ISSN 2706-655X Vol.4, Issue 4: 53-60, DOI: 10.25236/IJFET.2022.040407

Parameter Fluctuation Modeling and Extreme Value Prediction of Coal Gasification Based on Jump Diffusion Model

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Abstract: *In order to accurately predict the random fluctuation of uncontrollable process parameters in coal gasification process and optimize operation parameters, a stochastic differential equation with jump was proposed to study the random dynamic sequence of process parameters changing with time. Considering the effect of emergencies, the jump process was introduced into the geometric Brownian motion model to simulate the jump caused by emergencies, and the stochastic differential equation with jump was established to simulate and predict the parameter fluctuation sequence. The results show that the method can accurately simulate and predict the random fluctuation sequence of uncontrollable process parameters and describe the random fluctuation process of parameters, which lays a foundation for the study of its influence on the gas production performance of coal gasification.*

Keywords: *Coal Gasification, Operating Parameters, Noise Factor, Stochastic Differential Equation with Jump, Monte Carlo Simulation*

1. Introduction

In recent years, the increasing concern of coal utilization on environment and health has promoted the emergence of clean coal technologies [1-4]. In the process of coal gasification production, coal feeding speed, ash content, moisture and other key process parameters are affected by a variety of factors, such as coal lock bucket of gasifier and bridge of feeder, non-standard operation, different batches and coal degradation[5-7]. Under normal working conditions, it fluctuates randomly rather than keeping constant. Even due to the occurrence of emergencies, there is an extreme value exceeding the limit, which leads to the unstable operation of gasifier and even the occurrence of shutdown accident, affecting the gasification performance. Therefore, it is very important to optimize the control of gasification process and guarantee the smooth operation of gasification process to scientifically model the dynamic change of process parameters, accurately depict the random fluctuation of these process parameters and timely predict the possible over-limit extreme value.

Many researchers have discussed the optimization of coal gasification. Most of the simulation studies are based on Aspen Plus simulation software as an experimental platform to analyze the impact of various operating parameters on the gasification index [8-16]. In the other part of the study, some other test methods were used to analyze the influence of process parameters on gasification performance [17-18]. However, most of the existing research results focus on the deterministic modeling and optimization of gas gasification performance, and the influence of process parameter fluctuation on the stability of coal gasification production system has not been considered.

Therefore, considering the random jump thoughts, this paper aiming at uncontrolled technology parameters in coal gasification with jump stochastic differential equation is put forward, considering the incident to the influence of process parameters, based on the traditional model of geometric Brownian motion process of introducing the "jump" to simulate the incident caused by the jump, to truly describe the process of technological parameters of random fluctuations It lays a foundation for the study of its influence on gas production performance.

2. Construction of Jump Diffusion Model of Uncontrollable Process Parameters in Gasification Process

2.1. Basic theory of stochastic differential equations

Stochastic differential equation was originally proposed to solve the stock price fluctuation prediction problem, mainly used in the study of sample sequence. It is widely used to describe uncertain dynamic behaviors in physics, economy and finance. The basic form of stochastic differential equation is as follows:

$$\frac{dP(t)}{P(t)} = \mu(t)dt + \sigma dW \tag{1}$$

Where, P is the dynamic sequence to be predicted, μ is the rate of change of the TTH element in the sample sequence relative to the previous element, σ is the fluctuation of the rate of change, is the standard deviation of the rate of change, and W(t) is the Wiener process or Brownian motion.

Under ideal conditions, geometric Brownian motion can fit stochastic wave process well. Due to the influence of various emergencies, such as the significant influence of human factors, environmental factors, machine factors, etc., the process parameters appear large and irregular jump, resulting in the appearance of extreme values. Therefore, on the basis of the traditional geometric Brownian motion model, the "jump" process is introduced to simulate the jump caused by sudden events, so as to describe the random wave process truly. Considering the asymmetry of real statistical data, an asymmetric exponential jump diffusion model is established.

2.2. Jump Diffusion Model of Coal Gasification Process Parameters

2.2.1. Uncertainty Analysis of Process Parameters

After the coal is ground into pulverized coal, it will be transported by inert gas nitrogen. The feeding speed is the flow rate of pulverized coal in the transportation process. When oxygen and water vapor transport is stable, the feed speed determines the oxygen to coal ratio and steam to coal ratio, thus affecting the gasification performance. Ash content refers to the waste residue generated after coal combustion. Higher ash content of coal means low combustion efficiency, which is not conducive to improving coal gas efficiency. In addition, the coal with high ash content is easy to slagg in the gasifier, resulting in poor permeability of the bed and uneven distribution of gasifier, resulting in accidents. At present, the content of coal ash fluctuates greatly due to many reasons. Moisture is the moisture content of coal. Excessive moisture content of coal will lead to incomplete drying of coal powder, which will increase the heat required for drying and reduce the gasification efficiency. The proper moisture content can prevent the thermal cracking of coal and be beneficial to gasification. Moisture content in coal fluctuates from batch to batch and from coal deterioration.

2.2.2. Construction of Jump Diffusion Model for Coal Gasification Process Parameters

Uncontrolled during the process of coal gasification process parameters will be influenced by all kinds of emergencies, such as: human factors, environmental factor, machine factor, etc., thus appeared irregular jumping sharply, therefore, it is necessary in the traditional Brownian motion model on the basis of introducing the "jump" process to simulate the jump caused by emergencies. Continuous fluctuation is represented by geometric Brownian motion, and the fluctuation of extreme value of process parameters caused by emergencies is discontinuous jump, which is represented by composite Poisson process. Write S as the fluctuation sequence of process parameters to be predicted. The jump diffusion model is as follows:

$$\frac{dS_t}{S_t} = \mu dt + \sigma dW_t + (e^{J_u} - 1)dN_u(\lambda_u) + (e^{-J_d} - 1)dN_d(\lambda_d) \tag{2}$$

Where, S is the dynamic sequence of process parameters to be predicted, μ is the change rate of the t element relative to the last element in the sample sequence, σdW is the fluctuation of the volatility, σ is the standard deviation of the change rate, Wt is the Wiener process or Browne motion, Ju and Jd represent the jump amplitude up and down in the jump direction respectively. All obey exponential distribution and their density functions are as follows:

$$f(J_u) = \begin{cases} \frac{1}{\eta_u} e^{\frac{-J_u}{\eta_u}}, J_u > 0, \eta_u > 0, \\ 0, J_u \leq 0 \end{cases} \tag{3}$$

ISSN 2706-655X Vol.4, Issue 4: 53-60, DOI: 10.25236/IJFET.2022.040407

$$f(J_d) = \begin{cases} \frac{1}{\eta_u} e^{\frac{-J_d}{\eta_d}}, J_d < 0, \eta_d > 0, \\ 0, J_d \geq 0 \end{cases} \tag{4}$$

Here, η_u and η_d describe the mean of jumps, respectively; $dN_u(\lambda_u)$ and $dN_d(\lambda_d)$ are poisson counting processes of λ_u and λ_d respectively.

$$p(dN_u(\lambda_u) = 1) = \lambda_u dt, p(dN_u(\lambda_u) = 0) = 1 - \lambda_u dt$$

$$p(dN_d(\lambda_d) = 1) = \lambda_d dt, p(dN_d(\lambda_d) = 0) = 1 - \lambda_d dt$$

After logarithmic transformation of Equation (1) using ITO's lemma, the following form can be obtained:

$$d \ln S_t = \left(\mu - \frac{1}{2}\sigma^2\right) dt + \sigma dWt + J_u dN_u(\lambda_u) - J_d dN_d(\lambda_d) \tag{5}$$

The jump diffusion model of process parameter fluctuation dynamic sequence S is simplified as follows:

$$\mathrm{S_t} \approx \mathrm{S_{t-\Delta_t}} \cdot \exp\left\{\left(\mu - \frac{1}{2}\sigma^2\right) \Delta_t + \sigma\sqrt{\Delta_t}\varepsilon_t + B_t^u J_t^u - B_t^d J_t^d\right\} \tag{6}$$

2.3. Process parameter jump point identification and model parameter estimation

2.3.1. Lee-Mykland hop recognition theory and algorithm

Lee and Mykland proposed a jump recognition method. Based on this method, test statistical variable L(i) was constructed to test whether there is a jump from ti—1 to ti at ti moment:

$$L(i) \equiv \frac{\log S(t_i)/S(t_{i-1})}{\hat{\sigma}(t_i)} \tag{7}$$

Among them

$$\hat{\sigma}(t_i)^2 = \frac{1}{k-2} \sum_{j=i-k+2}^{i-1} \left|\log S(t_j)/S(t_{j-1})\right| \left|\log S(t_{j-1})/S(t_{j-2})\right| \tag{8}$$

Is the time-point variance of the point estimated by real double-power variation, S(ti) is the value of the process parameter at ti. The statistical variable L(i) asymptotically follows a normal distribution with a mean value of 0 and a standard deviation of $\frac{1}{C^2}$, where $c = \sqrt{\frac{2}{\pi}}$.

Lee and Mykland gave the rejection domain of jump recognition, and proved that if there is no jump in the time interval (ti-1, ti), then when δ T →0:

$$\frac{\max|L(i)| - C_n}{S_n} \to \psi \tag{9}$$

ψ is a cumulative distribution function, Meet the $P(\psi \leq x) = exp(-e^{-x})$, and $C_n = \frac{(2\log n)^{0.5}}{c} - \frac{\log(\pi) + \log(\log n)}{2c(2\log n)^{0.5}}$, $S_n = \frac{1}{c(2\log n)^{0.5}}$, $C = \sqrt{\frac{2}{\pi}}$, where n is sample size and K is window size.

By constructing the above test statistical variables, the corresponding test results were obtained when the significance level α was given. The jump recognition steps of process parameter value sequences are given below.

1) Calculate statistical variable L(i) for the ith data using Equations (8) and (9).

2) choose a significance level of alpha calculation threshold, it is a x cumulative distribution function, meet the P (ψ≤β^*) = exp ($-e^{-\beta^*}$) = 1-α.

3) if $\frac{|L(i) - C_n|}{S_n} > \beta^*$, then it is determined that there is a jump in the period of (ti-1, ti), otherwise there is no jump.

Repeat the above 3 steps for each site until all samples are tested

2.3.2. Parameter Estimation

Lee-mykland hop identification method was used to identify the jump point and jump moment in the fluctuation sequence of uncontrollable process parameters, which were separated from the diffusion process to obtain the jump sequence R_t^i I and the continuous sequence R_t^c. Because R_t^c is missing some data, the diffusion part is incomplete. In order to smooth the data and make the continuous sequence data smoother, we select the mean value of the data at 6 moments before and after the jump point to replace the data and obtain the modified diffusion process. The diffusion part follows normal distribution, and the modified data obtained by this method still follows normal distribution, and the maximum likelihood is used to estimate the parameters.

(1) Estimation of jump frequency

For Poisson counting with a strength of λ :

$$P(\xi = k) = \frac{\lambda^k e^{-\lambda}}{k!}, \mathrm{k} = 0,1,2 \cdots$$

The maximum likelihood estimate λ of Poisson distribution is: $\widehat{\lambda_l}(\xi_1, \xi_2, \cdots, \xi_n) = \bar{\xi} = \frac{1}{n}\sum_{i=1}^{n} \xi_i$,Where$\xi_1, \xi_2, \cdots, \xi_n$ are sample points.

Hop identification in this paper detects the jump sequence R_t^J in the sample, and the hop amplitude greater than 0 is m_1, and that less than 0 is m_2. The hop frequency can be estimated as $\hat{\lambda}_u = \frac{m_1}{n}, \hat{\lambda}_d = \frac{m_2}{n}$, where n indicates the number of sample points.

(2) Estimation of jump amplitude

As for the exponential distribution, it is simplified to log likelihood function $\ln(\hat{\lambda}) = n \ln \hat{\lambda} - \hat{\lambda} n \bar{x}$ and the maximum likelihood estimate of λ can be obtained as follows:

$$\hat{\lambda} = \frac{1}{\bar{x}} = \frac{1}{\frac{1}{n}\sum_{i=1}^{n} x_n} \tag{10}$$

Where x1,x2,…,xn are sample points.

For the jump rate sequence R_t^i, the modified continuous diffusion sequence can be obtained by using the above method, denoted as

$$\mathrm{R}_{t'} = \frac{1}{6}(\mathrm{R}_{t-3} + \mathrm{R}_{t-2} + \mathrm{R}_{t-2} + \mathrm{R}_{t+1} + \mathrm{R}_{t+2} + \mathrm{R}_{t+3}) \tag{11}$$

If $R_t^J$is subtracted from $R_{t'}$according to the time, the amplitude is obtained. The amplitude greater than 0 is m1, denoted as J_i^u(i=1,2,⋯,m1); the amplitude less than 0 is m2, denoted as J_i^d(i=1,2,⋯,m2). The estimates for the jumps up and down are:

$$\hat{\eta}_u = \bar{J}^u = \frac{1}{m_1}\sum_{i=1}^{m_1} J_i^u, \hat{\eta}_d = \bar{J}^d = \frac{1}{m_2}\sum_{i=1}^{m_2} J_i^d \tag{12}$$

(3) Parameter estimation of diffusion process

The maximum likelihood estimates of the mean and variance of the normal distribution are:

$$\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i = \bar{x} \tag{13}$$

$$\hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2 \tag{14}$$

The modified continuous diffusion process yield sequence $R_{t'}$, Calculate the mean value and standard deviation by using Equations (9) and (10) respectively.

3. Empirical Analysis

In the process of coal gasification, the fluctuation of coal feeding speed, ash content, moisture and other process parameters will have a bad effect on gas production performance, especially the instability of coal feeding speed will reduce the quality of gas production. In order to better describe the variation rules of these process parameters, taking coal feeding speed as an example, the stochastic process modeling and jump identification prediction of process parameters are carried out by using random jump process.

ISSN 2706-655X Vol.4, Issue 4: 53-60, DOI: 10.25236/IJFET.2022.040407

3.1. Data Sources

The process parameters are described as a diffusion process with exponential jump. In order to effectively estimate the frequency and amplitude of jumps in order to simulate and predict the authenticity of process parameters. According to previous literatures, taking coal feeding rate as an example, 1000 original data of coal feeding rate were selected (n=1000), as shown in Fig.1 (a). According to Fig.1 (a), it can be seen that the original data graph of coal feeding rate is not stable, and there are some extreme values, namely jump points.

Since the original data fluctuates greatly and is not stable enough, the logarithm of the original data is taken without changing the correlation and stability of the data. According to formula (15), the logarithmic difference sequence of coal feeding speed is derived from the original data, as shown in Fig.1 (b).

$$R_i = \ln S_i - \ln S_{i-1} \tag{15}$$

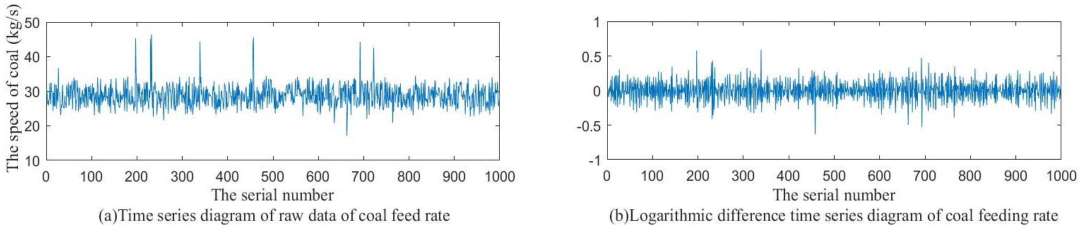

Figure 1: Time series diagram of coal feeding rate

The basic statistics of logarithmic difference sequence data of coal feeding speed calculated by Matlab are as follows. The skewness of the logarithmic difference series data of coal feeding rate is -0.0134, showing a left-biased distribution. The kurtosis coefficient is 3.6573, greater than the kurtosis coefficient 3 of the normal distribution, indicating that the logarithmic difference series of coal feeding velocity presents the characteristics of sharp peaks and thick tails. The above data show that the logarithmic difference sequence of coal feeding speed does not obey the normal distribution. Due to the existence of "jump", the original data shows the statistical characteristics of jump anomaly and sharp peak and thick tail.

3.2 Identification and Parameter Estimation of Process Parameter Fluctuation Jump

3.2.1. Jump Identification of Process Parameter Jump Diffusion Model

The Lee-Mykland hop identification method was used to conduct point-by-point test on the logarithmic difference sequence R_t of coal feeding speed. The significance level α=0.01 was selected to identify the jump sequence R_t^J, as shown in Figure 2 (a).

The six data before and after the jump point were used to replace the return rate of the jump point, and the modified continuous diffusion process sequence $R_t{'}$ was obtained, as shown in Fig. 2 (b).According to the difference between $R_t{'}$and the original data Rt, it can be concluded that the upward jump times m1 is 2, and the downward jump times m2 is 3.

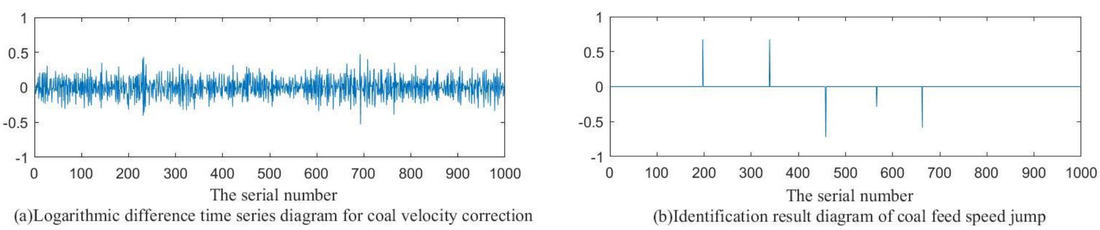

Figure 2: Time series diagram of coal feeding rate

The basic statistics of the corrected logarithmic difference series of coal feeding rate are given below. The mean value was 0.0002, standard deviation was 0.1395, skewness was -0.0250, and kurtosis was 3.0097.

It can be seen from the data obtained above that the modified logarithmic difference time series graph is basically stable. By comparing with the original sequence, it is found that the Lee-Mykland hop identification method can better identify the jump points in the sequence. On the other hand, the statistical characteristics of the revised sequence were observed, and the kurtosis decreased from 4.0813 to 3.0097, which was closer to the kurtosis value of the normal distribution.

3.2.2. Parameter Estimation of Process Parameter Jump Diffusion Model

After the jump identification of the logarithmic difference time series data of coal feeding speed, the second stage is entered, and the parameters of the logarithmic difference series of coal feeding speed are estimated according to the maximum likelihood method. The estimation results of parameters are obtained by matlab, as shown in 1.

Table 1: Parameter estimation results of coal feeding velocity jump diffusion model

parameter	μ	σ	λ_u	λ_d	η_u	η_d
estimate value	2.2223e-04	0.1399	0.0020	0.0030	0.6742	0.5295

As can be seen from the parameter estimation results in Table 1, the fluctuation rate of logarithmic difference series of coal feeding speed is 0.1399, the frequency of upward jump and downward jump are 0.0020 and 0.0030 respectively, and the amplitude of jump is between 0.5295 and 0.6742.

3.3. Analysis of Simulation Results

In order to test the effectiveness of the combined method of jump identification and parameter estimation in the process parameter jump diffusion model, monte Carlo simulation method is used to generate simulated logarithmic difference time series diagram below, and the effectiveness of the estimation method is tested by comparing with the real value. Because it is difficult to carry out mathematical derivation in theory, the method of simulation is often used to judge. Based on the established model (2) and parameters estimated from historical data, monte Carlo simulation method is used to generate simulated logarithmic difference time series diagram, and the validity of the estimation method is verified by comparing with the real value.

According to the

$$R_t = \ln S_t - \ln S_{t-\triangle t} = \ln\frac{S_t}{S_{t-\triangle t}} \approx \left(\mu - \frac{1}{2}\sigma^2\right)\triangle t + \sigma\sqrt{\triangle t}\varepsilon_t + B_t^u J_t^u - B_t^d J_t^d \tag{16}$$

The calculated parameters are substituted in respectively, and the corresponding logarithmic difference data sequence is simulated by Monte Carlo method in Matlab to generate Q-Q graph of simulated data and real data of coal feeding speed, as shown in Fig. 3 below.

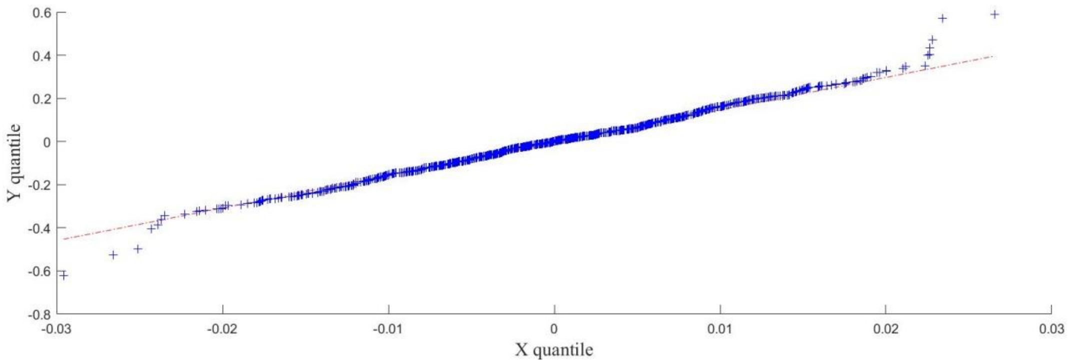

Figure 3: Q-Q diagram of simulated data and real value of coal feeding speed

As shown in coal feeding rate, Q-Q diagram of ash and moisture simulation data and real data can be obtained in the same way, as shown in Fig. 4 and Fig. 5 below.

ISSN 2706-655X Vol.4, Issue 4: 53-60, DOI: 10.25236/IJFET.2022.040407

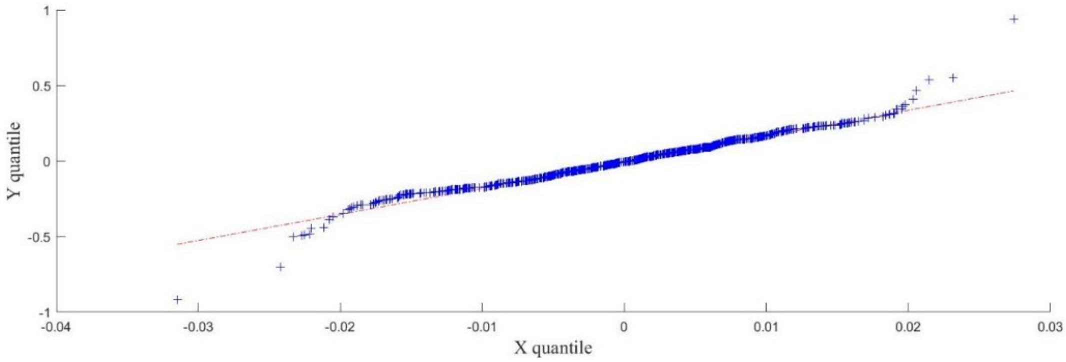

Figure 4: Q-Q diagram of ash simulated data and real value

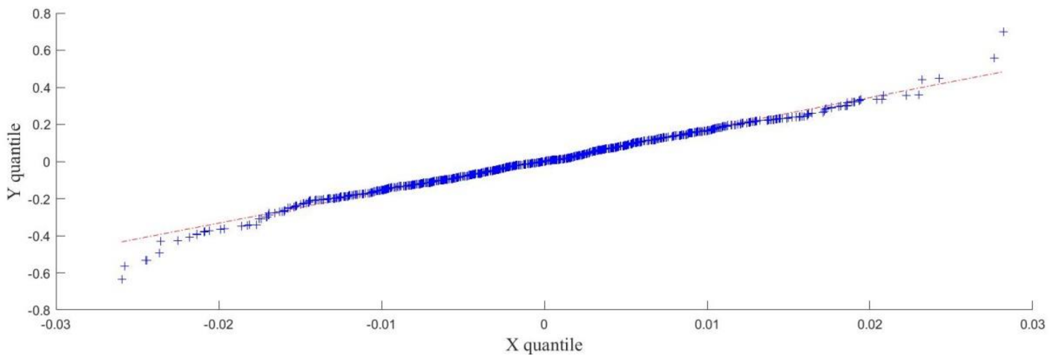

Figure 5: Q-Q diagram of water simulation data and real value

It can be seen from the Q-Q diagram of simulated data and real value that the fitting value of jump diffusion model of process parameters established in this paper is almost in a straight line with the real value, indicating that the fluctuation distribution of process parameter data simulated by stochastic differential equation model with jump is basically consistent with the real data distribution.

In this paper, we estimate the log-difference time series data of process parameters by using the combined method of parameter estimation of jump identification, which can not only estimate the parameters of jump diffusion model effectively, but also identify the time point of jump occurrence and the corresponding parameters. Finally, the effectiveness of the method is verified by Monte Carlo simulation.

3. Conclusion

(1)In order to predict the random fluctuation of process parameters more accurately, a jump process is introduced based on the traditional geometric Brownian motion model to simulate the jump caused by sudden events.

(2)The random fluctuation process of process parameters is described truly, which lays a foundation for the study of its influence on gas production performance. This method can identify the time point of jump and count the jump amplitude, effectively separate the "jump", and estimate the parameters of jump diffusion model effectively.

(3)The empirical results show that the time fluctuation sequence data of process parameters can be statistically analyzed and simulated by establishing stochastic differential equation with jump, which lays a foundation for the study of its influence on gas production performance and is worthy of further study and promotion.

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