Correction Model of Carbon Potential using AI Techniques and Mechanism Analysis

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***Abstract*—This paper investigates both the knowledge model and the mechanism model for correcting Carbon Potential Using an Oxygen Sensor (CPUOS). CPUOS is widely used and there exists a deviation between the true value and the measured value. Therefore it is very important to study the correction model for CPUOS. Experiments are planned and carried out to generate the necessary data. Based on the experimental data we get the knowledge model for CPUOS using Support Vector Machine (SVM). Under the guidance of the knowledge model, we build the mechanism model based on the carbon potential relevant theory. The knowledge model and the mechanism model are corrected and verified by the practical experience.**

***Keywords*—Carbon Potential, model, support vector machine, oxygen sensor**

I. INTRODUCTION

Oxygen probes are widely used as Carbon Potential (CP) sensor with the rapid development of oxygen probe manufacturing techniques. Compared to the other CP sensors, such as dewpoint meter, CO_2 infrared meter and resistance probe, the oxygen probe has some practical advantages. It may be used as a true "in-situ" device. The response rate is fast and local fluctuations or point-to-point variations are easily observed. Probe design based on the SIRO2 Sensor is simple and permits easy maintenance or refurbishing. Thus, it is widely used in the atmosphere control for carburizing, carbonitriding, bright quenching, bright annealing, bright normalizing and control for endothermic, drop-feed, nitrogen, direct atmosphere under protected atmosphere. Oxygen probes are suitable for multi- purpose chamber furnace, continuous gas carburizing furnace, pit-type gas carburizing furnace.

But the conventional measurement techniques for Carbon Potential Using an Oxygen Sensor (CPUOS) are not so satisfying. The control accuracy of carbon potential are affected by several factors, such as other atmosphere component[1], the change of the temperature, the deviation between the practical reaction and the balanced reaction, the system errors of oxygen probe and temperature meters. There exists a deviation between the measured carbon potential and the true carbon potential[2]. In order to improve the control technique of carbon potential, it is necessary to study the factors that cause the deviation and study the correction model for the oxygen sensor approach so as to obtain the more accurate value of carbon potential.

In this paper, we obtain both the knowledge model and the mechanism model for correcting the CPUOS approach. The remainder of this paper is organized as follows. Section II will provide some background knowledge of carbon potential and SVM. In section III, we select the input/output variables according to the practical experience and record the relevant data. In section IV, we analyze the influencing factors and get the knowledge model using SVM for correcting the CPUOS approach. Under the guidance of the knowledge model, in section V, we build the mechanism model based on the carbon potential relevant theory. In section VI, we obtain the more overall correction models combining the knowledge model, the mechanism model and the practical human experience. Section VII gives some summary and future work.

II. PRELIMINARIES OF CP USING AN OXYGEN SENSOR AND SVM FOR REGRESSION

For the readers' convenience, some background knowledge on controlling carbon potential using the Oxygen probe[3][4][5][6] and SVM[7][8][9] for regression is firstly provided in this section.

A. Carbon Potential using an oxygen sensor

When the electrodes of the oxygen probe are exposed to different oxygen partial pressures an electric potential (E) is developed. E is related to oxygen partial pressure (P_{O_2}), and P_{O_2} is related to CP. Thus CP could be indirectly measured through the voltage E outputted by the oxygen probe. Therefore we briefly introduce the relationship between E and P_{O_2}, P_{O_2} and CP. For more detailed information about measuring CP using an oxygen probe please refer to [3][4][6].

1) The relationship between voltage and oxygen partial pressure[3].

The sensor is an oxygen concentration cell. It comprises a membrane of stabilized zirconium oxide which, at high temperature, is a conductor of oxygen ions, two electrodes and leads to a voltage. Figure 1 gives the schematic diagram of an Oxygen probe[5].

When the electrodes are exposed to different oxygen partial pressures P' and P'' an electromotive force (emf) E is developed which following the Nernst equation

$$E = (RT/4F)In\frac{P'}{P''} \quad (1)$$

where $T(°K)$ is the temperature of the membrance, R is the gas constant and F the Faraday constant. The sense of the emf is such that the positive electrode is the one exposed to the higher oxygen partial pressure.

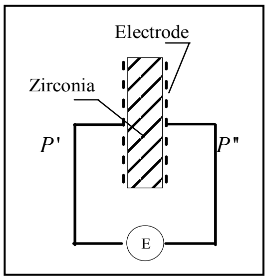


Figure 1. Schematic diagram of an Oxygen probe

The cell may be used to determine the oxyge partial pressure at one electrode (e.g. P'') provided that P' d T are known. P' is generally fixed by maintaining a c ıtrolled reference atmosphere, e.g. air, at the electrode.] an air reference is used, equation becomes

$$E = 4.96\times10^{-2}T\lg\frac{P_{ref}}{P_{O_2}}(mv) \quad (2)$$

2) Relationship between oxygen partial pressure ι d CP

The exchange of carbon between an equilibrium gas phase containing CO, O2, H20, H2, CH4 and N2 and a one-phase solid solution, such as austenite, is given by the following Equation[3].

$$CO = [C] + \frac{1}{2}O_2 \quad (3)$$

The equilibrium constant, K, for Reaction [3] is

$$K = \frac{P_{O_2}^{1/2}}{P_{CO}}\bullet\alpha_c \quad (4)$$

where α_c is the termodynamic activity of carbon, P_{CO}, P_{O_2} is the partial pressure of component CO,CO2.

In terms of atom fraction, the activity is given by the equation[6]:

$$\alpha_c = f_c C_P \quad (5)$$

where f_c is activity coefficient, C_p is carbon potentialt of carbon, a function of compositon and temperature.

Combining Equation（4），（5）, that is

$$C_P = \frac{K}{f_c}\frac{P_{CO}}{P_{O_2}^{1/2}} \quad (6)$$

Equation (6) provides the basis for relating P_{O_2} to CP. At a particular temperature, a given ratio $P_{CO}/P_{O_2}^{1/2}$ corresponds to a particular CP. When both T and P_{CO} do not vary, we can compute CP by P_{O_2}.

B. Support vector machine (SVM) for regression

In this section, we give the basic theory of SVM for regression estimation[7]. SVM, developed by Vapnik[8][9], is gaining popularity due to many attractive features and promising empirical performance. Originally, SVM is developed for pattern recognition problems. Recently, with the introduction of ε-insensitive loss function, SVM has been extended to solve nonlinear regression estimation, time-series prediction, system nonlinear identification and control.

We describe the linear function using the form $\langle\varpi\cdot x\rangle + b$. As to the non-linear case, we transfer the nonlinear problem into a linear problem by a nonlinear map $\phi(x)$ from the low dimensional input space to a higher-dimensional feature space. SVM approximates the function using the following form:

$$f(x) = \langle\varpi\cdot\phi(x)\rangle + b \quad (7)$$

The regression problem is equivalent to the following optimization problem:

$$\min \quad \frac{1}{2}\|\varpi\|^2 + C\sum_{i=1}^{l}(\xi_i+\xi_i^*)$$
$$s.t. \quad \begin{cases} y_i - \langle\varpi^T\cdot\phi(x_i)\rangle - b \le \varepsilon + \xi_i \\ \langle\varpi^T\cdot\phi(x_i)\rangle + b - y_i \le \varepsilon + \xi_i^* \\ \xi_i, \xi_i^* \ge 0 \end{cases} \quad (8)$$

where, minimizing $\|\varpi\|^2/2$ means minimizing VC dimension，and at the same time $f(x)$ approximates pairs (x_i, y_i) with ε precision. Thus, the above optimization problem is a realization of structure risk minimization (SRM) principle [5]. Therefore, the obtained regression estimation possesses good generalization ability. *C>0* is cost coefficient, which represents a balance between the model complexity and the approximation error. When the constraint conditions are infeasible, slack variables ξ_i, ξ_i^* should be introduced.

By solving Equation (6) the approximate function is obtained：

$$f(x) = \sum_{i=1}^{l}(\alpha_i - \alpha_i^*)K(x_i, x) + b \quad (9)$$

III. ACQUIRE THE RAW DATA

In order to investigate the influencing factors of CPUOS and the correction model, we select the relevant variables according to the practical experience. We measure and record the relevant data.

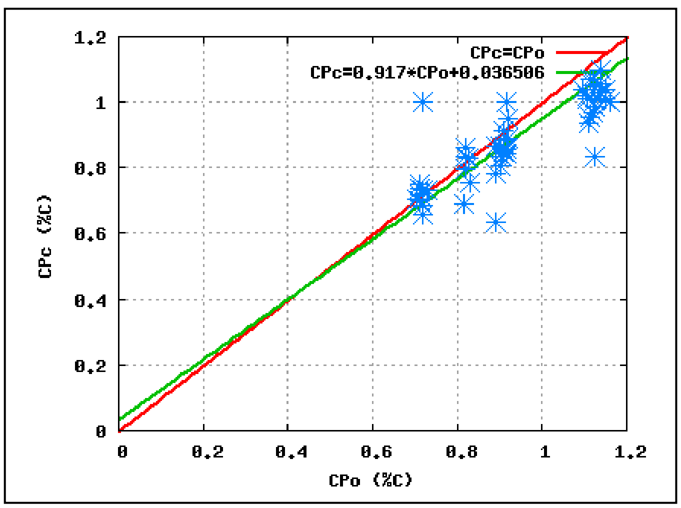
- CP obtained by the oxygen probe (C_{po}) which is the object to be corrected.
- CP measured by the steel foil (C_{pc}). The purpose of this work is to correct CPUOS and the steel foil approach represents an original definition of CP and leads to small error, so it can be regarded as the true value.
- Possible influencing factors for CPUOS. According to practical manufacturing experience, they could be the carburizing atmosphere (including CO, CO_2, CH_4, H_2) and the temperature.

In this experiment, atmosphere component is measured by MESA gas analyzer. The data are recorded and sent to the recorder system by a data acquisition system once a minute. The temperature is measured by the thermocouple.

IV. KNOWLEDGE MODEL OF CP CORRECTION

In order to investigate the influencing factor of CPUOS, we observe the relationship between CP by the oxygen probe C_{po} and the true CP value, that is CP by the steel foil C_{pc}. Figure 2 shows that C_{po} and C_{pc} is likely to be linear. In Figure 2, the slope of the fitting line is closed to 1, and there exists a bias.

Figure 2. Relationship between the CP by an Oxygen probe C_{po} and that



by a steel foil C_{pc}

For further study on the relationship between C_{po} and C_{pc}, we conduct quantitative analysis use SVM. The motivation of selecting SVM for modeling is that both linear and nonlinear models can be built using SVM. The other reason is the remarkable characteristics of SVM such as good generalization performance, and the absence of local minima.

Our purpose is to amend the CP by the Oxygen probe C_{po}, so C_{po} is the input variable. The steel foil approach represents the original definition, can be regarded as the true value, so CP by a steel foil C_{pc} is the output variable. In order to quantitatively analyze the relationship between the two CP value, we have built the linear model. we choose the linear kernel function: $K(x_i, x_j) = x_i^T x_j$. The linear model is $C_{pc} = 0.917 * C_{po} + 0.036506$.

For the purpose of validating the models, the data set is randomly split into 28 training samples and 27 test samples. The precisions of the methods are listed in Table 1. The first row is the error without amendment, that is, the error between the carbon potential using the oxygen and that using the steel foil. The second row is the error between the carbon potential after linear modification and that using the steel foil. The SVM models show that, after liner modification, the precision is improved, so the linear model is effective. In our experiment, the linear model performs a little better. The relation ship is likely linear.

TABLE I. THE PRESICION OF THE CORRECTION MODELS

	MAE (Mean Absolute Error)	**RMS (Root-Mean-Square)**
Without correction	0.047458	0.062793
Linear model	0.044675	0.051016

Figure 3 shows the error curves of the three methods: CP using the Oxygen probe, carbon potential after linear correction, carbon potential using the steel foil. The experimental results show that the carbon potential after linear correction is closer to the carbon potential using the steel foil, which also shows that the linear model is valid.

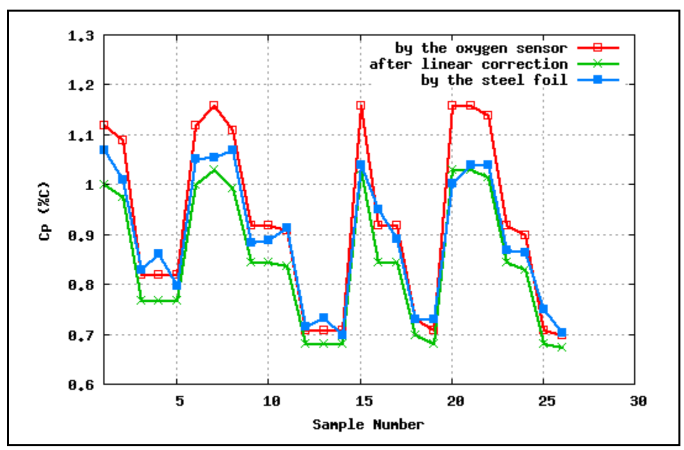


Figure 3. Curves of CP.

V. MECHANISM MODEL OF CP CORRECTION

In this section, we build the mechanism model about the relationship of the measured CP and the true CP. From the knowledge model, the linear relation is obvious; we can guess there exists certain relationships between the physical variables. We study the relationship between the physical variables in the measurement and computation process of using the oxygen probe in order to analyze the mechanism model.

In high temperature condition the carbon potential is a function of the oxygen partial pressure, the oxygen partial pressure is a function of the electric potential. Thus we mainly study the relationship among electric potential, oxygen partial pressure and carbon potential.

Revisit the relationship between electric potential E and oxygen partial pressure P_{O_2} and substitute P_{ref} =0.21 into Equation (2), we have

$$P_{O_2} = 10^{-\frac{20.161E}{T} - 0.6774} \quad (10)$$

Then focus on the relationship between carbon potential C_P and oxygen partial pressures P_{O_2} :

Define $K' = K/f_c$. Equation (6) can be represented as:

$$C_P = K' \frac{P_{CO}}{P_{O_2}^{1/2}} \quad (11)$$

Combining Equation (6) and (11), we have

$$C_P = K' P_{CO} 10^{\frac{10.0805E}{T} + 0.3387} \quad (12)$$

CO is affected by rich gas and balanced atmosphere, and varies in a large scope, so the deviation of CO should be considered. The deviation of E is another important influencing factor. The output of the oxygen probe is electric voltage, not electric potential, and affected by the internal resistance. The incremental format of Equation (12), that is, the practical value obtained by the oxygen probe C_{po} is:

$$C_{po} = K'(P_{CO} + \Delta P_{CO}) 10^{\frac{10.0805(E+\Delta E)}{T} + 0.33870} \quad (13)$$

Combing Equation（12）and（13）, we have:

$$C_P = kC_{po} + b \quad (14)$$

where

$$k = 10^{-\frac{10.0805\Delta E}{T}} ; b = -K' \Delta P_{CO} 10^{\frac{10.0805E}{T} + 0.33870} \quad (15)$$

C_P is the true CP value. CP by the steel foil C_{pc} is approximately equal to C_P.

VI. Summary and Future Work

Combining the knowledge model, the mechanism model and the practical experience, about the correction model on CPUOS, we draw the following conclusions:

1) Both knowledge model and the mechanism model show that the CP by the oxygen probe and the true value is linear relationship in a short period of time.

The result of the knowledge model:

C_{pc}=0.917*C_{po}+0.036506

where C_{pc} is the true CP value, i.e., CP by the steel foil, C_{po} is the value by the oxygen probe. It needs to be noted that the model varies according to the time and the work environment.

The result of the mechanism model:

$$C_{pc} = kC_{po} + b$$

where $k = 10^{-\frac{10.0805\Delta E}{T}} ; b = -K' \Delta P_{CO} 10^{\frac{10.0805E}{T} + 0.33870}$

2) The linear relationship is true only in a short period of time. ΔE is not a const value, the scope will vary. Therefore the model is linear in a short period of time and nonlinear in a long term. The linear relationship is meaningful, for it is easy to update for a linear relationship, only little data is enough to update the model; the nonlinear relationship shows that the model is not fixed, that means, in order to obtain the good result, the periodic updating is necessary. The linear model should be updated periodically according to the recent short-term data.

3）The mechanism model shows: the deviation is related to CO, and the higher the temperature is, the larger the deviation is; the higher the temperature is, the closer the rate of the line is close to 1, which means the error is more like translational error. This provide a theoretical foundation for the model correcting in the future under different temperature.

4）The future work will emphasize on temperature T , the deviation of the electric potential of the oxygen potential ΔE and K', the change rule of ΔE and K', and the further experimental verification.

VII. Acknowledgement

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