Study on the yield of cotton straw pyrolysis products based on nonlinear prediction and grey predictive analysis

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Abstract: With the increasing demand for renewable energy, this study focuses on the quality and yield of cotton straw pyrolysis products using cotton straw as an important biomass resource. Based on previous studies, this paper analyses the relationship between the mixing ratio of cotton straw pyrolysis combinations and the product yields, and finds that there is a nonlinear relationship between most of the product yields and the mixing ratios, so a polynomial nonlinear regression model is used for prediction. Due to the limited amount of data, the GM(1,1) grey prediction model was also introduced for comparison and evaluation in order to improve the accuracy of the model. The nonlinear regression model was established by Least Square Method, and then the GM(1,1) model was used to analyse the yield of products under different pyrolysis combinations. The results showed that the GM(1,1) model performed well in terms of prediction accuracy. Taking the DFA/CS combination as an example, the scatter plots of the raw data against the predicted values intuitively showed that the GM(1,1) model had a high degree of fitting, small prediction error and good prediction performance. This study is expected to provide a scientific basis for the efficient use of cotton straw pyrolysis products and the sustainable development of cotton straw.

1. Introduction

With the increasing global demand for renewable energy, biomass has received widespread attention as a mature renewable energy source. Cotton straw is an important biomass resource, rich in biomass components such as cellulose and lignin. Cotton straw pyrolysis is widely used for renewable energy production, but the quality and yield of the pyrolysis products are affected by a variety of factors such as pyrolysis temperature and catalysts [1-2]. Previous scholars have investigated the relationship between pyrolysis product yields and the mixing ratios of the corresponding pyrolysis combinations, and explored the effect of the mixing ratios of the pyrolysis combinations. Based on this conclusion, a nonlinear model was constructed between different product yields and pyrolysis combination mixing ratios[3-4], in which the primary-quadratic curve had the best fit. Therefore, a kinetic model for the pyrolysis reaction of cotton stalks was developed using polynomial

nonlinear regression as a model for the catalytic reaction mechanism. Building upon previous research, this paper focuses on predicting the yield or quantity of pyrolysis products. The data used in the paper were obtained from http://www.nmmcm.org.cn/.Based on previous studies, it can be found that there is a nonlinear relationship between most of the product yields or gas yields and the corresponding mixing ratios of pyrolysis combinations, so that polynomial nonlinear regression models can be used for prediction [5]. Meanwhile, due to the small amount of data, underfitting and overfitting can easily occur. Therefore, in order to improve the accuracy of the model, we also built a GM(1,1) grey prediction model for comparison and evaluation to ensure the correctness of the prediction results.

2. Establishment and analysis of the model

2.1 Nonlinear regression prediction model based on least square method

The least square method is a classical method for solving optimization problems. Its basic idea is to minimize the sum of squares of errors between the obtained unknown data and the actual data, so as to find the most suitable fitting function for the given data [6-7].

Let's take the conic curve $y = ax^2 + bx$ for example, according to the principle of least squares:

$$M = \sum_{i=1}^{N} (y_i - ax_i^2 - bx_i)^2$$
(1)

If the value of M is minimized, the partial derivative definition is:

$$\begin{cases} \frac{\partial M}{\partial a} = 0\\ \frac{\partial M}{\partial b} = 0 \end{cases}$$
(2)

Also because:

$$\begin{cases} \frac{\partial M}{\partial \alpha} = -2\sum_{i=1}^{N} (y_i - ax_i^2 - bx_i) * x_i^2 \\ \frac{\partial M}{\partial b} = -2\sum_{i=1}^{N} (y_i - ax_i^2 - bx_i) * x_i \end{cases}$$
(3)

If the above formula is 0, then:

$$\begin{cases} -2\sum_{i=1}^{N} (y_i - ax_i^2 - bx_i) * x_i^2 = 0\\ -2\sum_{i=1}^{N} (y_i - ax_i^2 - bx_i) * x_i = 0 \end{cases}$$
(4)

Deform the upper form to obtain:

$$\begin{cases} \sum_{i=1}^{N} y_{i} x_{i}^{2} &= \sum_{i}^{N} a x_{i}^{4} + \sum_{i}^{N} b x_{i}^{3} \\ \sum_{i=1}^{N} y_{i} x_{i} &= \sum_{i}^{N} a x_{i}^{3} + \sum_{i}^{N} b x_{i}^{2} \end{cases}$$
(5)

The results of solving *a* and *b* are as follows:

$$a = \frac{\sum_{i=0}^{N} y_i x_i^2 \sum_{i=0}^{N} x_i^3 - \sum_{i=0}^{N} y_i x_i^2 \sum_{i=0}^{N} x_i^2}{(\sum_{i=0}^{N} x_i^3)^2 - \sum_{i=0}^{N} x_i^2 \sum_{i=0}^{N} x_i^4}, b = \frac{\sum_{i=0}^{N} y_i x_i^2 \sum_{i=0}^{N} x_i^3 - \sum_{i=0}^{N} y_i x_i \sum_{i=0}^{N} x_i^4}{(\sum_{i=0}^{N} x_i^3)^2 - \sum_{i=0}^{N} x_i^2 \sum_{i=0}^{N} x_i^4}$$
(6)

In the nonlinear regression analysis, according to the above steps, the least square method is used to estimate the parameters and construct the polynomial curve [8]. Through many experiments, it was found that the nonlinear relationship between the yield of most products and the mixture ratio of pyrolysis combinations was more consistent with the nonlinear relationship of one single quadratic. Therefore, in this paper, the quadratic equation corresponding to the highest fit degree between different product yields and the mixture ratio of pyrolysis group is obtained. In addition, the product yield of the pyrolysis combination was predicted under the mixture ratio of 70/100 and 90/100. Some of the prediction results is as Table 1:

Product yield	DFA/CS(70/100)	DFA/CS(90/100)
Tar yield	11.752	11.492
Water yield	30.232	31.300
Char yield	29.527	29.798
Syngas yield	28.122	27.222

Table 1: Prediction results under the DFA/CS combination

2.2 GM (1,1) grey prediction model

Grey model defines grey derivative and grey differential equation based on concepts such as correlation space and smooth discrete function, and then establishes a dynamic model in the form of differential equation with discrete data columns. In other words, grey model is a model in the form of differential equation established by the generation of discrete random numbers into the generated numbers with significantly weakened randomness and more regular. This makes it easy to study and describe the changing process [9-10].

GM(1,1) grey prediction model is a prediction method based on grey system theory, which is mainly used to predict nonlinear dynamic systems with exponential growth or decay tendency.

Before establishing the GM(1,1) grey prediction model, it is necessary to carry out the level ratio test, and only through the level ratio test can the next step model construction be carried out. The step ratio test steps are as follows:

Original sequence $X^{(0)} = (x^{(0)}(1), x^{(0)}(2), ..., x^{(0)}(n))$, set $\lambda(k)$ is sequence $X^{(0)}$'s Stage ratio, then there is

$$\lambda(k) = \frac{x^{(0)}(k-1)}{x^{(0)}(k)}, k = 2, 3, \cdots, n$$
(7)

If satisfied:

$$\lambda(\mathbf{k}) \in \left(\mathbf{e}^{\frac{-2}{\ln+1}}, \mathbf{e}^{\frac{2}{n+1}}\right) \tag{8}$$

It indicates that the sequence has passed the level ratio test and a model of GM(1,1) can be established; otherwise, the data need to be processed to make it fall within the valid range.

If sequence $X^{(0)}$ Meet the above conditions, and $x^{(0)}(k) \ge 0$, after a cumulative generation post processing of the original sequence, you can get $X^{(0)}$'s Accumulate to generate a sequence:

$$\mathbf{X}^{(1)} = \left(\mathbf{x}^{(1)}(1), \mathbf{x}^{(1)}(2), ..., \mathbf{x}^{(1)}(n)\right)$$
(9)

Among:

$$\mathbf{x}^{(1)}(\mathbf{k}) = \sum_{i=1}^{k} \mathbf{x}^{(0)}(i) \quad \mathbf{k} = 1, 2, \dots, n$$
(10)

With the cumulative generating sequence, it is also necessary to use it to obtain the adjacent mean value sequence. The calculation formula of the adjacent mean value sequence is as follows:

$$z^{(1)}(k) = \frac{1}{2} \left(x^{(1)}(k) + x^{(1)}(k-1) \right)$$
(11)

By performing the above calculation on the sequence $X^{(1)}$. The sequence of adjacent means can be obtained:

$$Z^{(1)} = \left(z^{(1)}(2), z^{(1)}(3), ..., z^{(1)}(n)\right)$$
(12)

According to the above sequence, the first order differential linear equation, namely the gray differential equation, is established, and the mean form of the model and the corresponding whitening differential equation are obtained:

$$\mathbf{x}^{(0)}(\mathbf{k}) + \mathbf{a}\mathbf{z}^{(1)}(\mathbf{k}) = \mathbf{b}, \frac{\mathbf{d}\mathbf{x}^{(1)}}{\mathbf{d}\mathbf{t}} + \mathbf{a}\mathbf{x}^{(1)} = \mathbf{b}$$
(13)

Where a represents the development coefficient, b represents the grey action. Let \hat{a} be the parameter vector to be estimated, let $\hat{a} = \begin{bmatrix} a \\ b \end{bmatrix}$, Using the least square method to solve, we can get:

$$\hat{\mathbf{a}} = \left(\mathbf{B}^{\mathsf{T}}\mathbf{B}\right)^{-1}\mathbf{B}^{\mathsf{T}}\mathbf{Y}$$
(14)

Among B, Y respectively:

$$\mathbf{B} = \begin{bmatrix} -z^{(1)}(2) & 1 \\ -z^{(1)}(3) & 1 \\ \vdots & \vdots \\ -z^{(1)}(n) & 1 \end{bmatrix}, \mathbf{Y} = \begin{bmatrix} x^{(0)}(2) \\ x^{(0)}(3) \\ \vdots \\ x^{(0)}(n) \end{bmatrix}$$
(15)

The solution results are as follows:

$$\begin{cases} \hat{x}^{(1)}(k+1) = \left(x^{(0)}(1) - \frac{b}{a}\right)e^{-ak} + \frac{b}{a}, k = 1, 2\cdots, n \\ \hat{x}^{(0)}(k+1) = \hat{x}^{(1)}(k+1) - \hat{x}^{(1)}(k) \end{cases}$$
(16)

According to the above steps, using python programming to build and implement the GM(1,1) model, the final prediction results are as Table 2, Table 3 and Table 4:

DFA/CS	Tar yield	Water yield	Char yield	Syngas yield
0	19.46	26.84	29.21	24.490
10/100	16.651	27.530	29.161	26.809
20/100	15.703	27.954	29.209	27.138
30/100	14.809	28.385	29.257	27.471
40/100	13.966	28.823	29.306	27.808
50/100	13.171	29.267	29.354	28.149
60/100	12.421	29.718	29.403	28.495
70/100	11.714	30.176	29.451	28.844
80/100	11.047	30.641	29.500	29.198
90/100	10.418	31.114	29.548	29.556
100/100	9.825	31.593	29.597	29.919

Table 2: Prediction results of GM(1,1) grey prediction model under DFA/CS combination

Table 3: Prediction results of GM(1,1) grey prediction model under DFA/CE combination

DFA/CE	Tar yield	Water yield	Char yield	Syngas yield
10/100	34.420	27.420	21.430	16.730
20/100	40.041	19.819	24.636	15.738
30/100	41.348	18.928	24.609	15.121
40/100	42.698	18.077	24.582	14.528
50/100	44.092	17.264	24.555	13.958
60/100	45.532	16.488	24.528	13.411
70/100	47.019	15.747	24.501	12.885
80/100	48.554	15.039	24.474	12.380
90/100	50.139	14.363	24.447	11.894
100/100	51.776	13.717	24.420	11.428

Table 4: Prediction results of GM(1,1) grey prediction model under DFA/LG combination

DFA/LG	Tar yield	Water yield	Char yield	Syngas yield
10/100	18.06	15.3	58.170	8.470
20/100	13.213	19.064	57.278	10.708
30/100	11.851	19.809	57.233	11.055
40/100	10.630	20.584	57.188	11.414
50/100	9.534	21.389	57.143	11.784
60/100	8.551	22.225	57.098	12.166
70/100	7.670	23.094	57.053	12.561
80/100	6.879	23.997	57.008	12.968
90/100	6.170	24.936	56.963	13.389
100/100	5.534	25.911	56.918	13.823

Taking the DFA/CS combination as an example, the scatter line graph of the original data and the predicted value of each product yield is drawn, and it can be intuitively found that the fit degree of GM(1,1) gray prediction model is still high, the error between the predicted value and the actual value is small, and the prediction performance is good(figure 1).

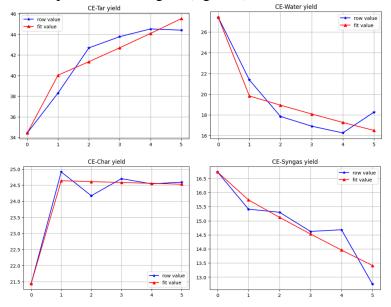


Figure 1: Prediction performance of GM(1,1) grey prediction model under DFA/CE combination

3. Conclusions

This study, dedicated to addressing the growing global demand for renewable energy, focuses on the quality and yield of cotton straw pyrolysis products, using cotton straw as an important biomass resource. An in-depth analysis of the relationship between the mixing ratio of pyrolysis combinations and the product yields reveals that there is a non-linear relationship between most product yields and mixing ratios. For this reason, a polynomial nonlinear regression model was used for prediction, aiming to improve the prediction accuracy.

With limited data, the study introduced the GM(1,1) grey prediction model and established a nonlinear regression model by Least Square Method as a means of analysing the product yields under different pyrolysis combinations. It was found that the GM(1,1) model performed well in prediction, and its high degree of fit and good predictive performance were verified by plotting scatter plots of DFA/CS combinations. A systematic and in-depth study reveals the superiority of the polynomial nonlinear regression model and the GM(1,1) model in predicting the pyrolysis products of cotton straw.

This study is of great significance for the development of the renewable energy field and provides a scientific basis for the efficient utilisation of cotton straw pyrolysis products. By developing and analysing the prediction model, the study provides insights into the sustainable development and green energy production from cotton straw. Ultimately, the study is expected to promote the research and application of renewable energy and contribute important scientific and technical support to solving global energy problems.

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