

Data Modeling Technologies for Process and Quality Control

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Abstract

Due to progress in information technology and artificial intelligence, improvements of processes based on the analysis of accumulated big data are highly expected in the steel industry as well as in other fields. However, attainments of improvement in real processes require methodologies compatible with physical models based on fundamental principles and operational knowledge in factories. This article introduces data modeling technologies and their applications deploying the strength of developments in physical and statistical models.

1. Introduction

Along with the recent dramatic progress of information and artificial intelligence technology including machine learning, large-scale database systems collecting data through the high-speed network are now able to be built to produce added value from the analysis of big data. Also in the steel industry, data from control and production management systems have been collected and stored for many years, the data capacity and the storage period have greatly increased, and the system environment collecting and analyzing various information across different systems has been built. Improvement of quality or high productivity is expected by the effective use of these data concerning actual operations.

However, in the steel industry, various processes produce various types of products at high productivity with strict operation restrictions. Since many improvements based on technological developments and accumulated operation knowledge have already been made, attempts for further improvement of yield and high productivity may often result in unsatisfactory results by only applying statistical analysis or machine learning.

Nippon Steel & Sumitomo Metal Corporation has physical models developed over many years based on fundamental principles and operation knowledge based on the experience in factories. Further improvements of the processes require the combination of the physical model based on physical/chemical knowledge with statistical analysis and machine learning, and methodologies compatible with operational knowledge in factories. The research and development departments of instrumentation and control in Nippon Steel & Sumitomo Metal have continuously researched and developed data mod-

eling technologies taking advantage of the strength of both physical model and statistical model developments. This paper introduces these technologies and examples.

Quality measures in steel production include indexes indicated by quantitative values such as temperatures determining the metallurgical structure as well as product dimensions (thickness and width), and qualitative evaluation indexes such as acceptance judgment for product surface or internal defects. First, in Chapter 2, technologies for quantitative measures are introduced and in Chapter 3, technologies of quality improvement for qualitative measures are introduced.

2. Process Control with Data Modeling Technology

For quantitative quality measures indicated by values such as dimensions (thickness and width) of steel products and temperatures, predictions and process control by physical models based on physical/chemical principles have been widely implemented. However, application of physical models based on theories or experiments to real processes requires adjustments of the models to fit the actual equipment or process, and error adjustments of the physical and control models by regression as alternatives of the physical models have been widely used.

While physical models are highly persuasive with clear correlation of their configuration and formula with real processes, it is difficult to describe all phenomena and the accuracy may be unsatisfactory. In contrast, while it is easier for statistical models (including machine learning models) based on the real process data to obtain high accuracy, their correlation with the processes is not always

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clear (less descriptive). In addition, the problem is that their accuracy is not reliable for new operating conditions or products.

Therefore, technology of gray box modeling has been developed to ensure descriptiveness for the process and improve the accuracy by combining physical and statistical models. This gray box was named by mixing both the black box meaning low descriptiveness of the statistical model and the white box meaning high descriptiveness of the physical model.

Various types of methods are considered for gray box modeling. The popular methods used in actual operations are as follows:

First, as shown in Fig. 1(a), error of the physical model is adjusted with the statistical model to improve the prediction accuracy of the model. In this model, using the recorded data of the physical model prediction errors, the statistical model predicting the errors is created.

Then, Fig. 1(b) shows the type of method in which the statistical model sets the parameters of the physical model. This method is suitable for the case in which qualitative characteristics of the process are well described by the physical model but it is difficult to determine the parameters in a real situation. Parameters of the physical model are estimated from the operation records with some method and the statistical model predicting the parameters is created.

Although Fig. 1(c) shows the type of method in which only the statistical model is used in actual operation, improving descriptiveness of the statistical model by correlating with physical characteristics of the process and implementing physical knowledge in advance in building the statistical model are enabled.

Examples of the three model types above are introduced in the

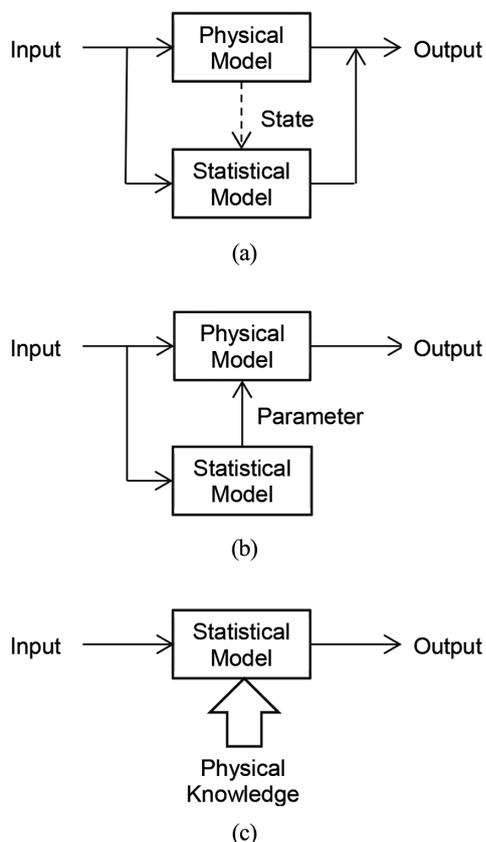


Fig. 1 Various configurations of gray box modeling

following sections.

2.1 Physical model adjustment technology with statistical model

First, we introduce an example of improving the accuracy for prediction of the steel pipe shrinkage factor in the medium diameter seamless mill at Wakayama Works, Nippon Steel & Sumitomo Metal to improve the prediction accuracy of the model by adjusting the physical model error with the statistical model.¹⁾

The medium diameter seamless mill was a state-of-the-art mill at the time of installation in 1997 under the concept of a simple and compact mill. As shown in Fig. 2, the reheating furnace that has been indispensable for conventional mill configuration was eliminated, and a very compact mill was achieved by placing the three-roll sizer that also has the extractor function immediately after the mandrel mill. However, problems that were not found in the conventional mill have appeared. The problem with the largest effect was fluctuation of the sizer finish temperature. To solve this problem, the development of a new control technology was started.

Figure 3 shows the system configuration of the developed outer diameter control system. The shrinkage factor of steel pipe depends on the average temperature of the steel pipe at the sizer delivery, but the inside temperature of the steel pipe cannot be measured. Therefore, predictive calculation is performed using the temperature simulator. The temperature simulator calculates the prediction of the temperature distribution inside the steel pipe using the records of the process and the transfer time from the heating furnace extraction to the sizer rolling as input. Inevitably, there are model prediction errors. Also, since the inside temperature of the steel pipe cannot be measured, adjustment to the predicted value of the temperature simulator is added using the actual shrinking factor as the valid value. In this case, the adjustment table for each stratum is maintained based on the analysis result of the error factor.

Figure 4 shows the concept of case-based modeling that models a plant based on the past experience, recorded values, and input/output relations. From the past cases stored in the database, only similar cases which are in the vicinity of the current operating conditions are selected, and model output is created by local modeling that minimizes the prediction error of the data in the vicinity. In this application, predictions of the conventional control model (temperature simulator) are used and only the remaining model errors are predicted by the case-based modeling technology.

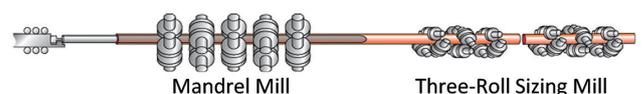


Fig. 2 Plant configuration of Wakayama Works seamless pipe mill

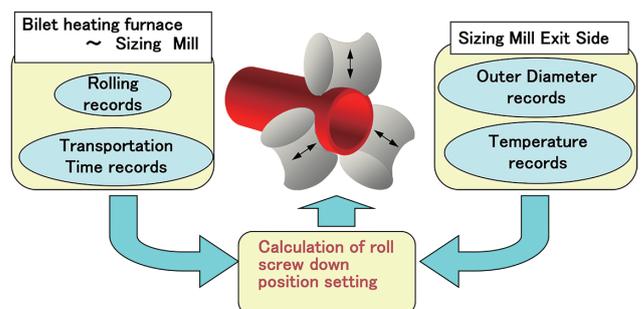


Fig. 3 System configuration of diameter control

Figure 5 shows the simulation verification result for investigating the effect of neighborhood setting on the prediction accuracy. Figure 5(a) shows the prediction accuracy of the sole physical model without adjustment. Figure 5(b) shows the accuracy when it is assumed that errors of the physical model are predicted using the concept of the case-based modeling to automatically generate the adjustment table values. This indicates that the prediction accuracy is improved by adding automatic adjustment compared to the conventional accuracy. When the area is set wider, the histogram curve becomes gradual (Fig. 5(c)). When the area is set narrower, the curve becomes steep (Fig. 5(d)). Even though the narrow area improves the prediction accuracy, it requires care for adverse effects are easily

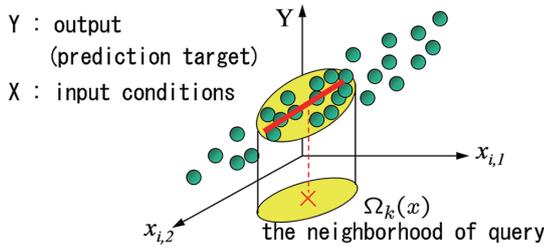


Fig. 4 Case-based modeling

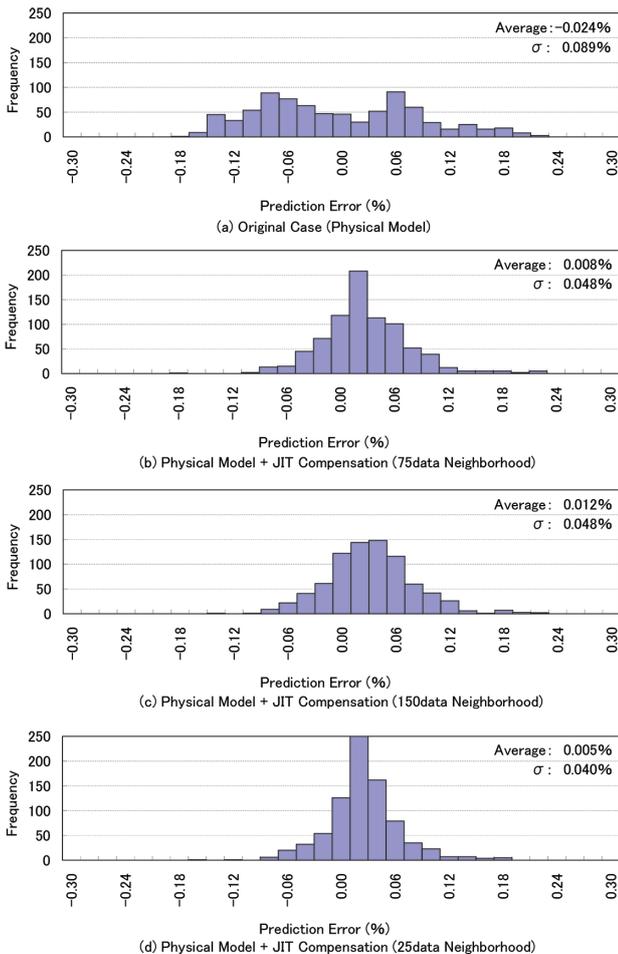


Fig. 5 Relationship between setting of neighborhood and prediction errors

caused by outliers included in the accumulated data.

2.2 Setting parameters of physical model with statistical model

As an example of the second type (Fig. 1(b)) of gray box modeling, development details of the converter blowing control model^{2,3)} are introduced.

The converter blowing control model instructs necessary blowing oxygen volume and cooling material input volume to achieve the specified target value of the molten steel temperature/carbon concentration measurement value at the end-point in blowing (end of the process) using the molten steel temperature and the carbon concentration measurement value obtained by substance measurement as the start point during blowing, and recursively estimates molten steel carbon concentrations and temperatures after the substance measurement. Usually, it consists of the oxygen balance equation (for estimation of carbon concentration) and the heat balance equation (for estimation of oxygen). Here, the oxygen balance equation is the target for review.

The oxygen balance equation is obtained by integrating the relationship between the decarburizing oxygen efficiency (η) and the molten steel carbon content ([C]) with respect to the blown oxygen volume (O_2) and [C]. As shown in Fig. 6, towards the end of blowing, for which this model is applicable to control, η reduces as [C] becomes smaller along with the progress of blowing. This is because the decarburization reaction ($[C] + 1/2O_2 \rightarrow CO \uparrow$) is changed from oxygen supply rate-limiting to carbon supply rate-limiting.

[C] when η starts reduction is called critical carbon concentration (C_{cr}). It is the value characterizing the decarburizing behavior at the end phase of blowing as well as the maximum decarburizing oxygen efficiency (k_2) during blowing. C_{cr} and k_2 vary under the effect of operating conditions including upper base blow gas conditions and slag volume. Therefore, it is important to evaluate C_{cr} and k_2 accurately in order to obtain the correct oxygen balance equation.

Next, the specific formula of the oxygen balance equation is derived. The relationship between η and [C] is expressed by Equation (1) using C_{cr} and k_2 .

$$f(C) = k_2 \times \left(1 - \exp\left(-\frac{(C - C_L)}{C_{cr}}\right) \right) \quad (1)$$

The oxygen balance equation of Equation (2) is obtained by integrating Equation (1).

$$\Delta O_2 = \frac{C_{cr}}{k_2} \left(\frac{1}{C_{cr}} (C_{SL} - C) + \ln \left(\frac{1 - \exp(-(C_{SL} - C)/C_{cr})}{1 - \exp(-(C - C_L)/C_{cr})} \right) \right) \quad (2)$$

In the frame of the gray box modeling, this oxygen balance equation corresponds to the physical model. Its parameters, C_{cr} and k_2 , are estimated by the statistical model.

In order to build the statistical model, the actual values of C_{cr}

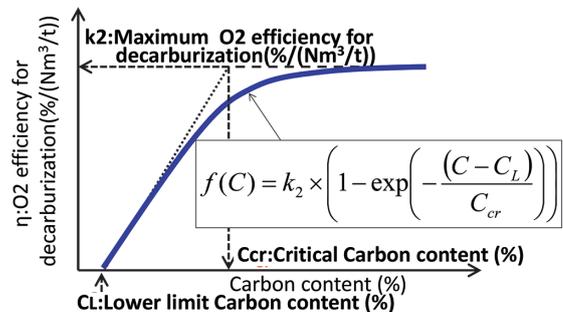


Fig. 6 Relation between O₂ efficiency for decarburization and carbon content

and k_2 are required. To this end, it is necessary to measure [C] during blowing in a short cycle. Even though it may be possible at the laboratory level, it is not realistic to obtain the number of samples required to build the statistical model with this method. In this way, using the operation record data (blowing oxygen volume, and blowing and end-point carbon concentration) of the actual plant, C_{cr} and k_2 are estimated (identified) by the mathematical programming problem described later. Assuming these estimates as the actual values, the statistical model is built. This mathematical programming problem is a non-linear optimizing problem consisting of the oxygen balance equation as the restrictive condition and the objective function minimizing the deviation of C_{cr} from the standard value obtained from conventional knowledge, etc. and the deviation of k_2 from the theoretical value. Solving this problem by sequential quadratic programming, reasonable values of C_{cr} and k_2 are obtained satisfying the oxygen balance.

Online calculation for the actual plant predicts C_{cr} and k_2 using the prediction equation obtained in advance, and, by applying these predicted values to the oxygen balance equation, sequentially calculates the necessary blowing oxygen volume and molten steel carbon concentration.

The prediction equation of C_{cr} and k_2 is built by the multiple regression model by setting C_{cr} and k_2 as the response variables that are identified by the mathematical programming with the recorded data of the past operation of the actual equipment and setting various operational conditions as predictor variables. Table 1 shows the estimated model parameters of the C_{cr} prediction formula and F values of operation factors obtained from the analysis of variance (the larger the F value, the larger the effect of the operation factor on C_{cr}). Table 1 shows that the F value of quicklime input is larger than other operation factors, that the sign of the parameter is positive, and that C_{cr} increases when quicklime input (\approx slag volume) is large. The result conformed to the knowledge of the conventional study (if slag volume increases, the decarburizing oxygen efficiency at the end of blowing is lower).

Figure 7 shows the relationship between the recorded values and estimated values of the end-point carbon concentration obtained from the oxygen balance equation applying the predicted values of C_{cr} and k_2 . The end-point carbon concentration was well estimated in a relatively wide range from low to medium carbon.

The converter blowing control model introduced in this paper is

being deployed to other steel works in Nippon Steel & Sumitomo Metal. It has been confirmed that the prediction accuracy improves when the oxygen remaining in the furnace obtained from the exhaust gas information is used for predictor variables. Further improvement of accuracy can be expected using machine learning, which has been remarkably developed in recent years, for building of the statistical model (prediction equations of C_{cr} and k_2).

2.3 Statistical model exploiting physical knowledge

There are many processes that use the control model created with regression, etc. from actual data because an appropriate physical model is not available, or even if it is available, it is difficult to adjust parameters for the real process. In order to improve the control accuracy and to reduce the maintenance load for such processes, the automatic building method of control models was developed.⁴⁾

Many statistical models used in actual operation use multiple models stratified by production conditions to meet non-linearity of the process. However, as building models including the stratum conditions depend on human experience and trial and error, the work load for model adjustment is high and the problem is deterioration of accuracy due to diversification of product types and other reasons. To this end, the method for building regression models, which automatically creates appropriate stratification using the operation

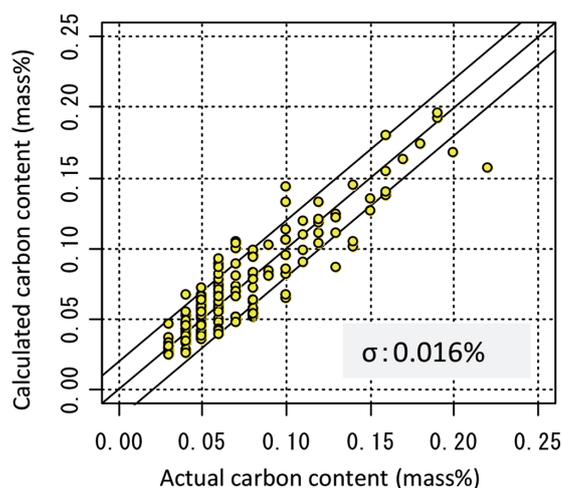


Fig. 7 Accuracy of carbon content estimation

Table 1 Results of regression of C_{cr}

No	Operational conditions	Parameters	t value	Pr (> t)	Df	Sum Sq	Mean Sq	F value	Pr (>F)	
1	(Intercept)	-0.1638	-1.3	1.88E-01	-	-	-	-	-	
2	Hot metal [Si]	-0.1250	-2.6	0.010338	1	0.2777	0.2777	53.7	3.09E-13 ***	
3	Hot metal [Ti]	0.1521	2.9	3.90E-03	1	0.033	0.033	6.4	1.16E-02 *	
4	Hot metal temp	0.0002	4.0	6.58E-05	1	0.0371	0.0371	7.2	7.42E-03 **	
5	Hot metal weight	-0.0007	-4.0	5.85E-05	1	0.2002	0.2002	38.7	5.66E-10 ***	
6	Lime	0.0067	9.5	2.00E-16	1	1.6034	1.6034	310.0	2.00E-16 ***	
7	Scale	0.0004	2.4	0.016748	1	0.0639	0.0639	12.4	4.46E-04 ***	
8	Sub material 1	-0.0004	-2.6	0.008235	1	0.1118	0.1118	21.6	3.49E-06 ***	
9	Sub material 2	-0.0038	-2.2	2.46E-02	1	0.0311	0.0311	6.0	1.43E-02 *	
10	Oxygen gas flow rate	0.0000	10.8	2.00E-16	1	0.6456	0.6456	124.8	2.00E-16 ***	
11	Bottom gas flow rate	-0.0018	-2.8	5.11E-03	1	0.0325	0.0325	6.3	1.23E-02 *	
Residuals					2710	14.0163	0.0052			

*: Pr < 0.05, **: Pr < 0.01, ***: Pr < 0.001

data in the past, was developed.

The model equation of the developed method is shown below:

$$\hat{y} = \sum_{i=1}^M \underbrace{(w_{i0} + w_{i1}u_1 + w_{i2}u_2 + \dots + w_{ip}u_p)}_{\hat{y}_i} \Phi_i(\bar{u})$$

The input variable space consisting of operation factor $\bar{u} = (u_1, \dots, u_p)$ is divided into the M number of local areas. In each local area, the relationship between quality y and operation \bar{u} is modeled by a linear equation. The full model is expressed as the sum of each local linear model \hat{y}_i with weight of the non-linear weight function $\Phi_i(\bar{u})$. $\Phi_i(\bar{u})$ indicates the contribution of local linear model \hat{y}_i . It takes the value of 1 in the area where \hat{y}_i is dominant, and takes the value close to 0 in the area where there is almost no effect. For any \bar{u} , $\sum_{i=1}^M \Phi_i(\bar{u}) = 1$ is satisfied. **Figure 8** is an example of weight functions that divide the space of two variables into 3 areas. Using such smooth weight functions at the area boundary, the full model also has continuous and smooth characteristics. As shown in **Fig. 9**, division of the input variable space into local areas is performed until a necessary model accuracy is obtained, starting from the entire space and sequentially selecting the division with the highest accuracy among methods dividing any area into two.

The selection of the division of the areas can be made among division candidate points dividing the area evenly or dividing the number of data in the area evenly. The division candidate points can also be provided from the preliminary physical knowledge or operation standard. The latter builds the model incorporated with preliminary knowledge and improves descriptiveness of the model.

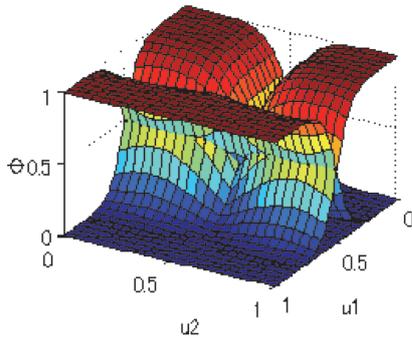


Fig. 8 Example of weight function

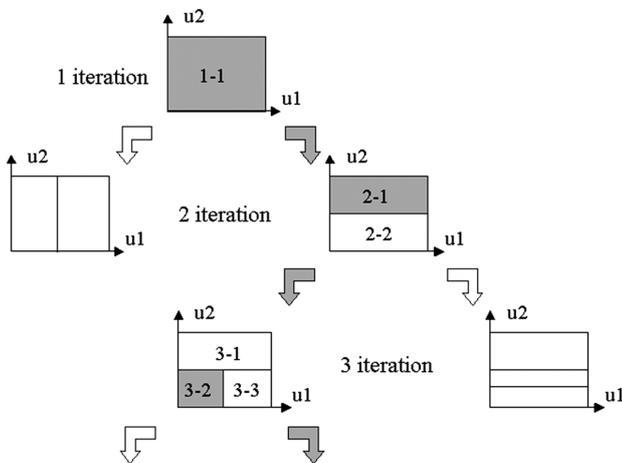


Fig. 9 Partitioning of input variable space

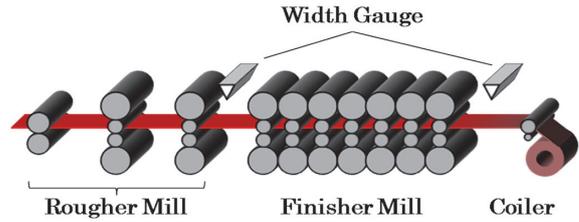


Fig. 10 Hot rolling process

Table 2 Comparison of model errors

Estimation error	Std. dev.
Conventional model	1.000
Proposed model	0.920

Values are rescaled

The proposed method was applied to the width variation prediction model in finish rolling of the hot rolling process (**Fig. 10**). The predicted value of width variation should be reflected to the target width at the rough rolling delivery. However, because the finish rolling condition is uncertain at the time of extraction from the reheating furnace when the rough rolling condition is determined, it was difficult to apply the physical model. Therefore, the multiple regression models (three strata for materials) have been conventionally used. As a result of the application of the developed method, the model consisting of six local areas ($M=6$) was automatically built and the width variation prediction accuracy improved by 8% (**Table 2**).

This method has been applied to the actual plant in the process reported, and achieved improvement of the control accuracy and reduction of the maintenance load. In addition, this technology can be widely applied to other processes, and application studies and applications to actual plants are in progress.

3. Optimization of Production Conditions by Statistical Approach

If the production quality is indicated by qualitative information such as “accepted” or “rejected,” a model indicating the relationship between the quality and the numerous numbers of operating conditions needs to be built first, and then it is necessary to determine the operating conditions optimizing quality conditions.

In addition, since probabilistic phenomena contribute greatly to quality in most cases, only the physical principles are insufficient for thorough description, and a statistical approach is necessary.

3.1 Quality improvement with PCA-LDA and DDQI

As a quality improvement action of the internal effect of bar and rod special steel, there is an example where the relationship between the qualitative quality information and the operating conditions was modeled with the principal component analysis-linear discriminant analysis (PCA-LDA) and the operating conditions were optimized with data-driven quality improvement (DDQI).^{5,6)}

In PCA-LDA, first, operation condition data $X \in \mathbf{R}^{N \times P}$ are compressed to R number of principal component score $T_R = XV_R (\in \mathbf{R}^{N \times R})$ with principal component analysis, PCA (N is number of data and P is number of operating conditions). $V_R \in \mathbf{R}^{P \times R}$ is called the loading matrix and is obtained by the singular value decomposition of X . Then, using linear discriminant analysis LDA in the space of the principal component score, discriminant axis $J \in \mathbf{R}^{N \times 1}$ that discrimi-

ates two classes of acceptance and rejection to the optimum degree is obtained.

$$J = T_R K_{PCA} = X V_R K_{PCA} = X K_{LDA}$$

Where, $K_{PCA} \in R^{R \times 1}$ is the vector indicating the discriminant axis for principal component score T_R , and converting it to the space of original operating condition data X gives discriminant coefficient $K_{LDA} = V_R K_{PCA} (\in R^{P \times 1})$.

The analyzed variables of operating conditions were 40 variables from secondary refining to blooming. From the data of 532 accepted samples and 208 rejected samples, the quality discriminant model was created by PCA-LDA with six principal components. As shown in Fig. 11, accepted samples and rejected samples were almost separated. The effect of each operating condition on quality can be calculated from discriminant coefficient K_{LDA} of LDA (Fig. 12). However, some operating conditions may not be independent of each other or some may be spuriously correlated with quality. It is necessary to pay attention to those with relatively large influence coefficients, make judgment to focus on those consistent with physical knowledge and operation knowledge, and, finally, to verify with tests in the laboratory room or with the actual plant.

Furthermore, it is possible to construct a quality model (quality model quantifying the qualitative quality) $Y = T_R K_{PCR} (Y \in R^{N \times Q})$ (Q is the number of quality variables) with principal component regression (PCR), which is essentially equivalent to this discriminant model, and obtain the operating conditions that improve yield with DDQI. Although the operating conditions to be obtained should achieve quality equivalent to the target acceptance rate as desired quality, the operating conditions cannot be uniquely determined since the number Q of the quality variables is less than the number R of the principal component in most cases. To this end, the quadratic form of the evaluation function on operating conditions is provided to determine the operating conditions by the optimizing problem. In this case, the feasible range of operating conditions is set to the restrictive condition and the easiness of changing each operating condition is incorporated in the weight of the evaluation

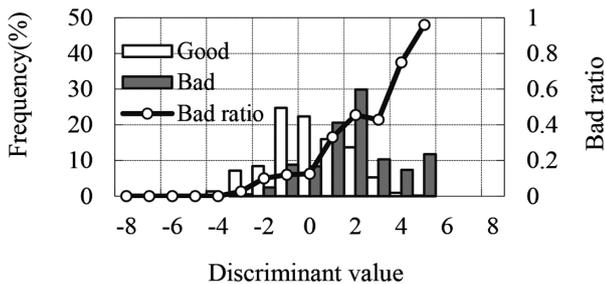


Fig. 11 A result of linear discriminant analysis

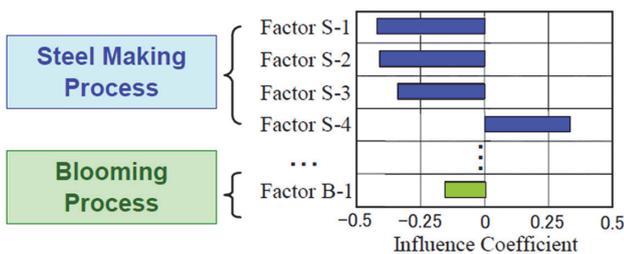


Fig. 12 Examples of influence coefficients for quality

function.

Table 3 shows partial results of estimated operating conditions using DDQI for the analysis example above, considering easiness of operating condition change, cost, etc. It shows the estimated value of operating conditions (S-1, S-5, B-1) that give an improved acceptance rate by 10% and 20% compared to the base condition. Since the confirmation test in the actual plant also gives the improved results generally conforming to the estimation results in Table 3, validity and effectiveness of this method were then confirmed.

3.2 Quality improvement by general linear model

The example in the previous section describes the binary of acceptance judgment as the linear discriminant model. There is another example that uses the generalized linear model (GLM) as a method to model a more general quality index.^{7,8)} GLM models prediction \hat{y} of response variable y using reversible and differentiable link function ℓ of linear predictor S that is a linear equation of predictor variables x_i , and enables analysis conforming to the probability distribution of actual quality data.

$$S = c_0 + \sum_{i=1}^I c_i x_i, \hat{y} = \ell(S)$$

Link function ℓ is set according to the target quality data. Table 4 shows examples of effective GLM for typical quality analysis of steel products. For continued values such as thickness, multiple regression with ℓ as the identity function may be used. For a coefficient value such as the number of defects, Poisson regression with ℓ as the exponential function may be used. For a ratio such as the acceptance rate, logistics regression with ℓ as the logistic function may be used.

To determine the optimal operating conditions for the product quality using GLM, linear predictor S is decomposed into the sum of S_1 consisting of controllable variables and S_2 consisting of non-controllable exogenous variables.

$$S_1 = c_0 + \sum_{i=1}^J c_i x_i, S_2 = \sum_{i=J+1}^I c_i x_i \tag{3}$$

To obtain the operating conditions that minimize the number of defects or reject rate, the operation condition at the point where S_1 is minimal within the variation range of the recorded data of controllable variables should be the optimal value. Quality ($=S$) for the optimal operating condition is estimated by substituting S_2 with the average of the recorded data.

Table 3 Recommended points to improve the quality

Factors	Yield		
	Base	10% up	20% up
S-1	3.6	5.0	6.6
S-5	2.9	4.2	5.5
B-1	87	89	92

Table 4 Effective GLMs in analysis of qualities of steel products

Quality	Accuracy of sheet gauge	Number of defects	Acceptance ratio
Sort of data	Continuous	Count	Ratio
Regression	Normal	Poisson	Logistic
Distribution of the objective	Normal	Poisson	Binary
Link function ℓ	S	$\exp(S)$	$[1 + \exp(-S)]^{-1}$

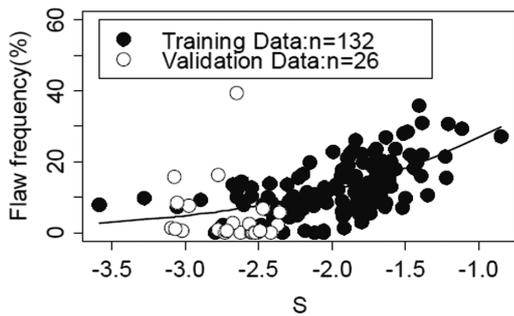


Fig. 13 Result of analysis using GLM

For a steel product type, logistic regression of the flaw rate of each product lot was performed using the operating conditions from continuous casting to blooming.

Figure 13 shows the relationship between the value of linear predictor and the flaw rate. Matching of the data plot (●) used for regression with the link function (logistic function) was good. Figure 14 is the plot of the relation of S_1 and S_2 in Equation (3). From the minimum value of S_1 (-2.0) within the variation range of the recorded data of controllable variables and the average value (-1.3) of recorded data of S_2 , the quality for the optimal operating condition was estimated to be $S = -3.3$. Changing the conditions that greatly give influence on the regression accuracy toward improvement of the quality based on the optimal operating condition estimated in this method, improvement of the flaw rate was confirmed as shown by the white circles (○) in Fig. 13 and Fig. 14.

4. Conclusions

The actions of process control and quality improvement exploiting data in the steel production process were introduced. These are a part of the actions performed at Nippon Steel & Sumitomo Metal. According to each process characteristic, accuracy of the physical model or operational knowledge in factories, various technology developments and improvements have been implemented.

The data collection and storage systems from the production

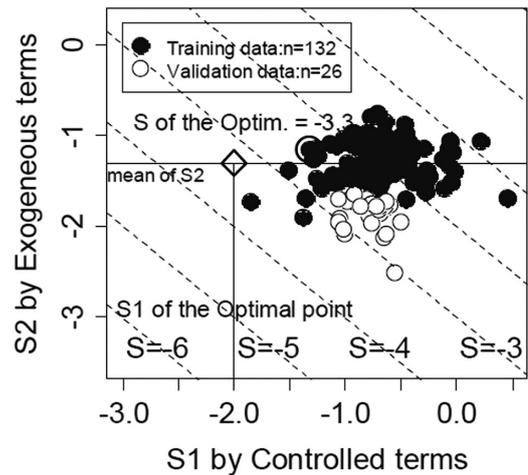


Fig. 14 Derivation of the optimal operational point

management systems and the process control systems have been continuously expanded and further use of data is expected. The artificial intelligence technology including machine learning continues to be developed. We continue to make efforts for improvement of the operation by incorporating and combining such latest technologies with the process and operational knowledge.

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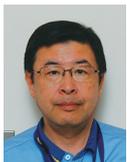
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