Prediction and Analysis of O3 Based on the ARIMA Model

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Abstract: Despite of the small amount in the atmosphere, ozone is one of the most critical atmospheric component as it protects human beings and any other life on the earth from the sun´s high frequency ultraviolet radiation. In recent decades, the global ozone depletion caused by human activities is well known and produces an " ozone hole" , the most direct consequence of which is the increase in ultraviolet radiation, which will affect human survival, climatic environment, ecological environment and other important adverse impacts. Due to the implementation of the Montreal protocol and other agreement, the total amount of ozone depleting substance in the atmosphere has been prominent reduced, which will lead to a new round of regional climate change. Therefore, predicting the changes of the total ozone in the future will have an important guiding significance for predicting the future climate change and making reasonable measures to deal with the climate change. In this paper, based on the ozone data of 1979 to 2016 in the southern hemisphere and ARIMA model algorithm, using time series analysis, we obtain prediction effect of ARIMA model is good by Ljung-Box Q-test and R^2, and the model can be used to predict the future ozone change. With the help of SPSS software, the future trend of the total ozone can be predicted in the future 50 years. Based on the above experiment results, the global ozone change in the future 50 years can be forecasted, namely the atmospheric ozone layer will return to its 1980´s standard by the middle of this century at the global scale.

Keywords: Ozone; Ozone Hole; ARIMA Model; Prediction Analysis.

1 Introduction

Ozone is a kind of filter of solar ultraviolet radiation, which can protect human, animal and plant from ultraviolet radiation damage[1]. However, with the intensification of human activities, especially the wide use of CFCs, halogenated hydrocarbons and other chemical substances, ozone depleting substance with a large number of catalytic action into the atmosphere and gathered in the polar area, and eventually the sun box shot and ozone photochemical reaction[2], and consume a lot of high-altitude ozone, which lead to a sharp reduction in the total amount of ozone in the atmosphere[3]. Due to a substantial decline in total ozone, the formation of a large area of ozone thin area over the Antarctic region, which is called the "ozone hole" by scientists[4]. The most immediate consequence of global total ozone reduction will lead to the increase of ultraviolet radiation[5], which will have an adverse impact on human survival, climate and environment, and so on. Excessive ultraviolet radiation on the skin will stimulate the skin to produce pigment that is " erythema effect" , if the UV radiation dose increases, it is easy to induce skin cancer; ultraviolet radiation can cause cataract, interfere with the body´s immune system, and endanger the respiratory.

Since mankind recognized the existence of ozone, the world began to observe and study the ozone, mainly including the change of the global total ozone latitude, the intranasal and seasonal variation of. The purpose of these works is to make people more aware of the changing trend of the ozone, guiding us to take appropriate measures to protect the ozone layer, human health and the survival of the environment. The prediction of global total ozone will provide an important theoretical basis and scientific guarantee for the reasonable response to global climate change.

Overall, the statistical classification model[6] and regression model[7] are widely used in the statistical prediction of the concentration of ozone. The classification model does not need to predict the statistical distribution of the forecast, the choice and the threshold value of the forecast factors are determined by the CART software according to the maximum correlation with the concentration of ozone. From a predictive point of view, CART is very valuable. Because it is very easy to operate, and allows for classification based on a small number of basic observations predicted.

Other researchers always used multivariate linear regression method [8] to predict ozone concentration, this method predicts the relationship between the dependent variable and the independent variable (ozone concentration) by selecting a factor that has a greater influence on the ozone concentration as a dependent variable. Because the dependent variable and the independent variable are usually nonlinear, it is obvious that the linear regression method cannot describe the relationship. The nonlinear regression method is used for the prediction of ozone. Because time series analysis has certain advantages in the change of ozone concentration and auto correlation, it has been widely used in the development of ARIMA model [9] based on the auto regression model.

Because ozone mainly exists in the stratosphere, the lower troposphere thickness in each dimension is not the same, the highest latitude low, can reach 17~18 km, mid latitude is about 11~12 km, and high latitude is only 8~9 km. Human emissions to the atmosphere of chlorofluorocarbons and other substances are most easily accessible over the polar regions. Cold is a key factor in the thinning of the ozone layer. The key research shows that, no matter what the nature of the particles in the clouds, the chemical reaction will occur in any form of chlorine transformation into active chlorine the clouds in the cold when the surface temperature dropped to minus 73 degrees Celsius. The particle will serve as a catalyst for the chemical reaction of active chlorine release, the ozone layer is much more damaging than other areas. This paper mainly illustrates the destruction on the Antarctic ozone layer.

Section 2 described the theoretical basis of prediction of total ozone time forecast. Section 3 established the ozone concentration prediction model based on ARIMA model and the application of this model to analyze and forecast the next 50 years the southern hemisphere and the global changes in the trend of ozone content.

2 The Theoretical Basis of Time Prediction of Total Ozone

2.1 Time Series Prediction

Time series analysis is an important part of multivariate statistical analysis, and time series analysis is a collection of observation data obtained in time sequence. A lot of data is presented in time series, such as the monthly throughput, freight dock road traffic times weekly report, the sequence number of admissions daily mean daily outpatient hospital, city sequence of air pollutants, the annual data series, area of the total industrial output value by demographic data, etc. The essential characteristic of time series is different from common data, which is the dependence or correlation between neighboring observations. The statistical analysis method of time series data is different from that of general data. In fact, the special techniques of time series analysis are almost based on the technique of self-correlation processing. The analysis of time series data can be used to understand the nature of things from a kinematic point of view, such as the differences between several time series, the periodicity between a longer sequence, and the prediction of future conditions.

2.2 The Establishment and Stabilization of Time Prediction

Before fitting the time series model to the data, it is important to observe and deal with the data until it is smooth. According to the sequence of data preprocessing, it will be divided into three steps: first, filled to the missing value data. Secondly, the data is defined as the corresponding time series. Finally, the stability of time series data is calculated and observed. If there is a variable in the data file. The value is collected at a certain time interval. To conduct a time series analysis, there is also a date variable that indicates the acquisition time.

2.3 ARIMA Model of the Time series analysis

2.3.1 Basic Concepts

In the prediction process, the average model (ARMA)、the autoregressive model for special cases and the moving average model (MA model) can be used to fit the stationary time series for predicting the future value of the time series[10]. However, in the actual forecast process, random sequences are often non-stationary. The differential operation for the random number series should be done firstly, namely ARIMA model which is a generalization of ARMA mode l[11].

The full name of ARIMA model is the autoregressive integrated moving average model[11], denoted as ARIMA (p, d, q), which is a famous time series model, proposed by Box and Jenkins in the early 1970s. So the prediction model also called Box-Jenkins model . In this model, AR is auto regressive, p is the autoregressive order, q is the moving average order, d for difference times In fact , ARIMA (p, d, q) model is the combination of the difference operation and ARMA (p, q) model , ARMA (p, q) can be replaced by ARIMA (p, d, q) model after d times differential operation.

2.3.2 Statistical Principle

(1) ARMA Process

Establish $\{x_t\}$ to be a zero mean stationary sequence, $\{a_t\}$ is white noise, $Ex_ta_t=0(t<s)$ is the mean sequence of time series, it is the time related sequence), conform to

$$x_t - \varphi_1 x_{t-1} - \varphi_2 x_{t-2} - \cdots - \varphi_p x_{t-p} = a_t - \theta_1 a_{t-1} - \theta_2 a_{t-2} - \cdots - \theta_q a_{t-q} \quad (1)$$

In Eq. (1), x_{t-p} represents the numerical value of time lag p time than the time t. $\{x_t\}$ is p order autoregressive moving average process of order -q, denoted by ARMA (p, q).

$\{x_t\}$ called ARMA (p, q) sequence, Non-negative integer p, q, respectively, known as the autoregressive order and moving average order, The parameter $\varphi_1, \varphi_2 \cdots \varphi_p$ are called the auto regressive coefficient, and $\theta_1, \theta_2 \cdots \theta_p$ are called the moving average coefficient.

When p=0, it is the ARMA (0, q) model

$$x_t = a_t - \theta_1 a_{t-1} - \theta_2 a_{t-2} - \cdots - \theta_q a_{t-q} \quad (2)$$

It is called Q order moving average model, denoted as MA (Q). When q=0, it is ARMA (P, 0) model

$$x_t - \varphi_1 x_{t-1} - \varphi_2 x_{t-2} = a_t \quad (3)$$

It is called as p order autoregressive model, denoted as AR (P).

Lead into the backward shift (delay) operator B, and let $B^k x_t = x_{t-k}, B^k a_t = a_{t-k}, B^k c = c$, ($c$ is a constant), and

$$\varphi(B) = 1 - \varphi_1 B - \varphi_2 B^2 - \cdots - \varphi_p B^p \quad (4)$$

$$\theta(B) = 1 - \theta_1 B - \theta_2 B^2 - \cdots - \theta_p B^p \quad (5)$$

The ARMA (p, q) model is abbreviated as

$$\varphi(B) = \theta(B) a_t \text{ or } x_t = \varphi^{-1}(B)\theta(B)a_t \quad (6)$$

(2) Identification of ARMA Model

Let ACF represents the autocorrelation function of $\{x_t\}$, and PACF represents the partial autocorrelation function of $\{x_t\}$. According to the method proposed by Box-Jenkins, using truncation of the sample autocorrelation function (ACF) and partial autocorrelation function (PACF) to preliminary identify the order number of ARMA model. The specification is as shown in Table 1.

Table 1 Identification of ARMA model

model	the sample autocorrelation function(ACF)	partial autocorrelation function(PACF)
AR(p)	Tailing	p-order truncation
MA(q)	q-order truncation	Tailing
ARMA(p,q)	Tailing	Tailing

The above table is an important basis for judging the form of time series model and fitting the model. According to the ARMA (p, q) sequence, the parameter of p, q can be initially recognized. Then, the identification process is repeated to find out the best combination p, q value.

(3) Nonstationary Time Series

Deficit a first-order differential operator for $\nabla = z_t - z_{t-1}$, and the difference operator ∇ and delay operator B are related as:

$$\nabla = 1 - B, \nabla^2 = (1 - B)^2, \nabla^d = (1 - B)^d \tag{7}$$

In Eq. (7), d is the order of difference.

Seasonal difference: seasonal difference in the k generally take a cycle, such as the monthly data for $k=12$, quarterly data for $k=4$, and so on, the seasonal difference of the operator

$$\nabla_k = x_t - x_{t-k} \tag{8}$$

Set up $\{z_t\}$ as a stationary sequence, $\{x_t\}$ as a (p, q) ARMA sequence, d is a positive integer, and $x_t = \nabla^d z_t, t>d$, the formula is as follows.

$$\varphi(B)(1 - B)^d z_t = \theta(B) A a_t \tag{9}$$

(4) Seasonal ARIMA Model

Time series are usually periodic, or seasonal trends. Using the ARIMA model to deal with this kind of seasonal trend can lead to excessive parameters and complex model. A seasonal product model can be used to obtain the parameters of the model. The seasonal product model is expressed as ARIMA (p, d, q, sp, sd, sq), in which, sp indicates the autoregressive coefficient, sd represents the difference of the order, usually for first order seasonal difference; sq represents the seasonal model of moving average parameters. If the monthly data, to describe the characteristics of the year, then $sd = 12$; if the log information, to describe the weekly feature, then $sd = 7$.

2.3.3 Modeling Steps of ARIMA Model

Making ARIMA model actually includes 3 stages, which are the pattern recognition stage, the parameter estimation and testing phase, and the prediction application stage. The first two stages often need to be repeated. The identification of ARIMA model is to determine the order of p, d, q, sp, sd, sq, mainly depending on the autocorrelation function (ACF) and partial autocorrelation function (PACF) to judgment and estimation. A good identification model should have two elements: one is the model of the residual is white noise series, through the residual white noise test, and the other is the simplicity and model parameter fitting optimization index of excellent balance, there is one point to note is that the form of the model should be easy to understand.

3 Establish and Analyze the Ozone Concentration Prediction Model

3.1 Ozone Concentration Prediction Model

3.1.1 Fill the Missing Value

Based on the southern hemisphere ozone data information in order to find missing data in 1995. Missing value in time series analysis can´t use delete ways to solve, this will lead to the destruction of the original time series periodic, but unable to get the correct results[12]. In 1979 ~ 2016 the lowest ozone concentration is as shown in Table 2.

Table 2 The minimum ozone concentrations from September 21st to October 16th 1979~2016

year	Ozone concentration
1979	225.0
1980	203.0
1981	209.5
1982	185.0
1983	172.9
1984	163.6
1985	146.5
1986	157.8
1987	123.0
1988	171.0
1989	127.0
1990	124.2
1991	119.0
1992	114.3
1993	112.6
1994	92.3
1996	108.8
1997	108.8
1998	98.8
1999	102.9
2000	98.7
2001	100.9
2002	157.4
2003	108.7
2004	123.5
2005	113.8
2006	98.2

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year	Ozone concentration
2007	116.2
2008	114.1
2009	107.5
2010	128.0
2011	106.2
2012	139.1
2013	132.5
2014	128.6
2015	116.5
2016	124.3

Here with the help of SPSS software to deal with the data in Table 1, it is observed by lack of data in 1995.

In order to fill in the missing data, the mean sequence method is chosen to fill the final effect after processing is shown in Table 3.

Table 3 in 1979 ~ 2016 the lowest ozone concentration data fill the missing value

year	O3	O3_1	year	O3	O3_1
1979	225.0	225.0	1998	98.8	98.8
1980	203.0	203.0	1999	102.9	102.9
1981	209.5	209.5	2000	98.7	98.7
1982	185.0	185.0	2001	100.9	100.9
1983	172.9	172.9	2002	157.4	157.4
1984	163.6	163.6	2003	108.7	108.7
1985	146.5	146.5	2004	123.5	123.5
1986	157.8	157.8	2005	113.8	113.8
1987	123.0	123.0	2006	98.2	98.2
1988	171.0	171.0	2007	116.2	116.2
1989	127.0	127.0	2008	114.1	114.1
1990	124.2	124.2	2009	107.5	107.5
1991	119.0	119.0	2010	128.0	128.0
1992	114.3	114.3	2011	106.2	106.2
1993	112.6	112.6	2012	139.1	139.1
1994	92.3	92.3	2013	132.5	132.5
1995	.	131.9	2014	128.6	128.6
1996	108.8	108.8	2015	116.5	116.5
1997	108.8	108.8	2016	124.3	124.3

3.1.2 Define the Variable of Date

Date module can generate cyclical and date of time series variables. Using " define date" dialog box to define the variable of date needs the data window read in a certain time sequence data files. It cannot repeat with the system default time variable names. Otherwise the date variables will be covered with the same name. System default variable name includes date, year, quarter, month, year, month, quarter, year, day, week, day, hour, day, etc.

3.1.3 Crate the Time Sequence

Smoothly on the condition of time series analysis based on sequence, it can be seen whether the mean square error no longer changes over time. Autocorrelation coefficient is related to time interval only and has nothing to do with that time. In time series analysis processing, the first difference and second order difference are often used to examine the time series. Sometimes, it needs to choose a suitable time sequence model of the original time series data to convert the logarithmic transformation or square, etc. This requires to create a new time series variable in the time series data files. The resulting sequence diagram is shown in Figure 1. The blue line is the curve of the actual value, and the green line is the fit values.

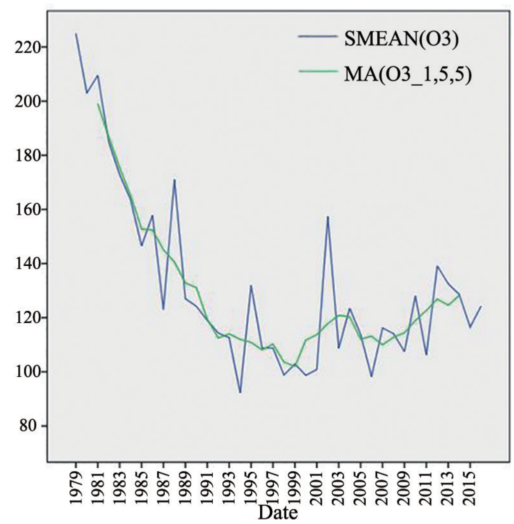

Fig. 1 Sequence diagram

3.2 Analysis of Global Ozone Trends from 1997 to 2016

By analyzing the time sequence diagram fitting generated for each year of the corresponding data, it can be obtained from the 1997 southern hemisphere ozone concentration began to decline around 2000 began to ease, 2004-2016 years, the amount of atmospheric ozone at a global scale in the overall on the rise, which shows that the atmospheric ozone layer on the global scale developed by regaining momentum. Overall, this linear trend shows that the total amount of atmospheric ozone in the global scale began to rise, confirmed that the ozone layer began to restore the forecast.

3.3 Forecasts of Ozone Levels over The next 50 Years

3.3.1 Using SPSS Software to Analysis the Data

First, the nature of the data sequence is observed. Using the SPSS software to make the time sequence diagram and observe the characteristics of the data sequence[13]. The timing diagram is shown in Figure 1 which shows that the data sequence appears to be relaxed after 2004. So it may be a stable time series. Then, the further analysis of autocorrelation and partial autocorrelation are executed. The output results are shown in Figure 2 and Figure 3.

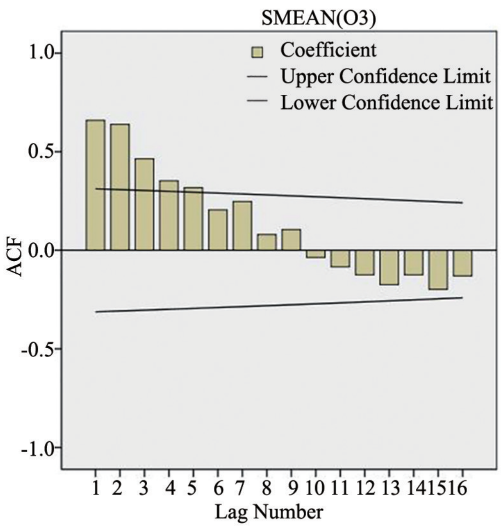

Fig. 2 Auto correlation diagram of ozone concentration

As can be seen from Figure 4, the autocorrelation function showed a typical tailing. The data correlation with time interval is decreased. From Figure 5, it can be seen that this data sequence has a short-term correlation, which further determines the sequence of the smooth. The data sequence autocorrelation and partial autocorrelation function, and pattern recognition rules 1, can determine the autoregressive order number *p*. Time series becomes stationary time series, which is the number of differential d and the moving average order. That is, ARIMA (p, d, q). Next, the ARIMA method is used to fit the model[14][15], and the final results are shown in Table 3, Table 4, Table 5, Figure 5, and Figure 6.

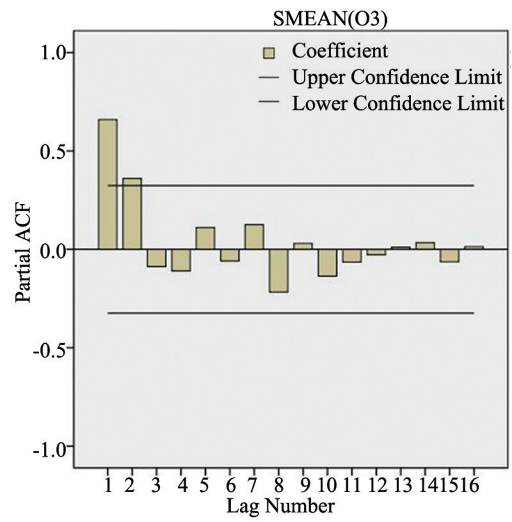

Fig. 3 Correlation diagram of ozone concentration

Table 4 Model Statistics

model	Number of Predictors	Model Fit statistics		Ljung-Box Q(18)			Number of Outliers
		R-squared	Normalized BIC	Statistics	DF	Sig.	
SMEAN(O3)-Model_1	0	0.651	6.406	16.219	17	0.508	2

Table 4 is a model of the statistics table. It lists some of the model fit statistics, including the coefficient of determination (R), the standard BIC value and Ljung-Box statistics. From the results, the fitting effect is ideal. The reason, namely Sig.>0.05, is the use of automatic detection of outliers in SPSS software analysis and prediction. Correspondingly the results are more ideal.

Table 5 ARIMA Model Parameters

					Estimate	SE	t	Sig.
SMEAN(O3)-Model_1	SMEAN(O3)	No Transformation	Constant		148.720	30.901	4.813	.000
			AR	Lag 1	.935	.054	17.298	.000

Table 5 is the ARIMA model parameter table. From the results, it can be seen that AR (1) model parameters is 0.935 and the parameters are significant. The constant term is 148.720, it also significant. From the results, the fitting model is Xt+0.935 =148.720+at.

Table 6 Outliers

			Estimate	SE	t	Sig.
SMEAN(O3)	1988	Additive	45.947	11.851	3.877	.000
-Model_1	2002	Additive	52.501	11.852	4.430	.000

Table 6 shows the results of the selection of detecting outliers automatically. According to the results of sig> 0.05, the choice of the value of the rejection is correct.

Figure 4 is ARIMA (1, 0, 0) model fitting residual autocorrelation function and partial autocorrelation function. It can be seen that the residual autocorrelation and partial autocorrelation functions are 0 order trailing. The residual is not a correlation with white noise sequence. Therefore the correlation of the sequences has been fully fitted.

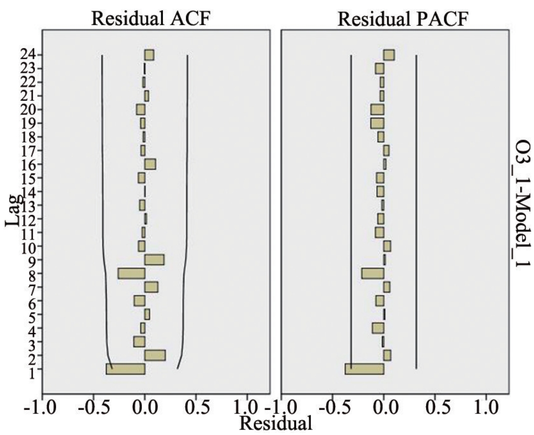

Fig. 4 Autocorrelation and partial autocorrelation function of ARIMA (1,0,0) fitting residual

3.3.2 Using SPSS Software to Predict the Ozone Level in the next 50 Years

Figure 5 shows the prediction results of ARIMA (1,0,0) model fitting, in which the red line is the observed value curve, and the fine blue line is the fitting curve. Through observation, it can be seen the predicted value curve can reflect the change of ozone content in the next 50 years, but it is too smooth that not close to the actual value curve. According to the data and combined with our experience, the predicted value curve should be up and down, and tend to be stable. The predicted curve is shown in Figure 6. Through the repeated verification of the value of p, d, q in ARIMA (p, d, q), it can be seen that the prediction results are better when ARIMA (p, d, q) = ARIMA (5,0,5). Finally, the ARIMA (5,0,5) model is selected to fit the results as the predicted value curve of ozone content in the future 50 years. The true prediction curve is shown in Figure 7.

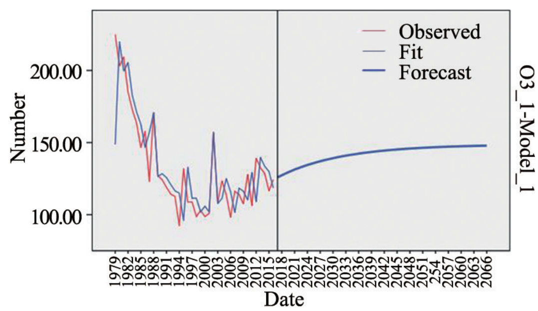

Fig. 5 Time sequence diagram of the observed and predicted values(AARIMA(1,0,0))

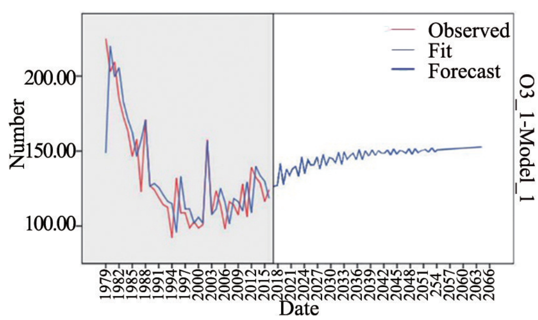

Fig. 6 The maginary prediction curve

The following conclusions can be drawn through the analysis of the above results shown in the timing chart of the observed and predicted values in Figure 5~Figure 7:

(1) Long term changes in the southern hemisphere and the trend of the total ozone extraction rate based on the discovery of atmospheric ozone have suddenly experienced 3 different phases, namely 1979-1994 total ozone decline phase, 1995-2005 transition phase and 2006~now ozone layer recovery phase. At the same time, the implementation of the Montreal agreement in 1986 effectively controlled the global total ozone decline rate.

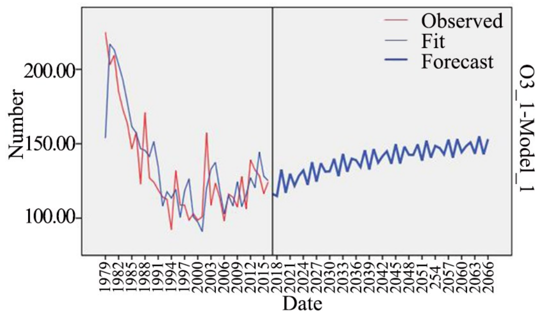

Fig. 7 Time sequence diagram of the observed and predicted values (ARIMA(5,0,5))

(2) The predicted results show that in 2040 the ozone layer in the southern hemisphere will be restored to the level of 1980 and remained within a stable level only considering the human factors of the Montreal agreement. The current due to the ozone hole caused by regional climate change will likely be reversed.

4 Conclusions

In recent decades, due to human activities caused by the global stratospheric ozone reduction has been confirmed by many observational facts.The most immediate consequence of the reduction of the ozone layer is the increase of short wave ultraviolet radiation in the near surface, which will have an important impact on the survival of human beings, climate and environment, and so on.

The research results of this paper is divided into two parts.

Firstly, from the southern hemisphere 1979~2016 in September 21st to October 16th the lowest ozone concentration data in the first part analyzes the characteristics of temporal and spatial variation of ozone. The results show that the atmospheric ozone content experienced a decline stage transition stage and rising stage. At the same time, it is found that the change of total ozone in the southern hemisphere is mainly affected by human factors, especially the implementation of the Montreal agreement.

The second part is the use of time series analysis of ARIMA modeling. With the help of SPSS software, it is predicted the total atmospheric ozone for the next 50 years. The predicted results show that the ozone layer in the southern hemisphere in 2040 will be restored to the level of 1980.

This proposed mode has the following advantages:

(1) By using time series analysis to establish the ARIMA model to predict the future 50 years of total ozone. The prediction method does not need to understand the physical mechanism of ozone concentration evolution as fully as numerical traditional prediction methods. The method of mathematical statistics can not affect the complexity of time series completely due to the external random factors, but directly according to the objective law extracted from the time series forecast to avoid the subjectivity and randomness of prediction and improve the precision and reliability of forecast.

(2) The application of prediction model of the southern hemisphere ozone analysis can approximate the consistent conclusion of total ozone in the northern hemisphere, so the application of the ARIMA model can accurately predict the next 50 years the global total ozone. And the prediction model only needs the ozone concentration time series, and does not need other meteorological data. It is convenient to use and has strong applicability.

(3) Using SPSS to carry out the auxiliary data operation can save a lot of physical and mental work, greatly improve the efficiency of the work.

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