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Research on the establishment and application of the model for the identification of ancient glass products based on principal component analysis

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Abstract: *In order to distinguish the ancient and foreign glass products in China, repair the weathered glass products and better protect the ancient glass products, the impact of surface weathering on the two kinds of glass and the main components of the two kinds of glass are explored. The principal component analysis method is used to analyze 14 indicators of 18 samples of high potassium glass and 49 samples of lead barium glass respectively, and the model between different glass types and chemical composition is established. The correctness of the model is verified by linear regression test with SPSPRO software. The results show that the five main components of high potassium glass are silicon dioxide, sodium oxide, potassium oxide, calcium oxide and magnesium oxide. The six main components of lead barium glass are silicon dioxide, sodium oxide, potassium oxide, calcium oxide, magnesium oxide and aluminum oxide. Through sensitivity analysis and error analysis, the mathematical model proposed in this paper is reasonable and effective, and it has certain theoretical guiding significance for the identification and research of the composition of ancient glass products.*

Keywords: *Principal component analysis, Glass products, Control variable method, SPSSPRO*

1. Introduction

Glass products have become an essential part of human life, and the development history of glass can be traced back to the two rivers in 2500 BC [1]. Glass is mainly an artificial product of silicate materials. With the continuous development of archaeological work in China, it has been discovered that ancient Chinese glass products were mainly produced on the Silk Road [2]. Gan Fuxi focused on discussing the impact of transportation and tribal exchanges between China and foreign countries during the original historical period on the origin and development of ancient Chinese glass during the pre-Qin period [3].There are currently two different opinions in the academic community regarding the origin of ancient glass in China. One is the “foreign theory”, which means that China’s early glass products were “imported products’ imported from the West, and China’s early glass manufacturing technology was introduced from the West. Another is the “self creation theory”, which means that early glass products in China were produced by ancient laboring people using their own technology [4].

Since the 1980s, archaeologists have attached great importance to the study of ancient glass, which has made the study of ancient glass more comprehensive. However, it cannot be denied that there are still certain problems to be solved in the study of ancient Chinese glass, especially the impact on the surface weathering degree of different types of glass. Liu Song *et al*. used portable X-ray fluorescence spectroscopy to quantitatively analyze the surface of glass samples and pointed out the changes in the content of the main flux at different parts [5]. Li Qinghui *et al*. combined proton induced X-ray emission and energy dispersive X-ray emission analysis techniques to classify ancient Chinese mosaic glass into PbO-BaO-SiO_2 glass, Na_2O CaO-SiO_2 glass, CaO-MgO-SiO_2 glass, and other categories [6]. Principal component analysis (PCA) is widely used in various industries. Yue Cuinan *et al*. used PCA and cluster analysis to analyze 18 physical and chemical indicators of 18 yellow tea samples under different conditions of suffocation and yellowing [7]. Xuan Shiyao *et al.* proposed an improved PCA evaluation model combining single factor index method. Niu Wenjing *et al*. analyzed the main aroma substances in Zanthoxylum bungeanum oil using PCA and established an aroma quality evaluation model for Zanthoxylum bungeanum oil. It can be seen that PCA plays a very effective role in analyzing

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and identifying the main components of substances.

This paper is based on existing research, using the 2022 Higher Education Cup Mathematical Modeling Competition question C as the prototype, and using PCA to explore the impact of weathering on two types of glass, as well as the main components of high potassium glass and lead barium glass. A mathematical model that meets its requirements is constructed, and the rationality and sensitivity of the logarithmic model are analyzed.

2. Data source and preprocessing

This article selects the relevant data from Question C of the 2022 Higher Education Cup Mathematical Modeling Competition, which comes from the data of 14 components from 69 cultural relics sampling points provided in Forms 1 and 2 of the attachment. Due to detection methods and other reasons, the accumulation of component proportions may not be 100%. In this question, data between 85% and 105% will be considered as valid data. Therefore, it is necessary to preprocess the given data to remove invalid data from the form to prevent erroneous data from affecting the results.

Import the types of glass artifacts from Attachment Form 1 into Form 2 using Excel software, and then automatically screen the types in Form 2 to classify high potassium and lead barium glass. Accumulate the sum of each component in Form 2, remove data with a sum less than 85% and greater than 105%, and obtain valid data. Use Excel functions to calculate the maximum, minimum, range of change, mean, standard deviation, and median. As shown in the table below, the maximum, minimum, range of change, mean, standard deviation, and median of weathered high potassium glass are given in Table 1, and the unweathered glass are shown in Table 2.

Table 1: High potassium glass (weathered).

Chemical composition	Maximum value	Minimum value	Range of Changes	Mean value	Standard deviation	Median
SiO_2	96.77	92.35	92.35-96.77	93.96	1.58	93.51
Na_2O	0	0	0	0	0	0
K_2O	1.01	0.59	0.59-1.01	0.82	0.16	0.83
CaO	1.66	0.21	0.21-1.66	0.87	0.45	0.83
MgO	0.64	0.54	0.54-0.64	0.59	0.05	0.59
Al_2O_3	3.5	0.81	0.81-3.5	1.93	0.88	1.72
Fe_2O_3	0.35	0.17	0.17-0.35	0.27	0.06	0.28
CuO	3.24	0.55	0.55-3.24	1.56	0.85	1.55
PbO	0	0	0	0	0	0
BaO	0	0	0	0	0	0
P_5O_2	0.61	0.15	0.15-0.61	0.34	0.16	0.35
ZrO_2	0	0	0	0	0	0
SnO_2	0	0	0	0	0	0
SO_2	0	0	0	0	0	0

Table 2: High potassium glass (unweathered).

Chemical composition	Maximum value	Minimum value	Range of Changes	Mean value	Standard deviation	Median
SiO_2	87.05	59.01	29.01-87.05	67.98	8.38	65.53
Na_2O	3.38	2.10	2.10-3.38	2.78	0.53	2.86
K_2O	14.52	5.19	5.19-14.52	10.18	2.60	10.00
CaO	8.70	2.01	2.01-8.70	6.40	1.92	6.72
MgO	1.98	0.52	0.52-1.98	1.30	0.47	1.38
Al_2O_3	11.15	3.05	3.05-11.15	6.62	2.39	6.19
Fe_2O_3	6.04	0.42	0.42-6.04	2.32	1.47	2.27
CuO	5.09	0.47	0.47-5.09	2.68	1.47	2.51
PbO	1.62	0.11	0.11-1.62	0.71	0.58	0.35
BaO	2.86	0	0-2.86	1.44	0.96	1.38
P_5O_2	4.5	0.16	0.16-4.50	1.53	1.36	1.10
ZrO_2	0.12	0.04	0.04-0.12	0.08	0.03	0.09
SnO_2	2.36	2.36	2.36-2.36	2.36	0	2.36
SO_2	0.47	0.36	0.36-0.47	0.41	0.05	0.39

Table 3: Lead barium glass (weathered).

Chemical composition	Maximum value	Minimum value	Range of Changes	Mean value	Standard deviation	Median
SiO_2	53.33	3.72	3.72-53.33	24.91	10.40	25.02
Na_2O	2.22	0.80	0.80-2.22	1.41	0.52	1.3
K_2O	1.05	0.14	0.14-1.05	0.39	0.25	0.32
CaO	6.40	0.37	0.37-6.40	2.80	1.57	2.93
MgO	2.73	0.47	0.47-2.73	1.13	0.54	1.11
Al_2O_3	13.65	0.45	0.45-13.65	2.97	2.58	2.38
Fe_2O_3	2.74	0.19	0.19-2.74	0.95	0.71	0.81
CuO	10.57	0.19	0.19-10.57	2.47	2.80	1.25
PbO	70.21	15.71	15.71-70.21	43.31	12.00	44.06
BaO	35.45	3.26	3.26-35.45	13.35	9.36	9.76
P_5O_2	14.13	0.07	0.07-14.13	5.72	3.98	5.88
ZrO_2	1.12	0.19	0.19-1.12	0.47	0.22	0.45
SnO_2	1.31	0.47	0.47-1.31	0.89	0.42	0.89
SO_2	15.95	1.96	1.96-15.95	8.88	6.62	8.81

Table 4: Lead barium glass (unweathered).

Chemical composition	Maximum value	Minimum value	Range of Changes	Mean value	Standard deviation	Median
SiO_2	75.51	31.94	31.94-75.51	54.66	11.57	54.61
Na_2O	7.92	0.92	0.92-7.92	3.87	1.98	3.05
K_2O	1.41	0.11	0.11-1.41	0.34	0.32	0.25
CaO	4.49	0.38	0.38-4.49	1.52	1.23	0.88
MgO	1.67	0.51	0.51-1.67	0.98	0.32	1.00
Al_2O_3	14.34	1.42	1.42-14.34	4.46	3.19	3.86
Fe_2O_3	4.59	0.17	0.17-4.59	1.54	1.20	1.27
CuO	8.46	0.11	0.11-8.46	1.57	1.96	0.70
PbO	39.22	9.30	9.30-39.22	22.08	8.03	20.12
BaO	26.23	2.03	2.03-26.23	9.00	5.70	8.99
P_5O_2	6.34	0.08	0.08-6.34	1.42	1.97	0.41
ZrO_2	0.91	0.12	0.12-0.91	0.36	0.21	0.30
SnO_2	0.44	0.23	0.23-0.44	0.36	0.09	0.40
SO_2	3.66	3.66	3.66-3.66	3.66	0	3.66

Table 5: Symbol Description.

Symbol	Meaning	Symbol	Meaning
x_1	SiO_2	x_8	CuO
x_2	Na_2O	x_9	PbO
x_3	K_2O	x_{10}	BaO
x_4	CaO	x_{11}	P_5O_2
x_5	MgO	x_{12}	ZrO_2
x_6	Al_2O_3	x_{13}	SnO_2
x_7	Fe_2O_3	x_{14}	SO_2

3. The relationship between weathering and glass type

After processing Attachment Table 1, we can find that it is mainly divided into four categories: high potassium weathering, high potassium weathering, lead barium weathering, and lead barium weathering. As with the previous processing method, Table 3 provides the maximum, minimum, range of variation, mean, standard deviation, and median values of each major component in weathered lead barium glass. Table 4 presents the maximum, minimum, range of variation, mean, standard deviation, and median values of each major component in unweathered lead barium glass. In order to more intuitively investigated the relationship between weathering and glass type, we now compare the components of high potassium glass and lead barium glass before and after weathering into a bar statistical chart, as shown in Figures 1 and 2.

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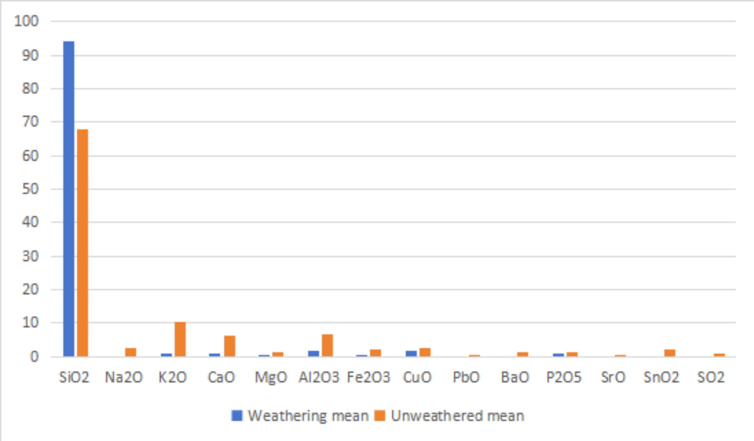

Figure 1: The average content of each component before and after weathering of high potassium glass.

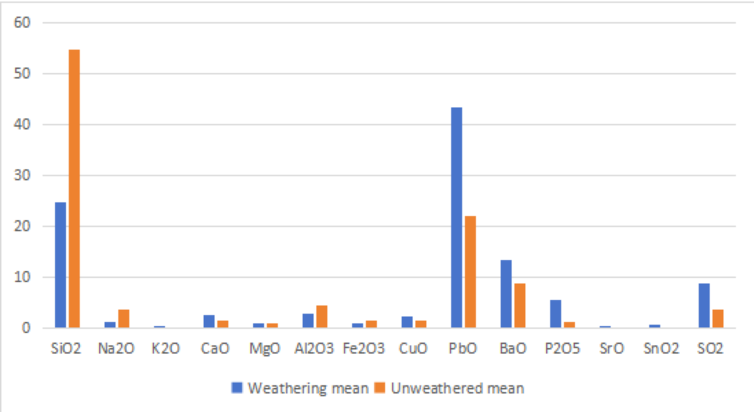

Figure 2: The average content of each component before and after weathering of lead barium glass.

Through the comparison between Figure 1 and Figure 2, we can intuitively see that when it is not weathered, the main content is silicon dioxide, with a small amount of other components. It can be preliminarily determined that it is a high potassium glass. When the content of silicon dioxide and lead oxide is high before weathering, it can be preliminarily determined as lead barium glass. After weathering, the content of silicon dioxide increases, and it can be preliminarily determined as a high potassium glass. After weathering, the content of silicon dioxide decreases and the content of lead oxide increases. We can preliminarily determine that it is a lead barium glass.

4. Model establishment and solution

The correlation matrix of PCA is composed of indicators of chemical composition in different glass types. Based on the PCA, the sum of different chemical composition combinations and cumulative feature root contribution rates is determined, and they are sorted to distinguish different types of glass. The specific steps are as follows.

4.1. Establish a model for high potassium glass

Step 1: Standardize data x to X.

From Attachment Table 2, it can be seen that there are a total of 18 samples and 14 indicators of high potassium glass, which can form a sample matrix n of size 18×14.All required symbols are explained in Table 5.

Calculate the mean by column$\bar{x}_j = \frac{1}{n}\sum_{i=1}^{n} x_{ij}$ and standard deviation $S_j = \sqrt{\frac{\sum_{i=1}^{n}(x_{ij}-\bar{x}_j)^2}{n-1}}$, then Calculate standardized data using standard deviation $X_{ij} = \frac{x_{ij}-\bar{x}_j}{S_j}$.

The obtained mathematical model can be expressed as:

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$$\begin{cases} F_1 = a_{11}X_1 + a_{12}X_2 + \cdots + a_{1j}X_j \\ F_2 = a_{21}X_1 + a_{22}X_2 + \cdots + a_{2j}X_j \\ \vdots \\ F_i = a_{i1}X_1 + a_{i2}X_2 + \cdots + a_{ij}X_j \end{cases} \tag{1}$$

Step 2: Calculate the sample covariance matrix.

$$R = \frac{\sum_{k=1}^{n}(x_{ki}-\overline{x_i})(x_{kj}-\overline{x_j})}{\sqrt{\sum_{k=1}^{n}(x_{ki}-\overline{x_i})^2 \sum_{k=1}^{n}(x_{kj}-\overline{x_j})^2}} \tag{2}$$

Step 3: Use SPSSPRO software to perform PCA on it, and obtain the variance percentage and cumulative contribution rate of the eigenvalues and feature roots.

Table 6: Explanation of total variance.

Component	Eigenvalue	Characteristic Root/Variance Percentage	Accumulate
X_1	5.400	38.573%	38.573%
X_2	2.430	17.359%	55.932%
X_3	1.715	12.253%	68.185%
X_4	1.649	11.777%	79.962%
X_5	0.949	6.775%	86.737%
X_6	0.644	4.601%	91.339%
X_7	0.513	3.666%	95.004%
X_8	0.302	2.16%	97.164%
X_9	0.195	1.392%	98.557%
X_{10}	0.111	0.795%	99.352%
X_{11}	0.061	0.435%	99.787%
X_{12}	0.018	0.129%	99.916%
X_{13}	0.007	0.051%	99.967%
X_{14}	0.005	0.033%	100.0%

Step 4: Analyze the table data to obtain the principal components. From Table 6, it can be seen that the cumulative contribution rate of the first five principal components is 86.737%. Therefore, only the first five components can be considered, which can effectively summarize the original variables, as shown in Table 7. Therefore, the expressions for each principal component are obtained as follows.

$$F_1 = 0.014X_2 - 0.152X_1 + 0.056X_{14} + 0.115X_4 - 0.013X_{13} + 0.126X_3 + 0.078X_9 + 0.137X_5 + 0.159X_6 + 0.154X_7 + 0.098X_8 + 0.126 \times X_{11} + 0.108X_{10} + 0.135X_{12}; \tag{3}$$

$$F_2 = -0.32X_2 + 0.171X_1 - 0.081X_{14} - 0.25X_4 + 0.132X_{13} - 0.209X_3 - 0.093X_9 + 0.136X_5 - 0.002X_6 + 0.067X_7 - 0.029X_8 + 0.23X_{11} + 0.147X_{10} + 0.208X_{12}; \tag{4}$$

$$F_3 = - 0.048X_2 - 0.072X_1 + 0.355X_{14} + 0.021X_4 + 0.264X_{13} + 0.166X_3 - 0.386X_9 + 0.193X_5 - 0.002X_6 - 0.004X_7 - 0.162X_8 + 0.055X_{11} - 0.368X_{10} + 0.025X_{12}; \tag{5}$$

$$F_4 = 0.28X_2 - 0.107X_1 - 0.353X_{14} - 0.137X_4 + 0.355X_{13} + 0.158X_3 + 0.185X_9 + 0.089X_5 + 0.056X_6 - 0.142X_7 - 0.366X_8 + 0.023X_{11} - 0.009X_{10} + 0.15X_{12}; \tag{6}$$

$$F_5 = -0.335X_2 + 0.077X_1 + 0.305X_{14} + 0.149X_4 + 0.457X_{13} + 0.173X_3 + 0.341X_9 + 0.129X_5 - 0.189X_6 - 0.336X_7 + 0.176X_8 - 0.413X_{11} + 0.314X_{10} + 0.037X_{12}. \tag{7}$$

Table 7: Principal Component Variance Interpretation Rate and Its Weights.

Name	Variance eXplanatory rate	Cumulative variance interpretation rate	Weight
Principal component 1	0.386	0.386	44.471%
Principal component 2	0.174	0.559	20.014%
Principal component 3	0.123	0.682	14.126%
Principal component 4	0.118	0.8	13.578%
Principal component 5	0.068	0.867	7.811%

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4.2. Establish a model for lead barium glass

Step 1: Standardize data *x* to *X*.

From Attachment Table 2, it can be seen that there are a total of 49 samples and 14 indicators of lead barium glass, which can form a sample matrix *x* of size 49×14.

Calculate the mean by column $\overline{x_j} = \frac{1}{n}\sum_{i=1}^{n} x_{ij}$ and standard deviation $S_j = \sqrt{\frac{\sum_{i=1}^{n}(x_{ij}-\bar{x}_j)^2}{n-1}}$, then calculated standardized data $X_{ij} = \frac{x_{ij}-\bar{x}_j}{S_j}$.

The obtained mathematical model can be expressed as:

$$\begin{cases} F_1 = a_{11}X_1 + a_{12}X_2 + \cdots + a_{1j}X_j; \\ F_2 = a_{21}X_1 + a_{22}X_2 + \cdots + a_{2j}X_j; \\ \quad\vdots \\ F_i = a_{i1}X_1 + a_{i2}X_2 + \cdots + a_{ij}X_j. \end{cases} \tag{8}$$

Step 2: Calculate the sample covariance matrix.

$$R = \frac{\sum_{k=1}^{n}(x_{ki}-\overline{x_i})(x_{kj}-\overline{x_j})}{\sqrt{\sum_{k=1}^{n}(x_{ki}-\overline{x_i})^2 \sum_{k=1}^{n}(x_{kj}-\overline{x_j})^2}}. \tag{9}$$

Step 3: Use SPSSPRO software to perform PCA on it, and obtain the variance percentage and cumulative contribution rate of the eigenvalues and feature roots.

Table 8: Total variance interpretation.

Total variance interpretation			
Ingredient	Characteristic root	Percent of feature root variance	Accumulate
1	3.576	25.54%	25.54%
2	2.949	21.062%	46.602%
3	1.665	11.89%	58.492%
4	1.085	7.748%	66.24%
5	0.908	6.483%	72.723%
6	0.841	6.004%	78.727%
7	0.747	5.338%	84.065%
8	0.618	4.416%	88.482%
9	0.564	4.03%	92.512%
10	0.365	2.605%	95.117%
11	0.350	2.499%	97.615%
12	0.206	1.472%	99.087%
13	0.123	0.88%	99.968%
14	0.005	0.032%	100.0%

Step 4: Analyze the table data to obtain the principal components. From Table 8, it can be seen that the cumulative contribution rate of the first six principal components is 78.727%, so we can only consider the first six components, which can effectively summarize the original variables.

$$F_1 = -0.242X_1 - 0.183X_6 - 0.1X_2 + 0.062X_4 - 0.082X_3 - 0.107X_5 + 0.151X_{14} + 0.178X_{10} - 0.08X_7 + 0.16X_8 + 0.127X_{11} + 0.156X_9 + 0.144X_{12} - 0.091X_{13}. \tag{10}$$

$$F_2 = -0.127X_1 + 0.094X_6 - 0.16X_2 + 0.272X_4 + 0.077X_3 + 0.216X_5 - 0.054X_{14} - 0.153X_{10} + 0.187X_7 - 0.12X_8 + 0.206X_{11} + 0.156X_9 + 0.085X_{12} + 0.109X_{13}. \tag{11}$$

$$F_3 = -0.02X_1 + 0.244X_6 - 0.07X_2 + 0.109X_4 + 0.275X_3 + 0.045X_5 + 0.316X_{14} + 0.337X_{10} + 0.103X_7 + 0.214X_8 + 0.009X_{11} - 0.316X_9 - 0.048X_{12} + 0.274X_{13}. \tag{12}$$

$$F_4 = -0.074X_1 + 0.252X_6 + 0.507X_2 - 0.016X_4 - 0.122X_3 + 0.37X_5 - 0.023X_{14} + 0.006X_{10} - 0.381X_7 + 0.094X_8 + 0.043X_{11} - 0.019X_9 + 0.521X_{12} + 0.126X_{13}. \tag{13}$$

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$$F_5 = 0.152X_1 + 0.062X_6 + 0.067X_2 + 0.156X_4 - 0.443X_3 + 0.232X_5 - 0.01X_{14} - 0.026X_{10} + 0.132X_7 + 0.28X_8 + 0.511X_{11} - 0.421X_9 - 0.239X_{12} - 0.451X_{13}. \quad (14)$$

$$F_6 = -0.037X_1 - 0.16X_6 + 0.241X_2 - 0.039X_4 + 0.746X_3 + 0.254X_5 + 0.18X_{14} - 0.016X_{10} + 0.007X_7 - 0.106X_8 + 0.04X_{11} + 0.014X_9 + 0.02X_{12} - 0.66X_{13}. \quad (15)$$

Table 9: Principal component variance interpretation rate with the corresponding weights.

Designation	The rate of variance interpretation	Cumulative variance interpretation rate	Weight
Principal component 1	0.255	0.255	32.441%
Principal component 2	0.211	0.466	26.753%
Principal component 3	0.119	0.585	15.103%
Principal component 4	0.077	0.662	9.842%
Principal component 5	0.065	0.727	8.234%
Principal component 6	0.06	0.787	7.627%

From Table 9, it can be concluded as follows.

$$F = (0.255/0.787) \times F_1 + (0.211/0.787) \times F_2 + (0.119/0.787) \times F_3 + (0.077/0.787) \times F_4 + (0.065/0.787) \times F_5 + (0.06/0.787) F_6. \quad (16)$$

4.3. Results and Analysis

PCA was conducted on the 14 components of high potassium and lead barium using SPSS PRO, and it was found that the main components of high potassium are silicon dioxide, sodium oxide, potassium oxide, calcium oxide, and magnesium oxide. The standardized data evaluation model is as follows:

$$F = (0.386/0.867)\times F1+(0.174/0.867)\times F2+(0.123/0.867)\times F3+(0.118/0.867)\times F4+(0.068/0.867)\times F5. \quad (17)$$

The main components of lead and barium are silicon dioxide, sodium oxide, potassium oxide, calcium oxide, magnesium oxide, and aluminum oxide

The standardized data evaluation model is as follows:

$$F = (0.255/0.787)\times F_1 + (0.211/0.787)\times F_2 + (0.119/0.787)\times F_3 + (0.077/0.787)\times F_4 + (0.065/0.787)\times F_5 + (0.06/0.787)\times F_6. \quad (18)$$

5. Model verification

Establish a linear regression model using SPSSPRO software and test it. The input variable is the content of high potassium silicon dioxide, and the dependent variable is whether the surface is weathered. Conduct linear regression analysis for detection. The VIF is less than 10 (as shown in Table 10), so the model has no multicollinearity problem, and the model is well constructed. The formula of the model is as follows.

$$y = 1.25 + 0.006*X_1. \quad (19)$$

Table 10: Results of the linear regression analysis.

Results of the linear regression analysis $n = 4$									
	Non-standardized coefficients		Standardization coefficient	t	p	VIF	R^2	Adjustment R^2	F
	B	Standard error	Beta						
Constant	1.25	2.168	-	0.577	0.622	-	0.026	-0.46	$F = 0.054$ $P = 0.838$
SiO_2	0.006	0.026	0.162	0.233	0.838	1.000			
Dependent variable: surface weathering									

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Figure 3: Sensitivity analysis between the true values and the predicted values.

Through sensitivity analysis, it was detected that the model is reasonable.

The input variable is the content of lead barium type silicon dioxide, the dependent variable is whether the surface is weathered, and linear regression analysis is conducted for detection. Since all VIFs are less than 10 (as shown in Table 11), the model has no multicollinearity problem and is well constructed. The formula of the model is as follows.

$$y = 1.505 + 0.006 * X_1. \tag{20}$$

Table 11: Results of the linear regression analysis.

Results of the linear regression analysis n = 4									
	Non-standardized coefficients		Standardization coefficient	t	p	VIF	R^2	Adjustment R^2	F
	B	Standard error	Beta						
Constant	1.505	1.668	-	0.902	0.462	-	0.011	-0.483	F = 0.022
SiO_2	0.006	0.042	0.105	0.15	0.895	1.000			P = 0.895
Dependent variable: surface weathering									

Through sensitivity analysis, it is detected that the model is reasonable, as shown in Figure 3.

6. Conclusions

This article first uses processed valid data to preliminarily determine the type of glass based on the chemical composition content and changes before and after weathering. Then, combining the changes in chemical composition of different glass types to form a correlation matrix for PCA, a model of PCA is established. The principal components of different types of glass can be obtained by solving the model. Finally, the accuracy of the model is tested through linear regression. This model can be used to distinguish between high potassium glass and lead barium glass, but for other types of glass, no relevant research has been conducted due to insufficient data. Through sensitivity analysis and error analysis, the mathematical model proposed in this article is reasonable and effective, and has certain theoretical guidance significance for the identification and research of ancient glass product components.

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