Numerical Simulation Study on the Impacts of Tropospheric O_3 and CO_2 Concentration Changes on Winter Wheat. Part II: Simulation Results and Analyses*

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ABSTRACT

With the rapid development of industrialization and urbanization, the enrichment of tropospheric ozone and carbon dioxide concentration at striking rates has caused effects on biosphere, especially on crops. It is generally accepted that the increase of CO_2 concentration will have obverse effects on plant productivity while ozone is reported as the air pollutant most damaging to agricultural crops and other plants. The Model of Carbon and Nitrogen Biogeochemistry in Agroecosystems (DNDC) was adapted to evaluate simultaneously impacts of climate change on winter wheat. Growth development and yield formation of winter wheat under different O_3 and CO_2 concentration conditions are simulated with the improved DNDC model whose structure has been described in another paper. Through adjusting the DNDC model applicability, winter wheat growth and development in Gucheng Station were simulated well in 1993 and 1999, which is in favor of modifying the model further. The model was validated against experiment observation, including development stage data, leaf area index, each organ biomass, and total aboveground biomass. Sensitivity tests demonstrated that the simulated results in development stage and biomass were sensitive to temperature change. The main conclusions of the paper are the following: 1) The growth and yield of winter wheat under CO_2 concentration of 500 ppmv, 700 ppmv and the current ozone concentration are simulated respectively by the model. The results are well fitted with the observed data of OTCs experiments. The results show that increase of CO_2 concentration may improve the growth of winter wheat and elevate the yield. 2) The growth and yield of winter wheat under O_3 concentration of 50 ppbv, 100 ppbv, 200 ppbv and the based concentration CO_2 are simulated respectively by the model. The simulated curves of stem, leaf, and spike organs growth as well as leaf area index are well accounted with the observed data. The results reveal that ozone has negative effects on the growth and yield of winter wheat. Ozone accelerates the process of leaf senescence and causes yield loss. Under very high ozone concentration, crops are damaged dramatically and even dead. 3) At last, by the model possible effects of air temperature change and combined effects of O_3 and CO_2 are estimated respectively. The results show that doubled CO_2 concentration may alleviate negative effect of O_3 on biomass and yield of winter wheat when ozone concentration is about 70-80 ppbv. The obverse effects of CO_2 are less than the adverse effects of O_3 when the concentration of ozone is up to 100 ppbv. Future work should determine whether it can be applied to other species by adjusting the values of related parameters, and whether the model can be adapted to predict ozone effects on crops in farmland environment.

Key words: ozone, carbon dioxide, winter wheat, effect, numerical simulation

1. Introduction

The crop yield loss and agricultural economic loss caused by ozone were assessed by the scientists based on substantial experimental and simulative study. The National Crop Loss Assessment Network (NCLAN) (Heck and Adams, 1983) was built in order to study impacts of ozone on crop growth and yield (such as cotton, wheat, soybean) by means of open top chambers and describe the relationship between ozone concentration change and crop yield with Wellbull function which has good effect to assess various crop yield loss (Larsen and Heck, 1984; Adams et al., 1989; Lesser et al., 1990). Based on 3-Dimensional Global Chemistry Mode (Chameides, 1994) and Model of Ozone and Related Tracers (MOZRT, Mauzerall et al., 2000),

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Chameides (1994) calculated ozone concentration in eastern North America, Europe, East China, Japan and so on, and estimated that about 10% to 35% of the world's grain production may occur in parts of these regions where ozone pollution may reduce crop yields. Kobayashi (1992) developed rice growth model considering impact of ozone on the light use efficiency of rice from the point of physiological mechanism in Japan. Marion and Farage (2000) built the models of acute ozone exposure effects on wheat leaf photosynthesis based on reactive oxygen scavenging process mechanism to describe the relationship between effective ozone dose and the decline in the maximum rate of carboxylation.

The experiments about impacts of ozone on crops have been conducted by means of open top chambers in China (Wang et al., 2000, 2002; Bai and Wang, 2002). Based on experimental studies impacts of ozone concentration change in the atmosphere and climate change on crops growth and yields are estimated numerically simulatively in the paper. Based on Modeling Carbon and Nitrogen Biogeochemistry in Agroecosystems (DNDC), the crop growth simulation in the former model is modified by adding the simulation about impacts of ozone on photosynthesis and leaf of winter wheat, coupling with the simulation about the impact of carbon dioxide on photosynthesis in order to build the updated DNDC model considering the impacts of ozone and carbon dioxide concentration change on winter wheat.

The structure and the modifying thread of the model have been described in another paper (Zheng and Wang, 2004). Based on updated DNDC model the growth and development and yield formation of winter wheat are simulated at different ozone and carbon dioxide concentrations and validated by experiment data. The results show that the model has good effect to describe the impacts of ozone and carbon dioxide concentration change on winter wheat.

2. Experiment data

The data about direct impacts of O_3 and CO_2 concentration change on winter wheat come from experiments conducted by Wang Chunyi et al. at Gucheng Agrimeteorological Station of Chinese Academy of Meteorological Sciences in 1999 and 1993. The experiment data about impacts of ozone concentration change on rice and rape conducted by Wang Chunyi et al. in 1999 and 2000 are also used in the paper. The experiments were conducted in the OTC-1 which was self-made by Wang et al. (2000). Winter wheat was planted in the pots with a diameter of 36 cm and a depth of 26 cm and transplanted to the open-top chamber at greening again in the second year after planted. The time of exposure was from 0900 BT to 1600 BT, 7 hours a day. The managements of all treatments were same and had no water and fertilizer stress and no plant diseases and insect pests. The details are described in Table 1.

3. Verification analysis

3.1 *Validation of the DNDC applicability*

Zhang (1999) has validated DNDC model based on experiment data of winter wheat in Tai'an Station of Shandong Province and the result was good. In order that DNDC can be applicable in North China

Table 1. Experiments about impacts of [CO_2] and [O_3] changes on winter wheat

Treatments		Station	Equipment	The time of exposure	Cultivar	The time of plant-harvest	Time to displace to OTCs
CO_2	350×10^{-6} 700×10^{-6}	Gucheng Station in Hebei Province	Open -top chambers (OTCs)	From April 6 to June 4, 1993	Winter wheat (Jingdong six)	From Oct. 1, 1992 to Jun. 7, 1993	Apr. 5, 1993
O_3	50×10^{-9} 100×10^{-9} 200×10^{-9} Based Air AA Carbon Filtrated CF	Gucheng Station in Hebei Province	Open -top chambers (OTCs)	From April 4 to June 3, 1999	Winter wheat (Jingdong six)	From Oct. 3, 1998 to Jun. 8, 1999	Mar. 31, 1999

and at Gucheng Station especially, the simulation of winter wheat growth is modified firstly. Based on the experiment data of winter wheat from 1992 to 1993 and from 1998 to 1999 under based atmospheric conditions (the concentrations of CO_2 and O_3 are 350 ppmv and 40 ppbv, respectively), the modified model is validated whether it is applicable at Gucheng Station.

The stem biomass and yields of winter wheat under based atmospheric conditions in 1993 and 1998 are simulated (Table 2). From Table 2, all differences between the simulated and the observed are under 10% except the yield in 1999, thus the error is acceptable and the simulating result is good.

Table 2. Simulated winter wheat stem biomass compared with the observed (kg hm^{-2})

Year	Simulated stem biomass	Observed stem biomass	Error(%)	Simulated yield	Observed biomass	Error(%)
1993	3646.7	4028.2	-9.5	4410.8	4078.0	8.2
1999	3776.5	3999.0	-5.5	5102.9	6290.0	-18.8

The winter wheat growth processes in 1993 and 1999 are simulated based on the former model and the updated model respectively and compared with the observed data in Figs. 1 and 2. From these, the peaks of leaf area index in the two years appear earlier in the former model than the observed because growth time through the winter is shorter and turns green earlier than the actual condition in the Gucheng Station. Leaf area index of winter wheat in earlier growth stage simulated by the former model is higher than the actual value and the biomass in earlier growth stage is more than the observed, but fewer in later growth step. This result shows that the simulation about assimilate allocation in the former model is not appropriate. The simulation about the change processes and the value of leaf area index and biomass in the modified model is close to the observed and can reveal the actual winter wheat growth condition in Gucheng Station, which laid a good base for modifying the model further.

3.2 *The results and validation of simulation about impacts of CO_2 on winter wheat*

The simulation about impacts of CO_2 concentration change on wheat photosynthesis is validated by the experimental data of winter wheat from 1992 to 1993.

The simulated results of winter wheat are compared with the observed when CO_2 concentrations are 500 ppmv and 700 ppbv, respectively in Figs. 3 and 4. The simulations of leaf area index changes are accordant with the observed so that the results are good. The aboveground biomass in the earlier growth period is close to the observed, but is more than the observed in the later growth, which shows the simulation about the degree of photosynthesis rising and assimilation enriching when CO_2 concentration increases is overestimated. The validation is not done further because there is lack of data.

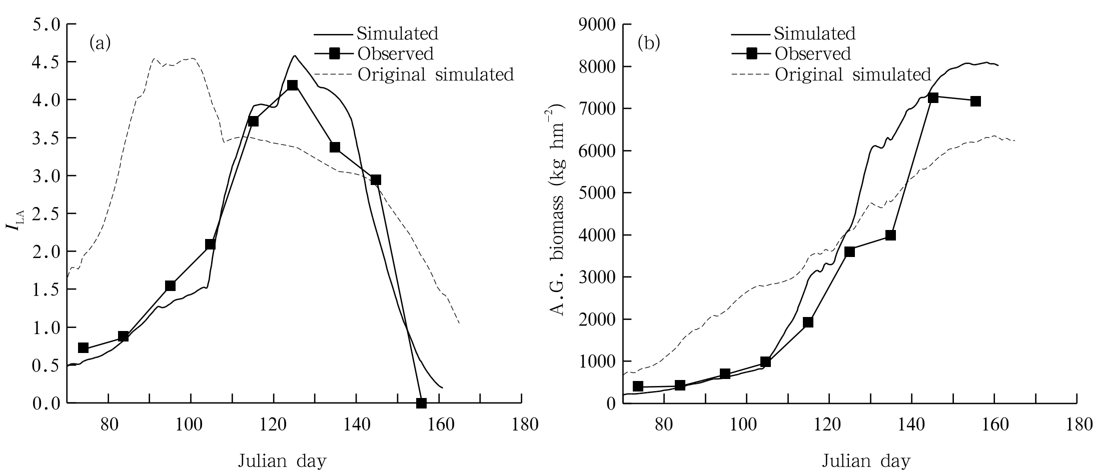

Fig.1. The simulated winter wheat I_{LA} and aboveground biomass compared with the observed in 1993.

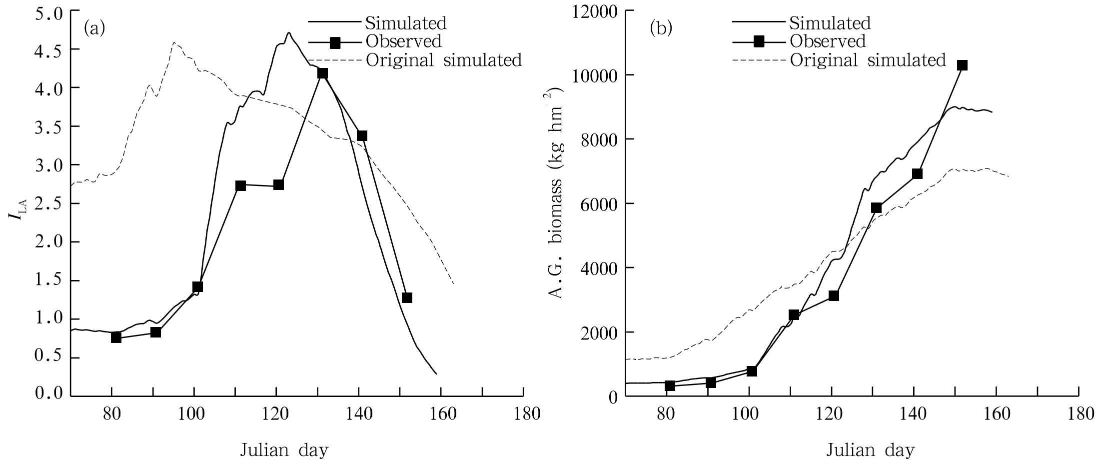

Fig.2. Winter wheat simulated I_{LA} and aboveground biomass compared with the observed in 1999.

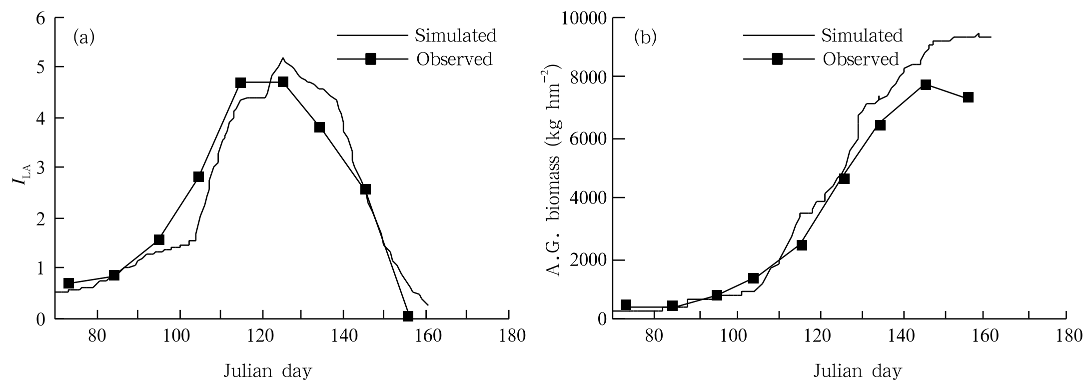

Fig.3. Winter wheat I_{LA} and aboveground biomass when [CO_2] is 500 ppmv.

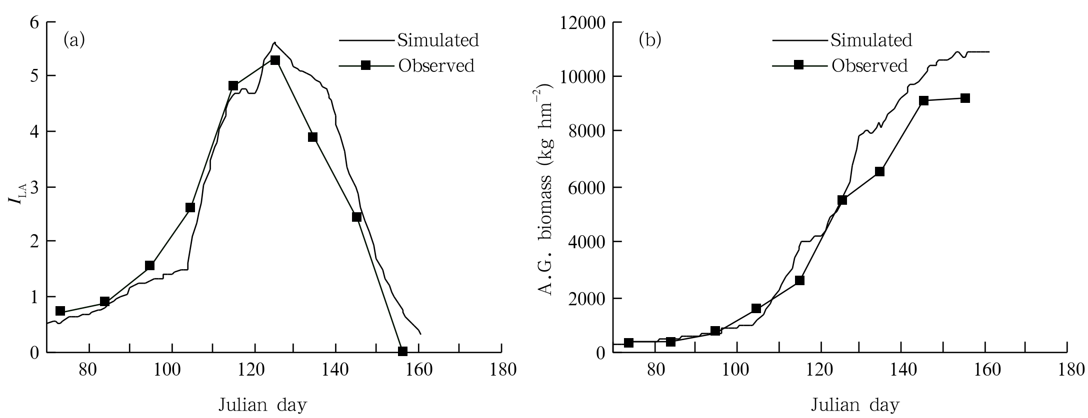

Fig.4. As in Fig.3, but for [CO_2] of 700 ppmv.

Impacts of CO_2 concentration increasing on winter wheat are simulated based on the growth and yield conditions of winter wheat at different CO_2 concentrations from Fig.1 to Fig.4. Changes of leaf area index as shown in Fig.5 indicate that during vegetative growth leaves grow slowly and impacts are not obvious; between vegetative and reproductive growth, leaves grow rapidly and CO_2 concentration more high, the rate more fast; during late growth, leaf area indexes are almost the same at three kinds of concentrations at last, which presents that the concentration of CO_2 is higher, and leaves senescence is faster. CO_2 concentration is higher, impacts on winter wheat leaves are more obvious based on variation and rate of leaf area change. By comparing among curves of winter wheat biomass change at different CO_2 concentrations, the result shows that growth trends are all accordant with crop growth actual condition but the biomass increases obviously at late growth as CO_2 concentration rising, and the concentration is higher, the rate is more quickly.

Impacts of CO_2 concentration change on winter wheat yield are presented in Fig.3. The result shows that winter wheat yield increases obviously as CO_2 concentration rising, but the degree of increment is more than the observed. The simulated is 15% more than the observed when CO_2 concentration is 500 ppmv and is 10% at 700 ppmv. The reason may be that the simulation is not accurate enough or the error comes from difference between assumptive growth condition and the actual. Based on Zhou (1999), he considered that winter wheat biomass maybe increase by about 20% when CO_2 concentration rises to 500 ppmv and about 30% at 700 ppmv. Therefore the result in this paper can be considered logical.

Table 3. Impacts of [CO_2] changes on winter wheat yields (kg hm^{-2})

[CO_2] (ppm)	The simulated and comparison (%)		The observed and comparison (%)	
350	4410.8	0	4078	0
500	5201.7	17.9	4225.8	3.6
700	6069.3	37.6	5202.7	27.5

3.3 *The result and validation of simulation about impacts of O_3 on winter wheat*

3.3.1 *Comparison between results of two different simulating methods*

The first method is based on impacts of O_3 on rice canopy light use efficiency of Kobayashi (1992) in Japan. The second is based on Liu et al. (2002) and the direct impact of ozone concentration change on crop is added in winter wheat photosynthesis simulation.

From the result of the first method, when O_3 concentration is 50 ppbv the simulation result is close to the observed. But as O_3 concentration increases the simulation result is not good. When O_3 concentration is 100 ppbv, the simulated leaf area index is overestimated obviously and the simulated value is twice more than the observed at 200 ppbv. The simulated biomass is less than the observed at 100 ppbv and the difference between the simulation and observation is more obvious at 200 ppbv. From the result of the second method, the simulated leaf area indexes are also more than the observed when O_3 concentrations are 100 ppbv and 200 ppbv but the biomass is close to the observed. Therefore the simulated result of the second method is better than the first method. The reason may be that the impact on rice is not suited to winter

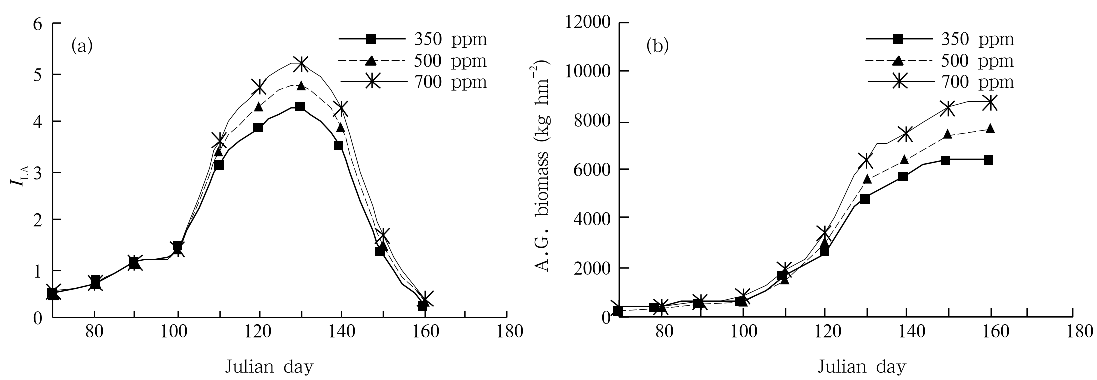

Fig.5. Impacts of [CO_2] increasing on winter wheat growth and yield.

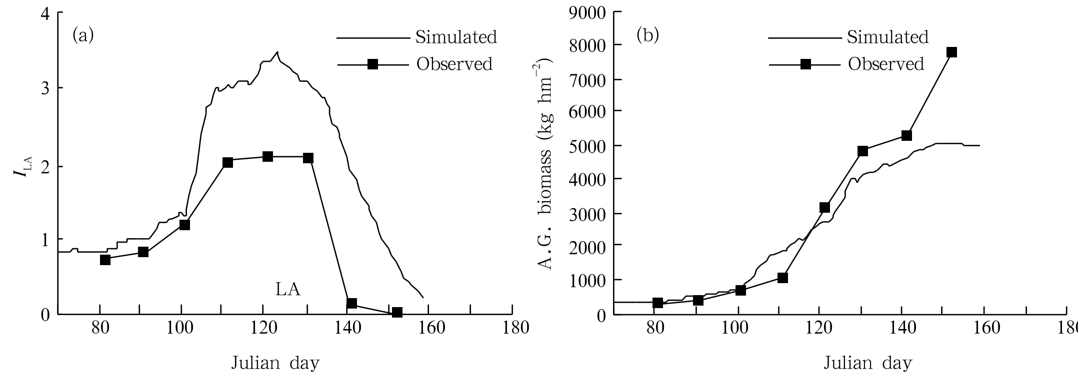

Fig.6. Simulated winter wheat growth and development when [O_3] is 100 ppbv by the first method.

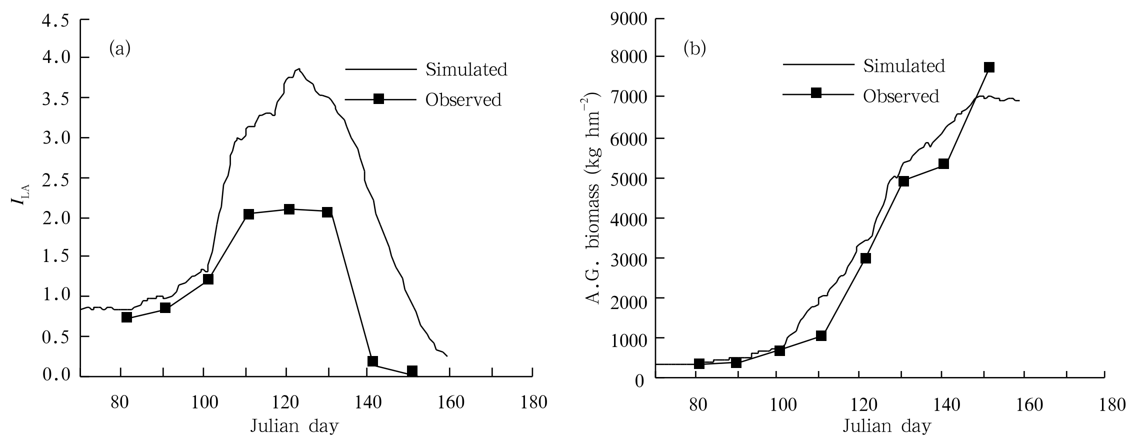

Fig.7. As in Fig.6, but for the second method.

wheat in the first method. Thus the second method is chosen to modify further.

3.3.2 *Impacts of O_3 on leaf as well as the further modification and validation of DNDC*

Results of simulation about direct impact of O_3 concentration change on photosynthesis reveal impacts of O_3 on winter wheat biomass and yield to a certain extent, but the result at high concentration is not very good. In order to simulate more exactly, the direct impact of O_3 on winter wheat is considered.

The simulations of winter wheat leaf area index and biomass are compared with the observed when ozone concentrations are 50 ppbv and 100 ppbv, respectively in Figs.8, 9 and 10. The results show that the simulated accords with the observed. Simulated leaf area index, organic biomasses, and growth curves are all closer to the observed than the simulation only considering the impacts on photosynthesis. Therefore the simulation of impacts on leaf is necessary and parameters are reasonable. But there are still some problems, e.g., at 100 ppbv and 200 ppbv, in the late growth period, the simulated rate of leaf area index decrease trails the observed, which shows that the model does not simulate the impact of ozone on leaf senescence appropriately; at high concentration, simulated biomasses of leaf and stem are more than the observed but spike is few in spite that simulated aboveground biomass is close to the observed. It may be the reason that the parameters are not correct all or that ozone affects assimilation allocation of winter wheat not considered. The study has not been performed furthermore because the mechanism is not clear.

From above-mentioned results, the model reveals impacts of ozone concentration increasing on winter

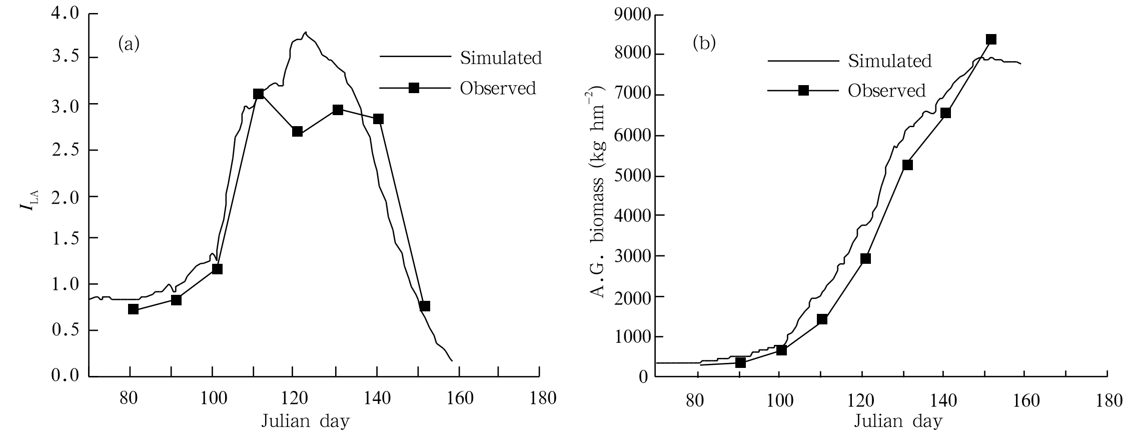

Fig.8. Simulated I_{LA} and aboveground biomass compared with the observed when [O_3] is 50 ppbv by considering O_3's damage to leaves.

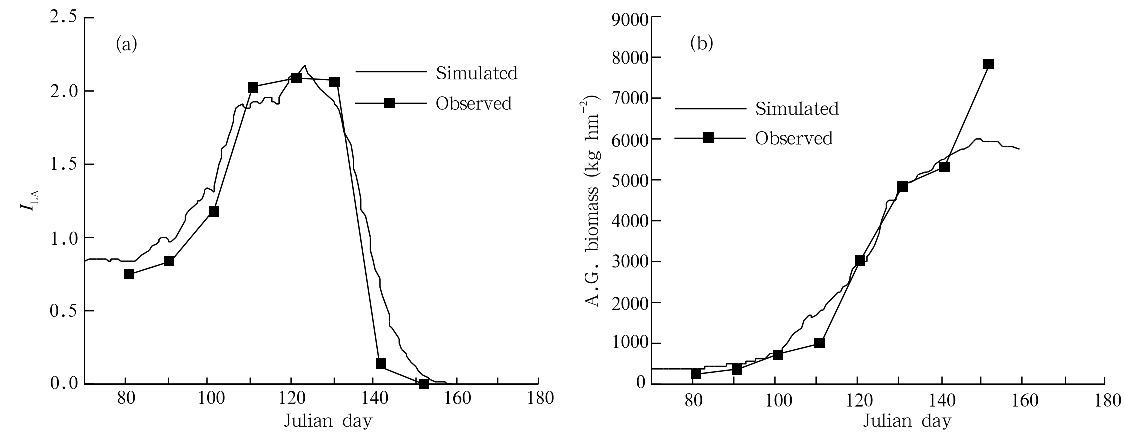

Fig.9. As in Fig.8, but for [O_3] of 100 ppbv.

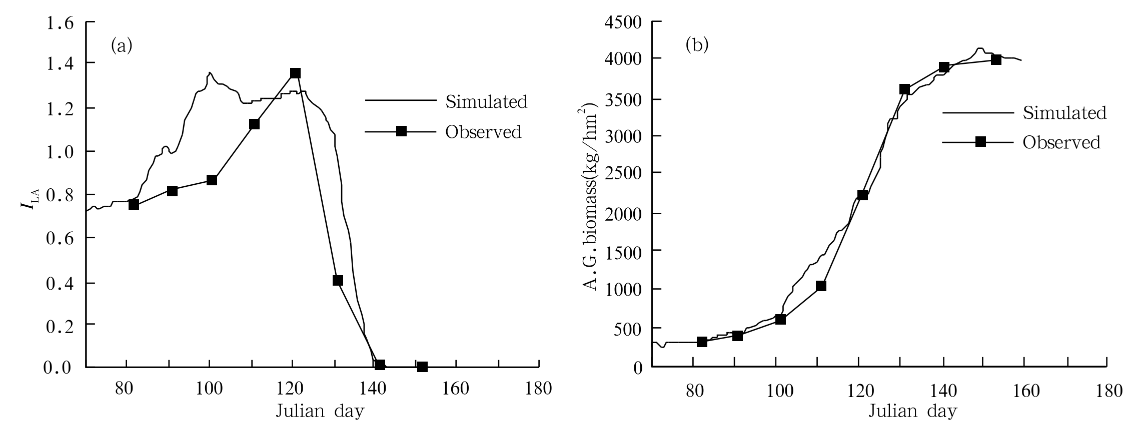

Fig.10. As in Fig.8, but for [O_3] of 200 ppbv.

wheat to a certain extent. At high concentration ozone, leaf is damaged severely and the biomass and yield of winter wheat decrease obviously at late growth period. The loss is as serious as ozone concentration rising. In Table 4 stem dry weights and yields of winter wheat and their variation at different ozone

Table 4. Impacts of $[O_3]$ changes on winter wheat yields (kg hm^{-2})

Treatment (ppbv)	Simulated stem biomass and variation (%)		Observed stem biomass and variation (%)		Simulated yield and variation (%)		Observed yield and variation (%)	
AA	3776.5	0	3999.0	0	5102.9	0	6290.1	0
50	3360.8	-11.0	2842.7	-28.9	4438.7	-13.0	5375.6	-14.5
100	2646.7	-29.9	2331.4	-41.7	3158.9	-38.1	2483.8	-60.5
200	1898.4	-49.4	1673.5	-58.2	2104.1	-58.8	1178.0	-81.3

concentrations are presented. When ozone oncentration is 200 ppbv, stem biomass and yield decrease by 50% and 60%, respectively, but compared with 60% and 80% of the observed, the simulation can not reveal enough the degree of injury and loss of impacts of high ozone concentration exposure on winter wheat.

Simulated results show that ozone concentration increase affects winter wheat leaf growth (leaf area index is lower than the measures in based atmosphere obviously) and biomass decreases; and high concentration exposure accelerates leaf senescence even dead and yield loss, which is accordant with the results of experimental observation. The experiments show that ozone exposure quickens wheat phenological development and shortens plant height, but because phenological stages are simulated based on temperature and plant height is not simulated, which cannot be revealed by the model. Impacts of ozone on wheat assimilate allocation are not considered in the model, which may be one reason that the simulation about total aboveground biomass is better than single organ.

4. Sensitivity analysis to temperature and O_3 and CO_2 concentration change

Sensitivity analysis can show whether calculated result is accordant with the presumptive result or the observation. The comparison of simulated results with the observed at different O_3 and CO_2 concentrations shows that the model is sensitive to O_3 and CO_2 concentration change and reflects the impacts on winter wheat quantitatively. Impact of temperature and inactive impact with O_3 and CO_2 are analyzed as follows.

4.1 *Impact of temperature on winter wheat*

Temperature is one of main factors studying climate change at present. We use the experiments when ozone concentration is 50 ppbv as a baseline for numerical experiments. The climate warming scenarios are assumed as daily average temperature increase and decrease by 1°C and 2°C, respectively, and precipitation is not changed. Then winter wheat phenological development, yield, leaf area index, single organ, and total biomass are simulated under different assumed temperature conditions.

From Table 5 and Fig.12, temperature increasing causes winter wheat growth rate to accelerate and development stage is shortened, and the result is contrary when temperature decreases, but the variation trend of ultima yield is not clear. Therefore winter wheat growth and development are sensitive to

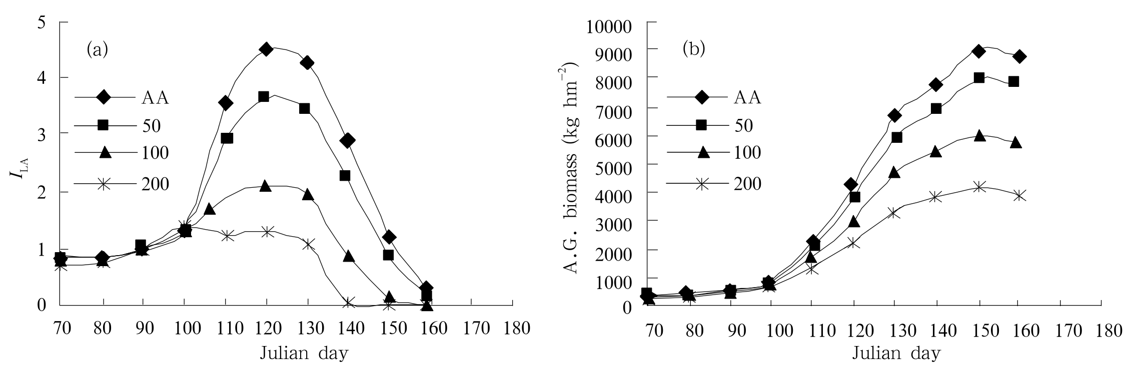

Fig.11. Impacts of $[O_3]$ changes on winter wheat yields (kg hm^{-2}). AA−based atmosphere; 50−ozone concentration 50 ppbv; 100−ozone concentration 100 ppbv; and 200−double CO_2 and ozone concentration 200 ppbv.

Table 5. Potential impacts of temperature change on winter wheat yield and development stage

		Yield and variation (%)		Development stage and variation (d)	
Temperature changed	+2°C	4358.9	-1.8	238	-11
	+1°C	4767	+9.4	244	-5
	0°C	4438.7	0	249	0
	-1°C	3785.9	-20.6	254	+5
	-2°C	4142.9	+9.4	259	+10

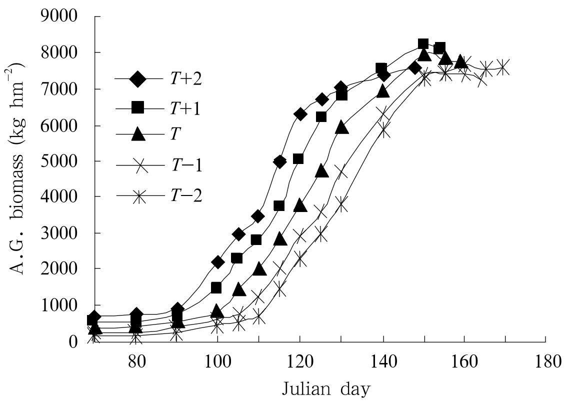

Fig.12. Potential impact of temperature change on winter wheat biomass.

temperature change. But the impact is complex. The main reason is that, temperature increasing leads to vernalization deferred in winter and turn green ahead in spring; at the same time, increased temperature also enhances photosynthesis, improves effective use of other resources (such as radiation, water, and fertilizer) and helps to accumulate dry biomass. But on the other hand, high temperature shortens crop growing duration, and stresses maturity so that negative effects may be more than obverse effects. Decreased temperature may cause vernalization ahead in winter and turn green deferred in spring and make against photosynthesis, but the probability of frost reduces when winter wheat grows again in spring because temperature increases steadily, at the same time grain filling stage may be extended and yield is enriched. If water stress and crop cultivar are considered the result is more complex. Therefore climate warming might have negative effects on winter wheat and other crops.

4.2 *Combined impact of O_3 and CO_2 concentration change on winter wheat*

With the rapid development of industrialization, urbanization, combustion of fossil fuel such as coal and oil and abundant fell of forest, tropospheric O_3 and CO_2 concentrations increase at striking rates. Ozone exposure has negative effect on crop and doubled CO_2 exposure has obverse effects on photosynthesis and yield of crop. The experiments in 1998−1999 are used as a baseline for numerical experiments that evaluates combined impact of O_3 and CO_2 concentration increasing on winter wheat. The scenarios include seven cases: (1) based atmosphere not considering O_3 and CO_2 concentration change, (2) the double level of CO_2 (700 ppmv) and O_3 concentration is 50 ppbv, (3) the double level of CO_2 and O_3 concentration is 70 ppbv, (4) the double level of CO_2 and O_3 concentration is 80 ppbv, (5) the double level of CO_2 and O_3 concentration is 100 ppbv, (6) the double level of CO_2 and O_3 concentration is 200 ppbv, and (7) the double level of CO_2 and not considering O_2 concentration change.

From Table 6 and Fig.13, compared with based atmosphere, the winter wheat leaf area index rises, biomass enriches and final yield increases by 34.6% because CO_2 concentration rising enhances photosynthesis and enriches assimilate allocation. When O_3 concentration is 50 ppbv, the obverse impact of doubled CO_2 exceeds the adverse impact of O_3 and the yield increases by 18.5%. When O_3 concentration is between 70 ppbv and 80 ppbv, the adverse impact almost counteracts the obverse impact, but if O_3 concentration goes on rising, the adverse impact would be greater than the obverse impact. When O_3 concentration reaches 200 ppbv, the winter wheat yield would be decreased by 45.3% because high O_3 exposure causes leaf and stem death and plants not to grow again.

5. Conclusions and discussions

The paper describes the development of a processes-oriented model, which combined the

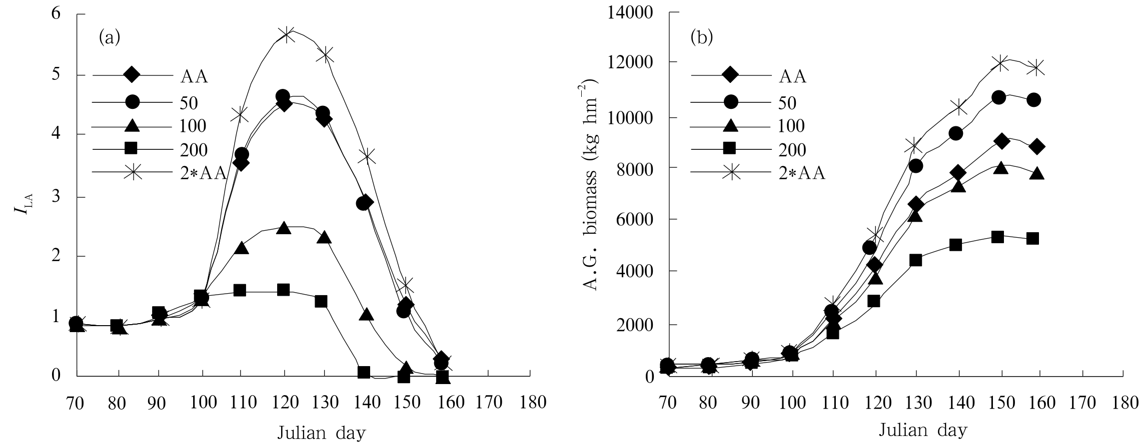

Fig.13. Combined impacts of $[O_3]$ and $[CO_2]$ changes on winter wheat I_{LA} and biomass. AA is Case 1; 50 is Case 2; 100 is Case 5; 200 is Case 6; and 2*AA is Case 7.

Table 6. Combined impacts of $[O_3]$ and $[CO_2]$ changes on winter wheat yield

$[CO_2]$(ppm)	$[O_3]$(ppb)	Yield (kg hm^{-2})	Variation (%)
350	Based concentration	5102.9	0
700	Based concentration	6870.0	+34.6
700	50	6049.3	+18.5
700	70	5254.9	+3.0
700	80	4890.5	-4.2
700	100	4262.3	-16.5
700	200	2792.6	-45.3

simulation about impacts of O_3 and CO_2 on crop with crop growth processes, and hence is able to predict crop biomass and yield loss dynamics simultaneously based on the modified DNDC and previous scientific studies. Through adjusting the DNDC model applicability, winter wheat growth and development in Gucheng Station are simulated well in 1993 and 1999, which is in favor of modifying the model further. Validation analysis shows that the model is able to capture winter wheat growth and development and yield at different O_3 and CO_2 concentration condition dynamics. Application analysis exhibits the sensitivity of the model to atmospheric O_3 and CO_2 concentration and temperature change. That shows the potential application of the model in researches of policy-making relating to climate change, greenhouse gas mitigation and trace gas effects and sustainable agriculture.

In the paper the model focuses on the simulation about impacts of O_3 on winter wheat. In comparison with several existing simulations, the modified DNDC model has main advantages: it is a mechanism model added impacts of O_3 in the crop growth process, and can be used for predicting impacts of climate change. The ozone-yield expose function (such as Wellbull function) may be more exact to estimate yield loss than the modified DNDC, but it is a statistic method and does not consider mechanisms of crop growth and impact of O_3 on crop. Photochemical model can predict ozone concentration and estimate crop yield and economic loss combined with ozone-yield expose, but it has not the mechanism of impacts of O_3 on crops either. Although rice growth model with impact of O_3 considers mechanism, but the simulation of crop growth process and impact of O_3 is simple relatively.

Based on experiments and simulations of model, the paper analyzes potential impacts of O_3 and CO_2 concentration change on winter wheat systematically.

Future work should determine whether the model can be applied to other species by adjusting the values of relating parameters and evaluate impacts of atmosphere sustaining ozone change on ecosystem by integrating with photochemical models. Because the study is still in primary stage and there are many problems of mechanism and methods which need to be studied and improved further:

(1) Mechanisms of impacts of O_3 and CO_2 on crops are very complicated and many questions are still not understood now. More mechanism researches are needed to provide theoretic bases for the development of models.

(2) Water stress, fertilizer shortage, and farming practices, are not considered in the experiments and the environment of crop growth is optimal except O_3 and CO_2 exposures, but the actual is not. Thus the interactive impacts of factors such as O_3, CO_2, temperature and precipitation and so on, and water stress, nitrogenous stress should be added in future work, which is true of actual ecosystem.

(3) The modified DNDC is validated only in Gucheng Station. It needs to be improved and validated further, and then to be used to other areas and wider regions. If the experiments which are used to build and validate the model were performed in the field in place of open top chambers, the model is more generic and closer to actual environment.

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