates the 2D fields of predicted temperature and solid fraction during cooling at a pouring temperature (T_P) of 700 °C. The temperature evolution follows the same trend observed in previous FE-simulation results, and the solid fraction develops accordingly. Solidification begins in the thinnest regions, where the temperature drops most rapidly, and then progresses toward the two casting hot spots: one at the bottom near the gating system and the other at the top. By approximately 200 s, the casting is fully solidified except for the riser. At the end of cooling, only the region adjacent to the gating system remains liquid.

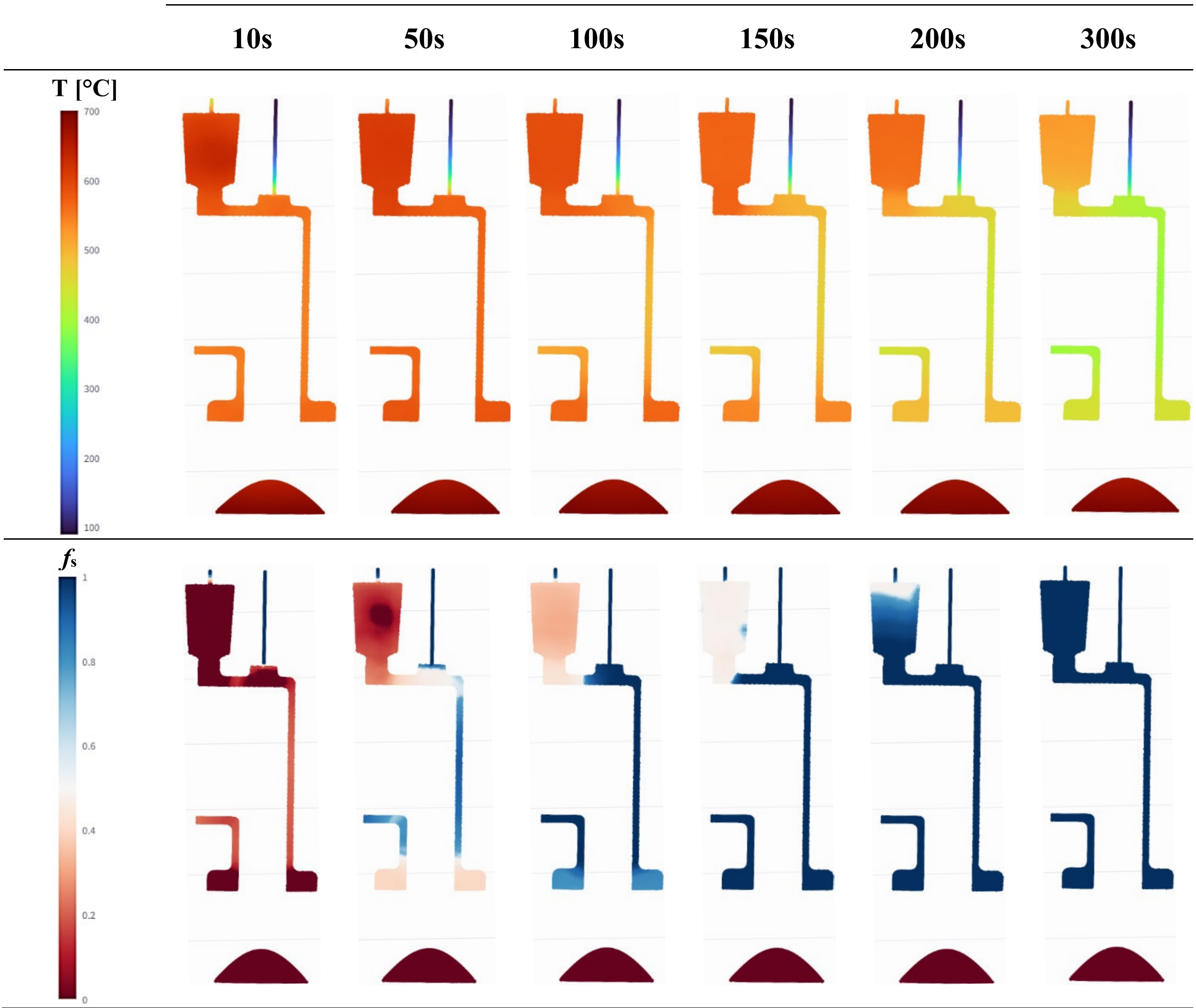

Fig. 7 ML-predicted spatiotemporal temperature and fraction solid (T_P = 700°C)

Conclusion

This study demonstrated that the developed ANN-based metamodel can accurately predict the spatiotemporal casting temperature field across a range of T_P values within the studied domain for a case produced using the LPSC process. A high-fidelity finite element (FE) model was first used to generate a database including nodal temperatures across the casting symmetry plane at different cooling times and for different T_P values. Three regression-based ML algorithms - polynomial regression, XGBoost, and ANN - were evaluated using early stopping and grid-search techniques. Among them, the ANN-based model demonstrated superior performance, achieving the lowest MAE (1.5 °C) and MSE (4.76 °C^2), as well as the highest R^2 value (0.99), and was therefore selected for thermal prediction of the casting during the cooling phase. The metamodel was validated through qualitative comparison with FE simulation results, demonstrating excellent predictive performance, with temperature deviation errors below 1% during the solidification process. A graphical user interface (GUI) was finally developed to visualize the predicted casting temperature field for different T_P values not used during the learning stage, as well as the corresponding solid fraction, which is computed with high accuracy based on the solidification curve of the aluminum alloy $AlSi_7Mg_{0.3}$.

The proposed metamodel reduces simulation costs and enables rapid, comprehensive 2D thermal analysis of the casting during the LPSC process, offering a potential alternative to time-consuming finite element (FE) simulations. Its demonstrated robustness in 2D spatiotemporal predictions can be readily extended to complex 3D geometries. Although this methodology can be applied in 3D, its use for geometries beyond the case study remains limited by the time required for process validation, which involves performing new FE simulations and fully retraining the metamodel.

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