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Data Engineering and Machine Learning for Solving the Inverse Problem Based on CAE Simulation Results

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ABSTRACT

The use of machine learning in solving direct forecasting problems is becoming an alternative to the use of comprehensive finite element modeling. However, the solutions of inverse problem by means of machine learning is conventionally not considered in the literature. Traditional approaches are based on iterative calculations that require multiple runs of models and do not work in real time, which limits the creation of digital doubles. **The objective of this study** is to solve the inverse problem by developing and verifying a Gaussian regression (GPR) model for determining the strain rate sensitivity index of superplastic material from the results of bulge tests based on the results of finite element calculations. The results of finite element modeling of the superplastic forming process in the ANSYS CAE package were used as a data source. 120 finite element simulations were performed, 40 for each of the three pressure modes. Two GPR models have been developed. One is for defining K with the Matern kernel, the second is for m with the RBF kernel. It is shown that replacing the RBF kernel with the Matern kernel ($\nu = 2,5$) reduces the median relative uncertainty of the forecast for parameter K from 50 to 16%. The following quality metrics were obtained on the test sample: $R^2 = 0.91$ for K and $R^2 = 0.92$ for m , the relative RMS error is 20% for K and 7% for m . **The developed model can be used** for non-destructive quality control, integration into digital twins, and optimization of superplastic forming processes.

Keywords: inverse problem; machine learning; Gaussian process regression (GPR); ANSYS; finite element modeling (FEM); CAE simulation; data engineering; superplastic forming (SPF)

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ОРИГИНАЛЬНАЯ СТАТЬЯ

Инженерия данных и машинное обучение для решения обратной задачи по результатам CAE-моделирования

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АННОТАЦИЯ

Применение машинного обучения в решении прямых задач прогнозирования становится альтернативой применению ресурсоемкого конечно-элементного моделирования. Однако применение машинного обучения для решения обратной задачи в литературе практически не рассматривается. Традиционные подходы основаны на итерационных расчетах, которые требуют многократных прогонов моделей и не работают в реальном времени, что ограничивает создание цифровых двойников. **Цель исследования** — решение обратной задачи путем разработки и верификации модели гауссовской регрессии (GPR) для определения параметров K и m по геометрии готового изделия на основе конечно-элементных данных ANSYS. В качестве источника данных использовались результаты конечно-элементного моделирования процесса сверхпластической формовки в CAE-пакете ANSYS. Было выполнено 120 конечно-элементных симуляций, по 40 для каждого из трех режимов давления. Общий объем данных, полученных из решений ANSYS, составил 7571 строку. Были разработаны две GPR-модели. Одна для определения K с ядром Matern, вторая для m с ядром RBF. Масштабирование данных выполнялось методом RobustScaler. Показано, что замена RBF-ядра на ядро Matern ($\nu = 2,5$) снижает медианную относительную неопределенность прогноза для параметра K с 50 до 16%. На тестовой выборке получены следующие метрики качества: $R^2 = 0,91$ для K и $R^2 = 0,92$ для m , относительная среднеквадратичная ошибка составляет 20% для K и 7% для m . Выполненный корреляционный анализ выявил наиболее значимое влияние давления формовки на параметр K ($r = -0,32$). **Разработанная модель может быть использована**



для неразрушающего контроля качества, встраивания в цифровые двойники и оптимизации режимов сверхпластической формовки.

Ключевые слова: обратная задача; машинное обучение; регрессия гауссовского процесса (GPR); ANSYS; конечно-элементное моделирование (КЭ-моделирование); CAE-система; инженерия данных; процесс сверхпластической формовки (СПФ)

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INTRODUCTION

In recent years, machine learning (ML) methods have found wide application in various fields, such as data analysis and control of technological processes. Their strength lies in their ability, by learning from experimental data, to identify complex nonlinear relationships between input process characteristics and output quality parameters [1, 2]. Therefore, predictive models built on these methods demonstrate high accuracy and can serve as an effective alternative to traditional approaches.

In particular, the significant potential of ML methods is revealed in the tasks of modeling and optimizing complex technological processes of metal forming by pressure. One of the promising areas for applying ML models is superplastic forming (SPF) — a technological process that makes it possible to produce parts of complex shape without welded seams due to the material's ability to undergo significant (up to hundreds of percent) strains without fracture [3–5].

For example, in [6], a method for intelligent design of superplastic forming process parameters based on an improved backpropagation neural network is proposed, which confirms the effectiveness of ML for complex technological tasks.

Numerical simulation of SPF is usually carried out using the finite element method (FEM), for example, in ANSYS or ABAQUS [7–9]. In this approach, an important aspect is the accuracy of describing the material deformation under superplastic conditions: the more accurate the model, the more reliable the calculation results. The key factor here is the parameters of the constitutive equations, in particular, the strain rate sensitivity index m and the strength coefficient K , which are introduced into the finite element model and determine the material response under external loads. The main difficulty when working with the constitutive parameters K and m is that they vary depending on many factors, such as temperature, grain size, and prior heat treatment. Therefore, there are no universal fixed values for these parameters. Direct methods for determining them (e.g., tensile tests) are labor-intensive and destroy the sample.

Earlier, in [10], the direct problem of predicting the geometric characteristics of a hemisphere obtained during the SPF process was solved. Within that work,

a Gaussian process regression (GPR) model was built based on finite element modeling in ANSYS, making it possible to predict the thickness at the pole s and the height of the inner ($UY1$) and outer ($UY111$) dome surfaces from the given parameters K , m , pressure p , and time t :

$$X_{direct} = [K, m, p, t] \rightarrow Y_{direct} = [s, UY1, UY111].$$

In [10], two pressure levels were considered: 0.29 MPa and 0.56 MPa. For the present study, in order to analyze the effect of pressure on the forming process in more detail, a third level — 0.9 MPa has been added to expand the applicability domain of the model and improve prediction accuracy over a wider range of loading regimes.

The ML model presented in [10] achieved high accuracy ($R^2 > 0.99$) on the validation set and demonstrated the possibility of replacing computationally expensive finite element modeling.

Unlike the direct problem, where the input parameters are known, the inverse problem of determining the constitutive parameters K and m from the geometry of the produced part remains less studied. Solving the inverse problem is important for creating digital twins, as it would allow refining the constitutive parameters without destructive testing, based on a single finished part.

Most of the problems considered that are solved using machine learning algorithms [11–13] are direct problems, whereas inverse problems are traditionally solved by iterative finite element calculations, which require significant computational resources and do not allow real-time operation.

The study conducted by the authors in [11] demonstrated the possibility of using ANNs for modeling complex technological relationships. In [11], a neural network was used to predict a set of mechanical properties of a cast alloy taking into account chemical composition, manufacturing technology, and heat treatment parameters. The study by authors [12] showed that a hybrid PSO-BP neural network predicts the thickness distribution of a part more accurately, especially in rounded areas, than the BP backpropagation algorithm, which confirms the possibility of using machine learning to analyze strain non-uniformity in SPF. In [13], the authors replaced direct finite ele-

ment calculations with a GPR surrogate model, which allowed them to reduce computational costs by a factor of 7–10 while maintaining high accuracy. Thus, direct problems of predicting geometry, properties, or thickness distribution in SPF are already being actively solved using ANN, PSO-BP, and GPR, whereas the inverse problem of reconstructing the constitutive parameters — the strain rate sensitivity index m and the strength coefficient K — from the geometry of the finished part remains virtually untouched in the literature, which defines its scientific and practical significance.

The aim of this work is to solve the inverse problem of superplastic forming by developing and verifying a GPR model for determining the parameters K and m from the geometry of the finished hemisphere based on ANSYS finite element data.

CONSTITUTIVE RELATIONS AND THEIR IMPLEMENTATION IN THE ANSYS CAE PACKAGE

In the classical formulation, superplastic forming is described by a power law relating the flow stress σ to the strain rate $\dot{\epsilon}$:

$$\sigma = K \cdot \dot{\epsilon}^m, \quad (1)$$

which is widely represented in the scientific literature [14–16].

In finite element modeling within the ANSYS CAE package, a different form of notation is used, adapted for the numerical calculation of deformation problems. ANSYS employs the Norton model, where the strain increment $\Delta\epsilon_{cr}$ over a time step Δt is expressed through the equivalent stress σ and the absolute temperature T :

$$\Delta\epsilon_{cr} = C_7 \sigma^{C_8} e^{-C_{10}/T} \Delta t. \quad (2)$$

C_7 is a scaling factor, C_8 is the stress sensitivity exponent, C_{10} is the temperature constant.

When modeling an isothermal SPF process, the temperature constant C_{10} can be set to zero ($C_{10} = 0$), which simplifies the exponential term to 1. Under constant temperature conditions, equation (2) reduces to:

$$\Delta\epsilon_{cr} = C_7 \sigma^{C_8} \Delta t. \quad (3)$$

This makes it possible to convert the parameters K and m into the ANSYS parameters C_7 and C_8 using the following formulas:

$$C_7 = \frac{1}{K^{1/m}}, C_8 = \frac{1}{m}, C_{10} = 0. \quad (4)$$

Since the original parameters K and m are more intuitive, the rest of this work will be based on them.

METHODOLOGY OF DATA GENERATION FOR SOLVING THE INVERSE PROBLEM

To build a model for determining the constitutive parameters K and m (1) from the hemisphere geometry, a dataset linking the input geometric features to the target parameters is required.

Because conducting physical experiments is expensive and time-consuming, the data were taken from finite element simulations of the superplastic forming process performed in the ANSYS CAE package.

To optimize computational resources while maintaining the required accuracy, an axisymmetric model was used. This approach transforms a three-dimensional problem into a two-dimensional one by exploiting the symmetry of the geometry and boundary conditions. It is widely adopted for modeling SPF of axisymmetric parts [15, 16] and provides acceptable accuracy with a significant reduction in computation time.

In ANSYS, the simulation began with constructing a geometric model of the blank and the cylindrical die (Fig. 1). The blank was defined as a deformable shell, while the die was represented as a rigid tool that determines the final shape of the part.

The parameters of the finite element model in ANSYS [8] were as follows:

1. Part geometry: sheet blank with initial thickness $s_0 = 1.2$ mm, round shape, diameter $D_s = 114$ mm; cylindrical die with diameter of $D_0 = 100$ mm.

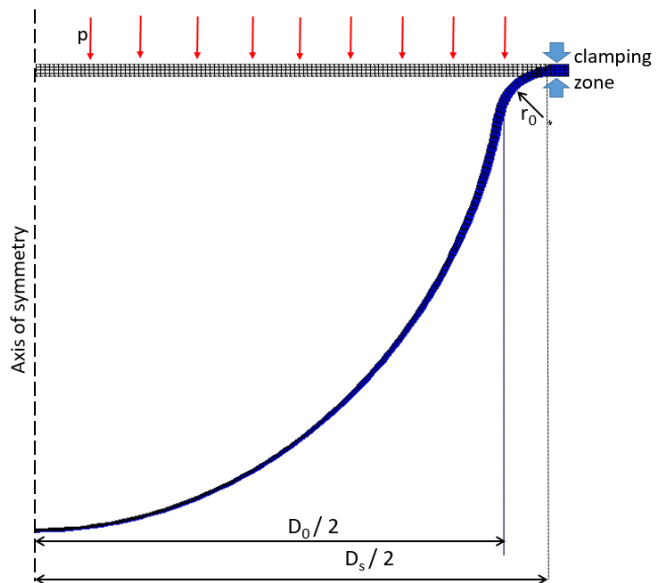
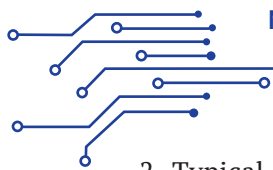


Fig. 1. Axisymmetric Finite Element Model with Mesh Overlay Before and After the Forming Process: D_0 – Diameter of the Cylindrical Die, D_s – Diameter of the Blank (Deformable Zone), r_0 – Entry Radius of the Die, p – Uniformly Applied Pressure

Source: author's calculations.



2. Typical mechanical properties of the alloy: Young's modulus $E = 70$ GPa, Poisson's ratio $\mu = 0.34$.

3. A 2D axisymmetric element PLANE183 was selected for the blank. CONTA172 and TARGE169 elements were used on the contact surfaces.

4. The blank mesh consisted of 2112 4-node elements.

5. Boundary conditions:

a) a uniform pressure p was applied to the top surface of the blank. Three experimental pressure levels were considered: $p_1 = 0.29$ MPa, $p_2 = 0.56$ MPa, and $p_3 = 0.9$ MPa;

b) blank constraints: a clamp is located in the contact zone between the blank and the die, therefore zero displacements were prescribed for both axes (All DOF = 0), and a symmetry condition $UX = 0$ was set on the axis of symmetry;

c) SPF process temperature: $T = 450$ °C.

6. For the mathematical model of the constitutive relationship, the Norton model was applied, following equation (2) and the parameter conversion (4).

The following parameters were varied to generate the training dataset:

1. The strain rate sensitivity index m was varied in the range typical for the superplastic state: $m = 0.3-0.7$.

2. The strength coefficient K was calculated for each value of m using equation (1).

3. Calibration of ξ and σ was performed by inverse modeling in ANSYS. The pressure histories $p(t)$ for each experimental case were set according to the input data. The parameters ξ and σ were varied within $\xi = 0.001-0.10$ s⁻¹ and $\sigma = 20-55$ MPa. The calibration criterion was the agreement between the calculated time to reach the experimental dome height and the actually measured time.

4. Forming pressure p : 0.29, 0.56 and 0.9 MPa following the experimental data from [8].

To capture the process dynamics and enlarge the training dataset without additional computational cost, intermediate forming parameters were recorded. For each ANSYS solution, the following quantities were saved at each time step:

1. Time t , s from the start of the process.

2. Current thickness s , m at the pole of the hemisphere.

3. $UY1$, m current height on the inner surface of the hemisphere.

4. $UY111$, m current height on the outer surface of the hemisphere.

The values of m within its typical range were sampled using the Latin Hypercube Sampling (LHS) method. LHS is a design of experiments technique that distributes points uniformly in a multidimensional parameter space with a limited number of simula-

tions. It was chosen because, for the same number of simulations, LHS produces more accurate models than the Monte Carlo method [17].

A total of 120 finite element simulations were performed, 40 for each of the three pressure levels. The total dataset obtained from the ANSYS solutions comprised 7571 rows.

For the inverse problem, the following data structure was adopted:

Input ($X_{inverse}$) = [s , $UY1$, $UY111$, t , p] → the Output ($Y_{inverse}$) = [K , m].

In this study, pressure p was included as an input feature, while only K and m were the target variables. If identifying p becomes necessary, the data structure can be modified by moving p to the target variables — a task that deserves a separate study.

DATA ENGINEERING AND FEATURE TRANSFORMATION WITH SCALING

Building a training dataset for the inverse problem involves several steps aimed at the correctness and efficiency of machine learning. The data from ANSYS were converted to CSV format and underwent the following steps:

1. To improve model stability and avoid loss of significance when dealing with very small numbers — for example, the height of the inner dome surface $UY1$ is on the order of 10^{-12} m, while the thickness s is down to 10^{-3} m — all linear dimensions were converted from meters to millimeters.

2. The superplastic forming process at the initial stage is characterized by an exponential growth of strains, followed by a slowdown. The time ranges from fractions of a second to thousands of seconds — on a linear scale, the data are distributed extremely unevenly. A logarithmic transformation of time, $\log t = \ln(t + \epsilon)$ ($\epsilon = 10^{-8}$), is applied in order to:

a) compress the dynamic range from 9 orders of magnitude to about 20 units;

b) maintain sensitivity to changes in geometry at the beginning of the process, when this is particularly important.

3. To evaluate the generalisation ability of the model, the data were randomly split into three parts:

a) 60% — training set;

b) 20% — validation set;

c) 20% — test set.

4. The input features differ in units of measurement and scales. For example, $UY1$ ranges from $3.7e-09$ to 49.7 mm, while pressure p ranges from 0.29 to 0.9 MPa. Therefore, scaling was applied using the RobustScaler method, which is robust to outliers and uses the median and interquartile range: $X_{scaled} = (X - median) / (Q75 - Q25)$, where $Q75$ and $Q25$ are the upper and lower quartiles.



Scaling was performed separately for the input features X and the target variables Y . To prevent data leakage from the test set into the training process, the scaling parameters (median and quartiles) were determined solely from the training set. These parameters were then applied to the validation and test sets.

5. When exporting data from ANSYS at the end of each simulation, duplicate rows were found, indicating that the limiting strain state had been reached. At that point, the geometric parameters stopped changing. To avoid overfitting, the model and to reduce the computational load, these duplicates were removed during the preprocessing stage. As a result, from 7571 original rows, 5505 unique values were selected (about 2066 duplicates removed, which is approximately 27% of the data).

JUSTIFICATION FOR CHOOSING THE MACHINE LEARNING

To solve the inverse problem of determining the constitutive parameters (1) from the geometry of the finished part, several machine learning methods were considered: artificial neural networks [18, 19], random forest [20], and Gaussian process regression (GPR) [13, 21, 22].

In this work, the GPR method was chosen to solve the inverse problem. This method offers several advantages confirmed in the scientific literature:

1. In [13], the authors demonstrated the effectiveness of using GPR under limited computational resources. They showed that applying GPR can reduce the number of direct finite element calculations by 70–90% compared to traditional methods, while maintaining high prediction accuracy ($R^2 > 0.96$). This result was achieved due to the ability of GPR to adaptively interpolate between training points and to quantify uncertainty, which is important for determining the constitutive parameters K and m .

2. The study [21] demonstrated that the GPR method has a built-in function for quantifying prediction uncertainty, which is essential for determining the constitutive parameters K and m from the geometry of the finished part. This method allows not only obtaining point estimates but also forming confidence intervals that characterise the reliability of identification.

3. The research presented in [22] showed that GPR effectively models complex processes whose outcomes depend on many heterogeneous factors, such as constitutive parameters, geometric features, and temperature regimes. The present study faces a similar situation: the geometry of the hemisphere after superplastic forming (SPF) is determined by five input parameters (s , $UY1$, $UY111$, $\log t$, p), which are in complex nonlinear relationships with the target characteristics K and m .

CONFIGURING THE GPR MODEL

The key element of a GPR is the kernel (covariance function). It determines how smooth the relationships between the data will be. In this study, two kernel configurations were tested.

First kernel configuration. Initially, it was assumed that the SPF process yields smooth relationships between the input parameters and the output characteristics. Therefore, the squared exponential kernel (RBF) was chosen for training, with the addition of a WhiteKernel to account for the errors in simulation and data export.

However, the analysis of the model training results showed that for the parameter K , the median relative uncertainty was about 50%, which is approximately twice the desired level.

Second kernel configuration. To improve the prediction accuracy for the parameter K , the Matern kernel ($\nu = 2.5$) was chosen, which corresponds to moderately smooth functions, as it is less sensitive to local variations.

For predicting the parameter m (where the relationships are smoother), the RBF kernel was retained.

For both kernels, a WhiteKernel component was added with a noise level of $1e-3$ (the value was determined experimentally).

The refined kernel configuration — Matern for K , RBF for m — yielded good results. $R^2 = 0.91$ for K and $R^2 = 0.92$ for m . For K , the median relative uncertainty decreased from 50 to 16%. Further hyperparameter optimization made no sense, as additional tuning no longer provided a significant improvement in quality.

RESEARCH RESULTS

The developed GPR model performed well in predicting the parameters of the constitutive relation (1). Table 1 presents the statistical characteristics of the target variables on the test set.

The coefficient of variation (CV) is calculated using the formula:

$$CV = \frac{\sigma}{\mu} \times 100\%,$$

where σ is the standard deviation of the actual values on the test set, μ is the mean actual value on the test set.

A CV value of 65% for the parameter K (see Table 1) indicates a significant spread of values of this parameter around the mean $\mu = 282.1 \text{ MPa} \cdot \text{s}^m$ in the original dataset. This is explained by the fact that the model was trained on a wide range of parameters of the constitutive relation (1): the values of the parameter m (0.3–0.7) and the corresponding K values were varied, as well as three pressure regimes p (0.29,

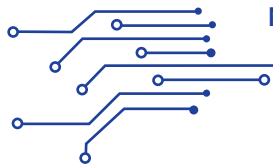


Table 1

Statistical Characteristics of the Target Variables in the Test Sample

Parameter	Mean (μ)	Standard deviation (σ)	Coefficient of variation (CV), %
K	282.1 МПа·с ^м	183.5	65.0
m	0.488	0.120	24.6

Source: Complied by the authors.

Table 2

Prediction Quality Metrics

Parameter	Set	R ²	RMSE	MAE	Relative RMSE, %
K	Validation	0.9346	44.9934	12.9657	—
	Test	0.9056	56.3923	16.1770	20.0
m	Validation	0.9363	0.0293	0.0116	—
	Test	0.9175	0.0343	0.0133	7.0

Source: Complied by the authors.

0.56 and 0.9 MPa). Table 2 presents the main quality metrics of the developed GPR model.

The relative RMSE (relative root mean square error) is calculated as:

$$\text{Relative RMSE} = \frac{\text{RMSE}}{\mu} \times 100\%,$$

where RMSE is the root mean square error, μ is the mean actual value of the target variable on the test set.

As can be seen from Figs 2 and 3, the actual and predicted values for K and m lie along the diagonal ($y = x$), indicating high prediction quality (see Table 2).

The scatter of points is slightly larger for K and denser for m , which corresponds to the difference in R².

Analysis of prediction quality for the parameter m :

1. The R² value exceeds 0.92 on the test set, indicating high prediction quality.

2. The low RMSE (0.0343) and MAE (0.0133) values also indicate high accuracy. The small difference between the validation and test sets confirms the absence of overfitting.

Analysis of prediction quality for the parameter K :

1. An R² value of ≈ 0.91 indicates good prediction quality of the developed model. The R² values on the validation (0.9346) and test (0.9056) sets are close,

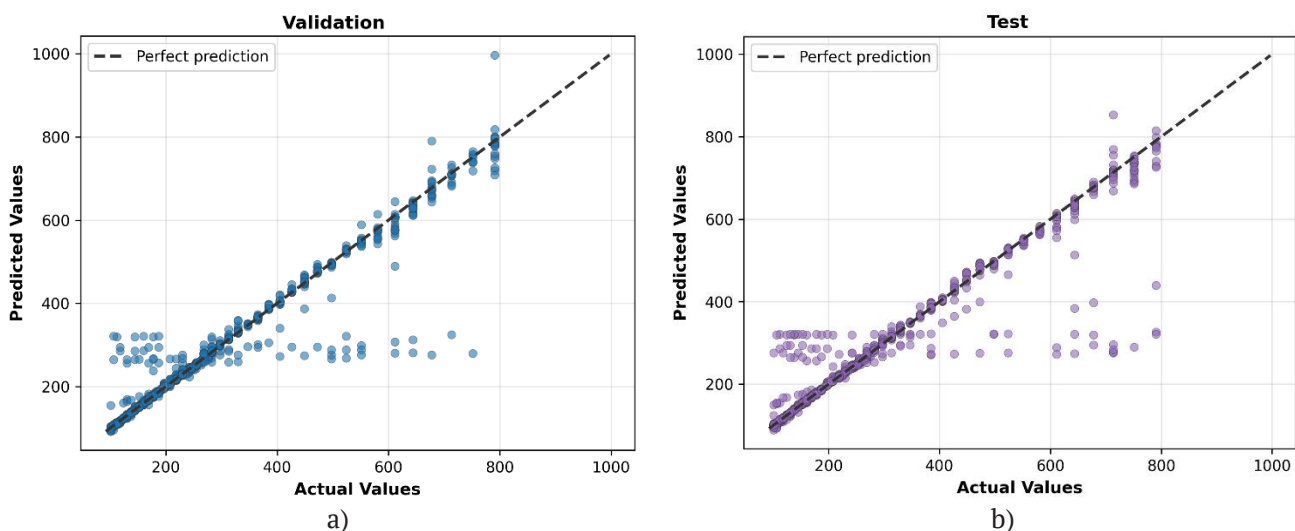


Fig. 2. Comparison of Actual and Predicted K Values (a – Validation set, b – Test set)

Source: author's calculations.

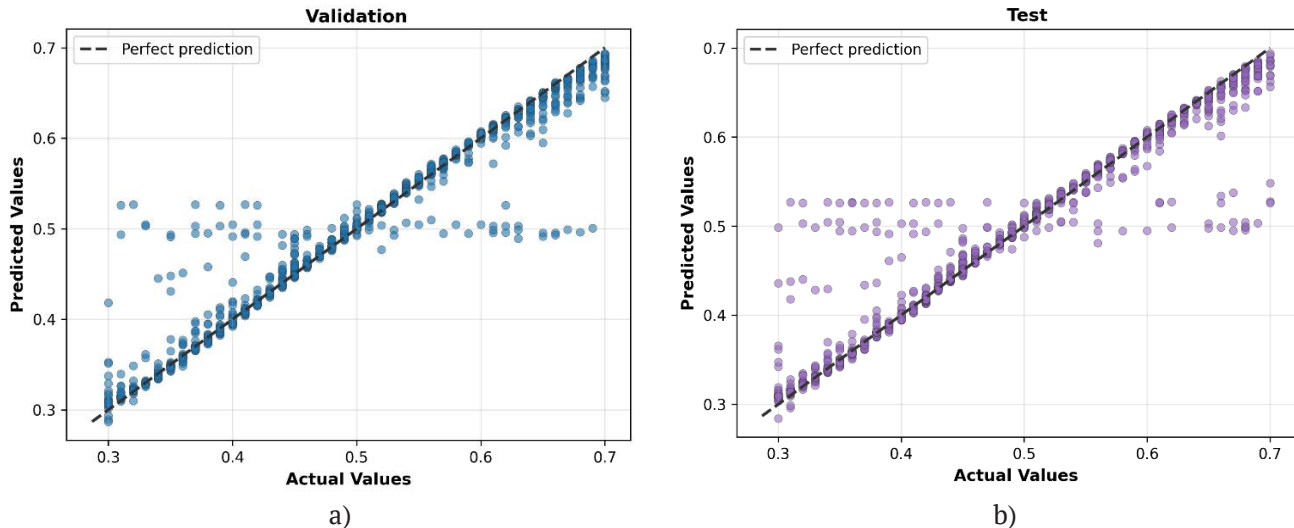


Fig. 3. Comparison of Actual and Predicted m Values (a – Validation set, b – Test set)

Source: author's calculations.

which indicates a good generalisation ability of the model and the absence of overfitting.

2. The obtained RMSE (≈ 56.4) and MAE (≈ 16.2) values require justification taking into account the scale of the data.

The mean value of the parameter K (see Table 1) on the test set is $\mu = 282.1 \text{ MPa}\cdot\text{s}^m$, and the standard deviation is $\sigma = 183.5$. Thus, the relative prediction error is:

$$\frac{RMSE}{\mu} \times 100\% = \frac{56.4}{282.1} \times 100\% \approx 20\%.$$

Thus, despite the high variability of the original data ($CV = 65\%$), the GPR model provides a relative prediction error for the parameter K of about 20%, which is a satisfactory result for the inverse problem of identifying the parameters of the constitutive relation (1).

To identify relationships between the parameters, a linear correlation analysis was performed. Its results are presented in Table 3 and Fig. 4.

Analysis of the correlation results (see Table 3 and Fig. 4):

1. Among all factors, pressure p has the most noticeable effect on K ($r = -0.32$). This is consistent with the physical principle of superplastic forming: the higher the strain rate, the lower the value of K should be.

2. The use of a logarithmic time scale made it possible to establish a weak correlation of the parameter K with the logarithm of time $\log t$ and thickness s (correlation coefficient $|r| \approx 0.12$). This result would not have been achievable using a linear time scale.

3. The values of $UY1$ and $UY111$ show little correlation ($|r| < 0.06$) with the target parameters K and m ,

Table 3

Correlations Between Input Features and Target Parameters (K, m)

Feature	With	
	K	m
Pressure p	-0.3199	-0.0091
Logarithm of time $\log t$	+0.1214	-0.0370
Thickness at the dome pole s	-0.1151	-0.0544
Dome height on the inner surface of the hemisphere $UY1$	+0.0587	+0.0062
Dome height on the outer surface of the hemisphere $UY111$	+0.0594	+0.0067

Source: Compiled by the authors.

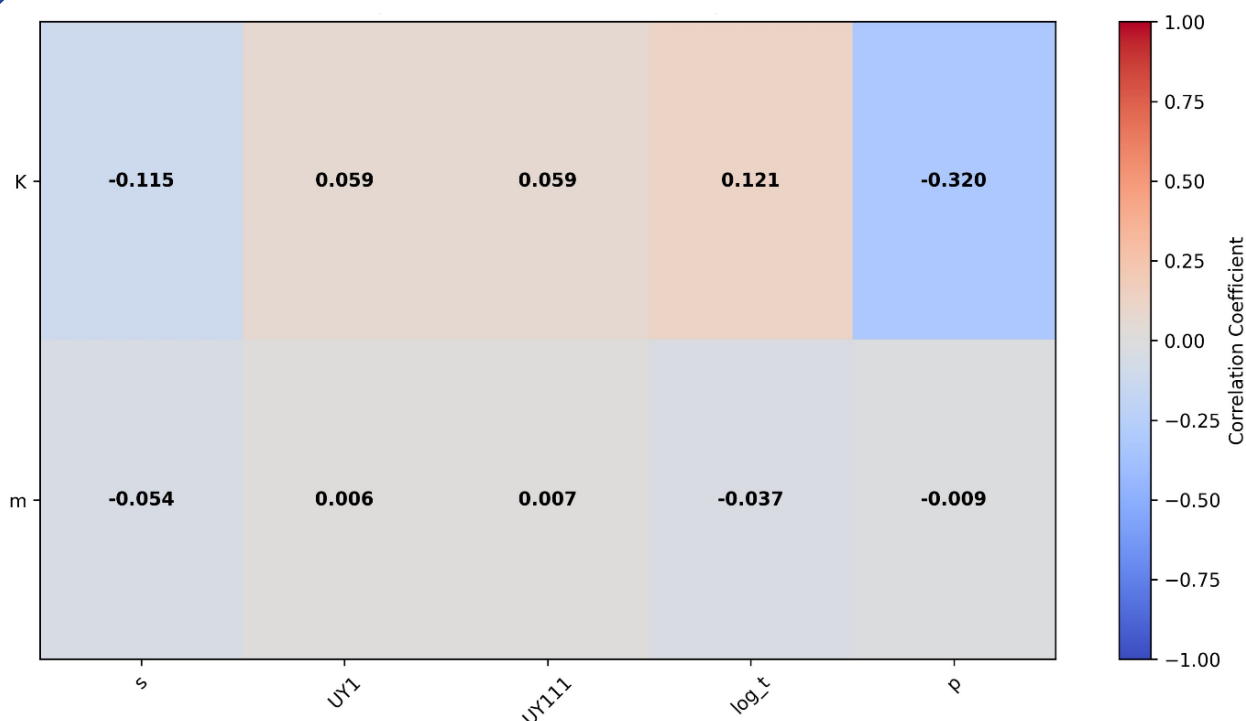
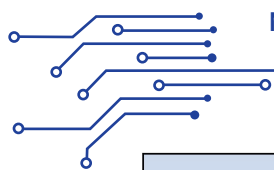


Fig. 4. Correlation Between Features and Target Variables, Data in mm Fors, UY1, UY11

Source: author's calculations.

which is justified in the case of solving the inverse problem, since they are not input characteristics.

4. The correlation results show that the parameter m correlates weakly with other features, which may be due to the fact that its value is almost independent of the input data within a linear model. Therefore, the choice of a nonlinear machine learning method, in particular GPR, to identify complex relationships is well justified.

CONCLUSIONS

To solve the inverse problem of determining K, m from the geometry of the finished hemisphere, a Gauss-

ian regression (GPR) model has been developed and tested.

The key result in determining the value of parameter K is the replacement of the RBF kernel model with Matern, which reduced the median relative uncertainty of the forecast from 50 to 16%. The correctness of choosing GPR to solve the inverse problem is further confirmed by the correlation analysis, which revealed the nonlinear nature of the relationships between the input geometric parameters and the target variables.

The model developed may be used for non-destructive quality control, integration into digital counterparts, and optimization of superplastic forming processes.

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