

Gaussian Process Regression for Product Geometry Prediction in CAE Modeling

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ABSTRACT

Superplastic forming is an advanced technology used in the aerospace and automotive industries, as well as in the medical sector, for fabricating complex seamless components. However, its application is limited by high costs and the extended duration of the process. While finite element analysis in CAE systems such as ANSYS provides accurate results, it is computationally expensive. While finite element analysis performed in CAE systems such as ANSYS provides high-fidelity results, its computational expense creates a need for fast and accurate predictive models capable of supplementing or replacing this approach in multi-criteria analysis tasks. Despite the increasing adoption of machine learning across various disciplines, the development of reliable predictive models for specific geometric characteristics of superplastically formed components remains an understudied research area. **The purpose of this study is** to develop and verify a Gaussian process based model for predicting key geometric parameters of a hemisphere during the superplastic forming. An additional objective was to create an initial dataset using data generated from numerical simulations. The Latin Hypercube Sampling method was employed to design the experiment and generate the initial dataset, enabling efficient variation of material parameters K , m and pressure regime within ranges typical for aluminum alloys. Based on data from 50 numerical simulations, a predictive model for the hemisphere's geometric characteristics was developed with Gaussian Process Regression with a composite kernel. Model hyperparameter optimization was performed using RandomizedSearchCV. The developed Gaussian Process Regression model demonstrated high accuracy, achieving a coefficient of determination greater than 0.90 on the validation set for all target variables: thickness at the pole, average height, and height difference. Analysis of the Mean Squared Error confirmed the models generalization capability and absence of overfitting. **This research is aimed** at integrating the model into a digital twin system for real-time optimization of process parameters. The main challenge in scaling this approach is the computational cost associated with generating the required training data.

Keywords: ANSYS; predictive modeling; machine learning; Gaussian process regression (GPR); mean squared error (MSE); finite element simulation; finite element method (FEM); superplastic forming (SPF)

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ОРИГИНАЛЬНАЯ СТАТЬЯ

Гауссовская регрессия для прогнозирования геометрии изделия по данным CAE-моделирования

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АННОТАЦИЯ

Для создания сложных бесшовных деталей в аэрокосмической промышленности, автомобилестроении и медицине перспективной технологией является сверхпластическая формовка. Однако применение технологии ограничено высокой стоимостью и длительностью технологического процесса. Применение конечно-элементного моделирования в CAE-системах типа ANSYS дает точный результат, но вычислительно затратное, потому возникает потребность в быстрых и точных моделях прогнозирования, способных заменить или дополнить данный метод в задачах многокритериального анализа. Несмотря на растущее применение машинного обучения в различных областях, построение надежных моделей прогнозирования для конкретных геометрических характеристик деталей, полученных в результате сверхпластической формовки, остается малоизученным. **Целью данного исследования** является разработка и верификация модели прогнозирования на основе гауссовского процесса для предсказания ключевых геометрических параметров полусферы, получаемой в процессе сверхпластической формовки. Дополнительная задача состояла в создании исходного набора данных на основе результатов численного моделирования. Для формирования исходного набора данных использовался метод выборки латинского гиперкуба, позволивший эффективно варьировать параметры материала K , m и режим давления в типичных для алюминиевых сплавов диапазонах. С помощью 50 симуляций была



разработана модель прогнозирования геометрических характеристик полусферы, основанная на методе регрессии гауссовского процесса с использованием составного ядра. Для оптимизации параметров модели применялся метод RandomizedSearchCV. Разработанная модель регрессии гауссовского процесса показала высокую точность, продемонстрировав коэффициент детерминации $R^2 > 0,90$ на валидационной выборке для всех целевых переменных (толщина в полюсе купола, средняя высота, разность высот). Анализ значения среднеквадратичной ошибки подтвердил обобщающую способность и отсутствие переобучения. **Проведенное исследование направлено** на интеграцию модели в систему цифрового двойника для оптимизации технологических параметров в реальном времени. Главная проблема масштабирования — это создание данных для обучения, которое требует больших вычислительных ресурсов.

Ключевые слова: ANSYS; модель прогнозирования; машинное обучение; регрессия гауссовского процесса (GPR); MSE; конечно-элементное моделирование; МКЭ; процесс сверхпластической формовки (СПФ)

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INTRODUCTION

Superplastic forming (SPF) is recognized as an advanced technology in industries such as aerospace, automotive, and medical manufacturing. SPF is a materials processing technique that enables extremely high plastic deformation without failure. It serves as an optimal solution for fabricating complex, seamless components. Recent reviews [1–3] discuss the increasing relevance of SPF across industries and summarize latest advancements.

The principal advantages of superplastic forming (SPF) include the capability to manufacture structurally complex components in a single operation and the potential for producing parts with larger overall dimensions.

Given the costs associated with tooling, materials, and energy, as well as the duration of the part manufacturing cycle, the application of preliminary computer simulation becomes evident. Conducting virtual trials helps to optimize process parameters and reduce the probability of defects in actual production.

During the virtual design phase, a critical task is the prediction of key output parameters, particularly the thickness distribution of the final product. To address this, the Finite Element Method (FEM) [4–6], implemented in specialized CAE software packages, is traditionally employed. For instance, using the ANSYS system enables the construction of a detailed mathematical model for investigation. However, despite its high accuracy, detailed finite element modeling is characterized by significant computational expense and long simulation times, which limits its applicability for tasks requiring rapid optimization and the analysis of extensive parameter sets. Consequently, a relevant and promising development direction is the application of machine learning methods as an alternative or supplement to the classical FE modeling.

The developed predictive models, trained on limited datasets obtained from preliminary high-fidelity FE simulations or physical experiments, are capable of identifying complex non-linear relationships between process input parameters (geometry, material properties, pressure regime) and output characteristics. Machine

learning algorithms, such as artificial neural networks, support vector machines, and ensembles of decision trees, enable the construction of predictive models that are orders of magnitude faster than traditional approaches in forecasting key process outcomes. This capability establishes the foundation for developing digital twins of the manufacturing process.

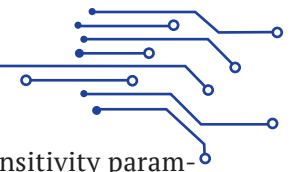
Machine learning algorithms demonstrate effectiveness in solving complex metal processing challenges, including defect prediction, rheological parameter identification, and process optimization [7].

The practical significance of applying machine learning algorithms is supported by the results of recent research. For instance, in the paper [8], the authors successfully employed machine learning methods, including artificial neural networks, to accurately predict the superplastic behavior of new multi-component alloys, such as Al-Mg-Fe-Ni-Zr-Sc. In the work [9], the authors demonstrate an approach where a multilayer feedforward neural network is used to establish correlative relationships between a wide spectrum of process parameters chemical composition, modifying additives, production methods, heat treatment regimes and the complex of mechanical properties in aluminum alloys.

The potential of machine learning is realized not only in predicting material behavior but also in solving applied technological challenges, such as product geometry control. A case in point is the research [10], where the authors demonstrated that a hybrid PSO-BP algorithm, used for predicting a thickness distribution in stiffening ribs after SPF, provides higher accuracy compared to a standard BP network. This underscores the practical value of employing machine learning methods for process optimization.

Thus, the analysis of research [7–10] reveals the advantages of integrating machine learning into the optimization of the SPF process.

The aim of the research is to develop and verify a Gaussian process-based prediction model for forecasting the geometric characteristics of a hemisphere produced by the SPF process. Primary focus is placed on predicting the thickness in the most critical area the pole of the



hemispherical dome. A dataset for training and validation was created based on the results of numerical modeling using the finite element method.

INITIAL DATASET FORMATION METHODOLOGY

To train the machine learning model, the source data comprised both experimental data from study [4] and the results of numerical modeling of the SPF process in ANSYS. The experimental data from [4] represent the results of a series of experiments on the superplastic forming of hemispherical domes from an aluminum alloy. The hemisphere was molded to a height of 50 mm, the initial thickness of the blank sheet was 1.2 mm. The molding was carried out through a cylindrical die with constant pressure of an inert gas. During the research, various pressure values were considered, including $p = 0.29$ MPa and $p = 0.56$ MPa.

In the research, the results of numerical modeling were used as the main data source, since conducting technological experiments is costly, and data from literary sources is insufficient to form a training sample.

To generate initial dataset, 50 solutions were performed in ANSYS. For each of the two pressure values [4], a series of calculations was performed with various combinations of key material parameters K and m included in the superplasticity equation and determining its deformation behavior:

$$\sigma = K \cdot \dot{\epsilon}^m,$$

where σ is the flow stress, $\dot{\epsilon}$ is the strain rate, K is the strength parameter, and m is the strain rate sensitivity parameter.

To create combinations of parameters K and m , the Latin Hypercube Sampling (LHS) method was used, which showed higher efficiency compared to the standard Monte Carlo sampling [11].

The initial data in the LHS method used were the ranges of parameter values $K = 100\text{--}300$ MPa·s ^{m} , $m = 0.3\text{--}0.7$, which correspond to typical values for aluminum alloys. A sample size of 50 parameter combinations was selected as a compromise between model accuracy and computational cost.

To form the initial data set (training, validation and test samples) from the results of numerical modeling, not only the final, but also intermediate values of the process parameters were used, such as time (t , sec), dome height (h , m) and thickness at the pole (s , m) to take into account the dynamics of the SPF molding for predicting changes in geometric parameters over time during the SPF process.

Dome height was measured at two distinct points: on the inner (UY_1) and outer (UY_111) surfaces at the pole of the hemispherical dome.

The following values were determined as input parameters (features) in the sample:

- 1) m — the material's strain rate sensitivity parameter;
- 2) K — the material's strength coefficient, MPa·s ^{m} ;
- 3) p — pressure, MPa;
- 4) t — time, sec.

The output parameters (target variables) are:

- 1) s — thickness at the pole, m ;
- 2) UY_1 — height at point 1 (inner surface), m ;
- 3) UY_111 — height at point 111 (outer surface), m .

FINITE ELEMENT MODELING OF HEMISPHERE SUPERPLASTIC FORMING USING ANSYS

The simulation of the hemispherical SPF process was performed using the ANSYS CAE system. To reduce computational cost while maintaining result accuracy, a simplified axisymmetric model was used.

The mathematical model was implemented as a boundary value problem of creep theory based on the Norton model, which describes the dependence of the strain rate on stress. According to the chosen model, the parameters of the K and m models were adjusted to describe the superplastic behavior of the material.

The Latin Hypercube Sampling (LHS) method was used to determine the values of the material parameters K and m , essential for the model, within ranges typical for aluminum alloys.

The following mechanical properties of the aluminum alloy were used to determine its elastic characteristics:

- 1) Young's modulus (E) = 70 GPa;
- 2) Poisson's ratio (μ) = 0.34.

To implement the numerical model in ANSYS, solid models of the blank and the die were created. The blank was modeled as a deformable shell, while the cylindrical die was defined as a rigid tool that determines the final shape of the product. The modeling process began by defining their geometric dimensions. The modeling scheme is presented below (Fig. 1).

Compliance with the limitations of the student version of ANSYS 10 required optimization of the finite element mesh. For the blank model, 2112 four-node elements were determined, distributed across four layers with 278 elements per layer. In the clamping zone, where deformations are insignificant, the mesh density was reduced to 25 elements per layer.

The initial mesh configuration (Fig. 2a) and its final state (Fig. 2b) after completion of the superplastic forming process through the cylindrical die are presented below (Fig. 2).

As can be seen from the Creep Strain Intensity distribution, the most critical zone in terms of localization of thinning is the dome pole (Fig. 3) of the hemisphere.

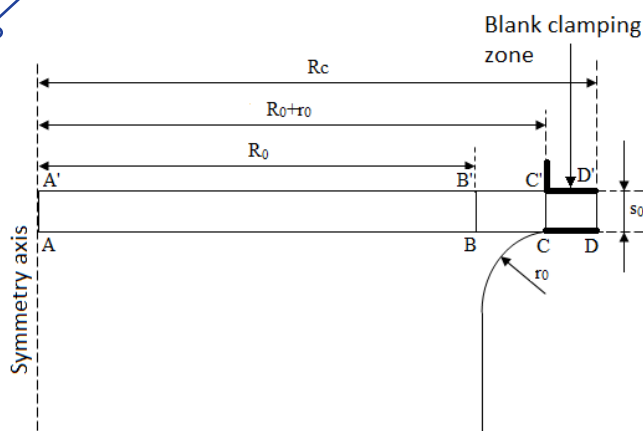
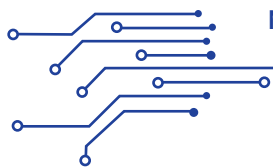
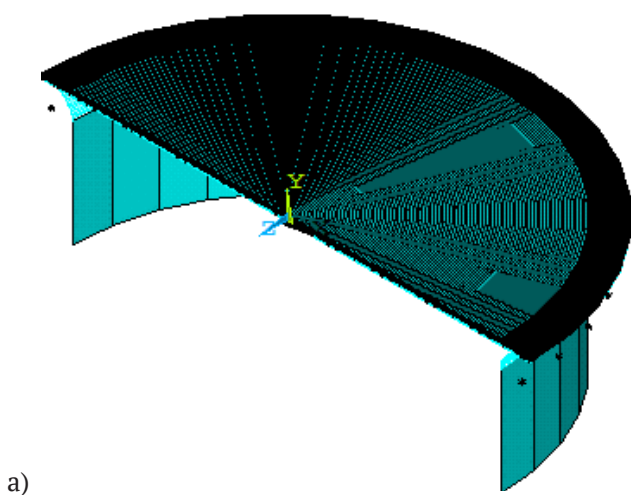
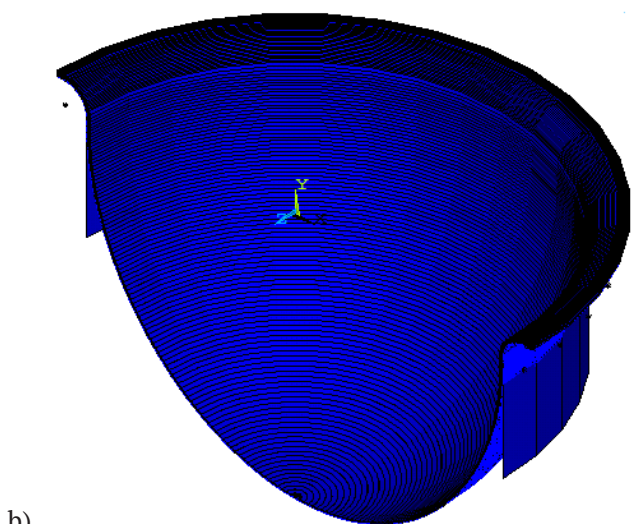


Fig. 1. Schematic Model of the Blank and Cylindrical Die: *ACC'A'* – the Deformable Zone, *CDD'C'* – the Clamping Zone, R_0 – the Die Radius, r_0 – the Die Entrance Radius, R_c – the Blank Radius, s_0 – the Initial Blank Thickness

Source: Compiled by the authors.



a)



b)

Fig. 2. Finite Element Mesh: a) in the Initial Configuration, and b) in the Final Deformed State

Source: Compiled by the authors.

SELECTION AND APPLICATION OF THE MACHINE LEARNING METHOD

To develop a predictive model for the geometric characteristics of a hemisphere produced by the SPF process, the following machine learning methods were considered: artificial neural networks [12, 13], random forest [14], and Gaussian Process Regression (GPR) [15, 16].

The GPR method was selected for predicting the geometric characteristics of the hemisphere for the following reasons:

- It provides not only a point prediction but also a variance estimate, enabling the construction of confidence intervals and quantitative assessment of the model's reliability, which is crucial in engineering applications.
- Nonlinear dependencies between material parameters, process conditions, and the resulting geometry are effectively approximated by GPR through the selection of an appropriate kernel function.
- The method demonstrates high accuracy for interpolation within the researched parameter range.
- The algorithm is suitable for training a model in conditions of a limited amount of data, which is typical for resource-intensive CAE simulations and shows more stable performance than deep neural networks.

To model complex relationships in the data, a kernel composed of the following components was selected [17]:

1. Radial Basis Function (RBF) kernel was used to model smooth, non-linear dependencies. This is appropriate because the SPF process is continuous, and its characteristics evolve smoothly with changes in input parameters.
2. ConstantKernel allows the model to automatically adjust the prediction scale to account for the actual variance in the data. This is necessary because the target parameters (height, thickness) vary within specific ranges.
3. WhiteKernel was incorporated to account for random errors inherent in the finite element modeling results, which are influenced by mesh density, time step, numerical solution methods, and other factors.

The kernels hyperparameters were optimized using the RandomizedSearchCV algorithm, which performed ten iterations with 2-fold cross-validation for the initial exploration of the parameter space.

The following methodology was applied to ensure the stability of the model:

1. RobustScaler was applied to scale all input features and output target variables to a comparable range. Unlike StandardScaler, it is more resistant to abnormal values, which are often found in real data and CAE simulations due to the use of median and interquartile range.

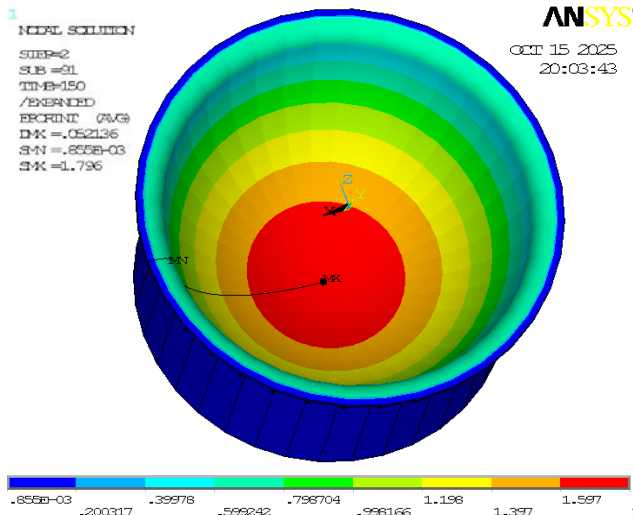
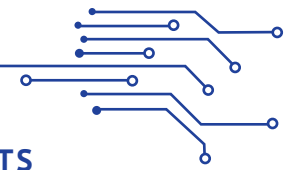


Fig. 3. Localization of Deformation and Thinning in the Pole of the Hemisphere Dome

Source: Compiled by the authors.

2. A combination of the alpha parameter (from $1e-8$ to $1e-2$) to protect against overfitting and the WhiteKernel trainable core so that the algorithm can independently estimate the noise level in the data during training.

3. The optimizer was configured with multiple restarts ($n_restarts_optimizer=5$). This strategy initializes the optimization process from different starting points to increase the probability of locating the global maximum of the likelihood function.

4. Three-stage data separation: creation of a training sample (60% of the total data), a validation sample (20%) and a test sample (20%).

5. Cross-validation to assess the generalizing ability of the model and its ability to predict on new data.

RESEARCH RESULTS

The effectiveness of the developed Gaussian process model was evaluated using standard regression analysis metrics: Mean Squared Error (MSE) and the coefficient of determination (R^2).

These metrics were calculated using the following formulas:

$$MSE = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2,$$

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y}_i)^2},$$

where y_i — is the actual value of the target variable; \hat{y}_i — is the value predicted by the model; \bar{y}_i — is the mean of the actual y values, calculated for the same sample used to compute R^2 .

The total initial dataset comprised 6250 samples, which were partitioned into three subsets:

- 1) 3750 samples (60%) for training;
- 2) 1250 samples (20%) for validation;
- 3) 1250 samples (20%) for testing.

Following hyperparameter optimization, the final Gaussian process kernel was determined as:

$$5.382 \times \text{RBF}(\text{length_scale} = 0.145) + \text{WhiteKernel}(\text{noise_level} = 1e-05).$$

The results of the evaluation of the forecasting model based on training, validation, and test samples are shown in *Table*.

The models performance during each hyperparameter optimization stage was assessed based on the coefficient of determination (R^2) calculated on the validation dataset. The model's final predictive

Table

Results of Gaussian Process Prediction for Hemispherical Geometric Characteristics

Target variable	Dataset	MSE, mm ²	R^2
Thickness (s)	Training	1.44×10^{-5}	–
	Validation	2.56×10^{-5}	0.9996
	Test	2.84×10^{-5}	–
Average height (h_{avg})	Training	0.065	–
	Validation	0.112	0.9994
	Test	0.124	–
Height difference (Δh)	Training	1.44×10^{-5}	–
	Validation	2.35×10^{-5}	0.9996
	Test	2.46×10^{-5}	–

Source: Compiled by the authors.

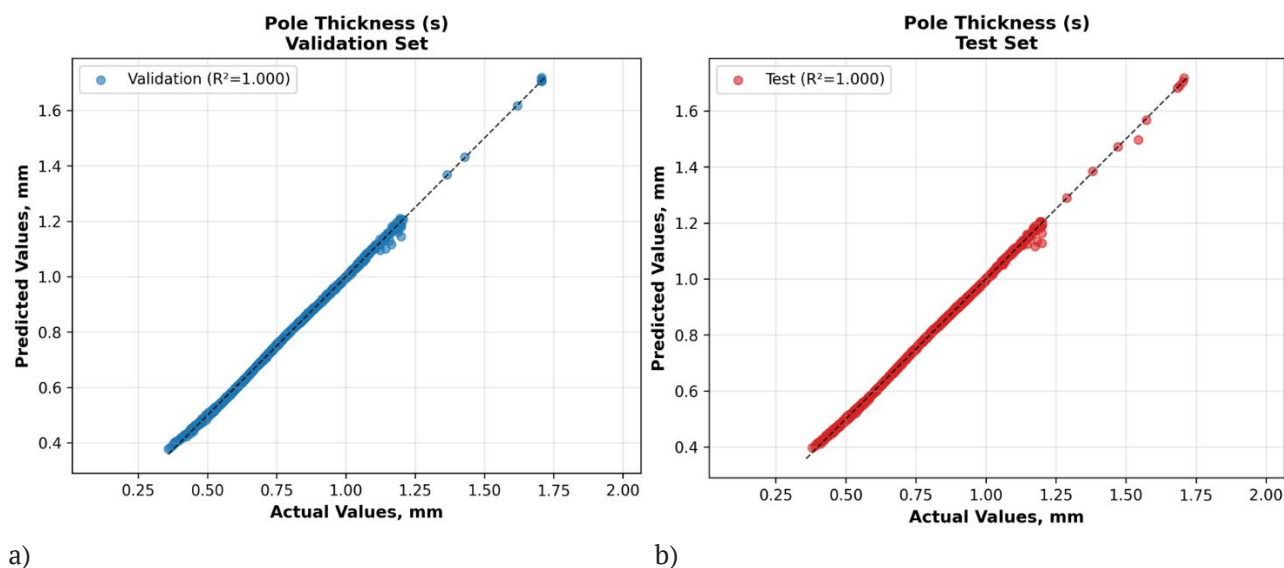
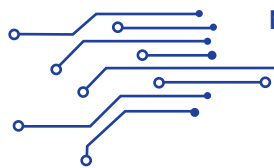


Fig. 4. Comparison of Actual Versus Predicted Thickness Values, s (mm): a) Validation Set, b) Test Set

Source: Compiled by the authors.

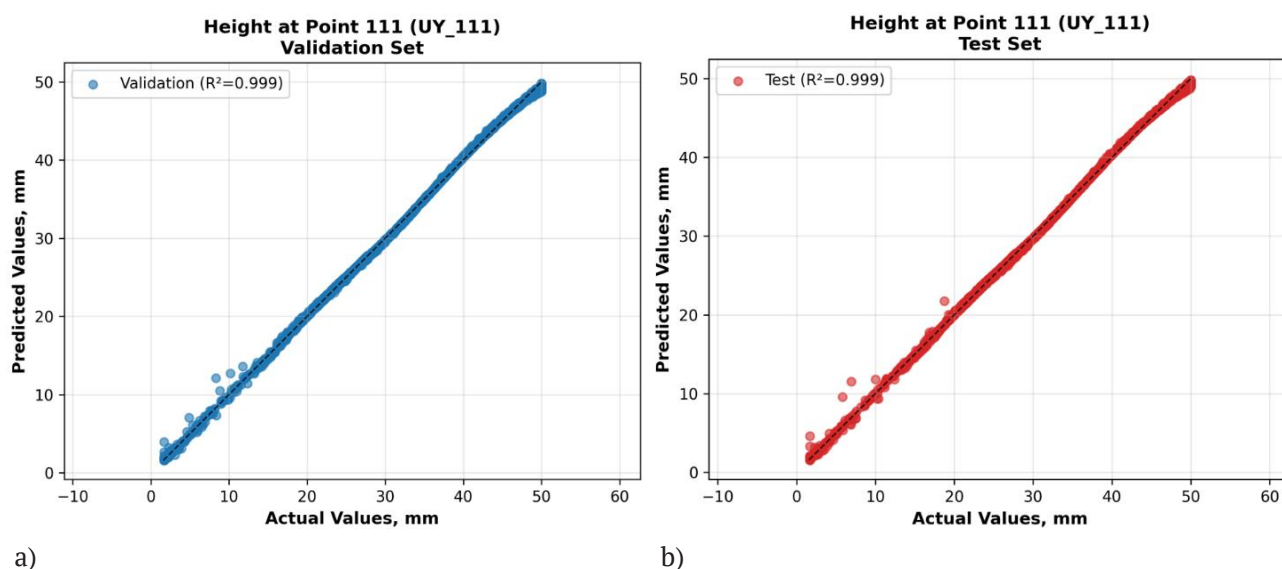


Fig. 5. Comparison of Actual Versus Predicted Height Values at Point UY 111: a) Validation Set; b) Test Set

Source: Compiled by the authors.

ability was evaluated on the test set using the mean squared error (MSE).

Prediction accuracy was visualized using scatter plots (Figs. 4, 5), comparing actual (x-axis) versus GPR-predicted (y-axis) values. The proximity of points to the $y=x$ bisector indicates model performance, with separate validation and test plots for thickness (Fig. 4) and height (Fig. 5). Point color intensity represents absolute error magnitude.

Two GPR prediction plots with confidence intervals were generated to visualize model uncertainty:

- 1) thickness (s) with confidence intervals (Fig. 6a);
- 2) height UY_1 with confidence intervals (Fig. 6b).

Both plots display time on a logarithmic scale.

DISCUSSION OF RESULTS

The results presented in Table demonstrate the performance of the GPR model for predicting the geometric characteristics of a hemisphere after superplastic forming. Analysis of the metrics reveals the following:

1. The MSE on the training set is slightly lower than on the validation and test sets, which is normal and indicates some degree of memorization of the training data. The nearly identical MSE values on the validation and test sets signify that the model has learned the underlying patterns rather than merely memorizing noise or specific cases from the training set.

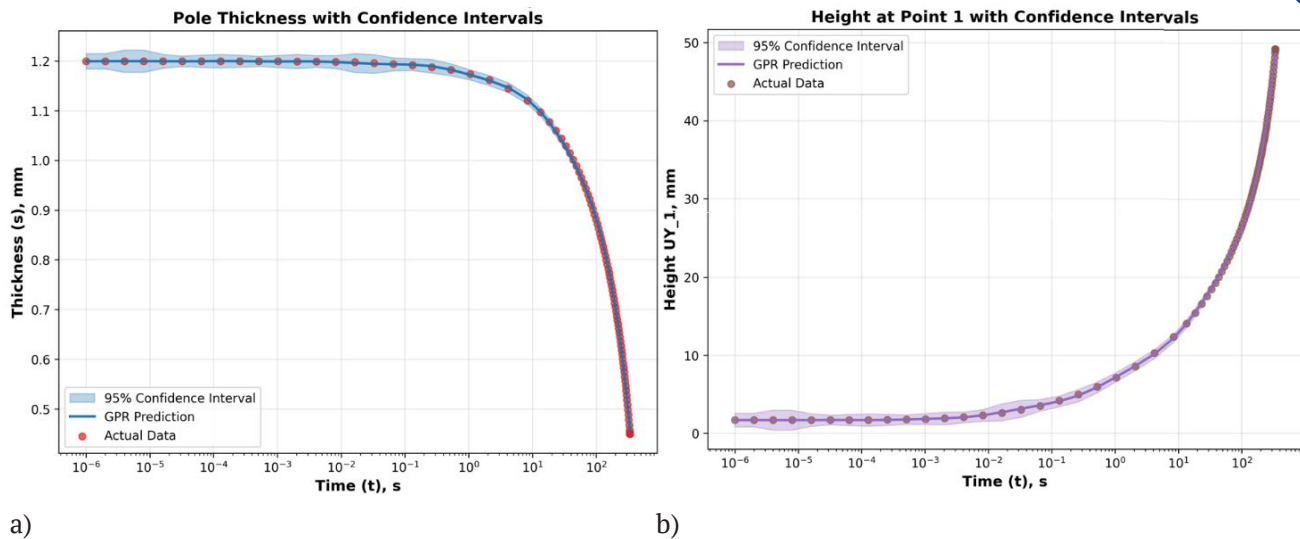


Fig. 6. GPR Uncertainty Plots for a Test Dataset Instance with Parameters $m = 0.471$, $K = 203.0 \text{ MPa}\cdot\text{s}^m$, $p = 0.29 \text{ MPa}$: a) Thickness Confidence Interval at Dome Pole; b) Height Confidence Interval at Location UY 1

Source: Compiled by the authors.

2. Analysis by target variables thickness (s), average height (h_{avg}), and height difference (Δh) with a validation set score of $R^2 \approx 0.9996$, indicates that the model explains approximately 99.96% of the variance in the target variable.

Analysis of the scatter plots (Figs. 4, 5) demonstrates that the GPR model is generally accurate and adequate, as evidenced by the dense point cloud along the bisector down to a thickness of 1.2 mm, which corresponds to the initial blank thickness.

The confidence intervals (Fig. 6) reveal a technological window where stable results can be expected. The consistent positioning of actual data points within the central region of these intervals indicates a controllable and robust process.

The wider confidence interval at the process onset likely reflects inherent uncertainty during the initial stage, potentially associated with challenges in simula-

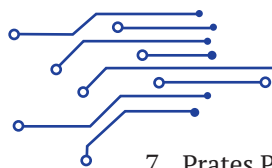
ting the early phase where plastic deformation just begins to develop in the material. The subsequent narrowing of the interval suggests that the deformation process has stabilized, exhibiting highly predictable behavior that is well-captured by the selected material model.

CONCLUSIONS

The developed Gaussian process model demonstrated high accuracy and reliability in predicting the geometry of hemispheres produced by superplastic forming. The high values $R^2 \approx 0.9996$ and the close agreement between errors on the validation and test sets confirm that the model successfully learned the underlying physical relationships without overfitting. Analysis of scatter plots and confidence intervals indicates a controllable and robust process, with the model adequately capturing its physics, particularly during the stable deformation phase.

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