Reply to Anonymous Referee #3

We thank the reviewer for the careful reading of the manuscript and helpful comments. We have revised the manuscript following the suggestion, as described below.

General comments:

Air pollution has been a serious problem in China in recent decades. While most of the previous studies have focused on the three major polluted regions with dense population – the Beijing-Tianjin-Hebei region, the Yangtze Delta region, and the Pearl River Delta region (as cited in the manuscript), there are many other cities which have also been experiencing heavy air pollution but with limited studies so far. Being the largest city in northwestern China, Xi'an is such an example. This study employed the WRF-CHEM model to investigate the ozone formation in Xi'an and surrounding areas during a heavy air pollution episode in August 2013. Simulated meteorological fields and near-surface ozone and PM_{2.5} concentrations showed reasonable agreement with measurements. Sensitivity studies were performed to evaluate the impact of aerosols and changes in anthropogenic and natural emissions on the surface ozone concentrations. Based on the simulation results, the authors concluded that ozone formation in Xi'an and surrounding areas varied from NO_x to VOC-sensitive regimes, constituting a dilemma for ozone control strategies. Although the conclusions are unsurprising, this study is comprehensive and presents some new data/results that are beneficial for future air quality studies in China. Therefore, I think the topic covered in this study is appropriate for ACP. However, the English needs to be improved a little bit before publication and more efforts are needed to highlight the significance and application of the results.

Specific comments:

1. This study focused on a three-day simulation episode in August 2013, which is too short to be representative of the prevalent meteorological conditions. It would be helpful if the authors could show time series of observational temperature, relative humidity, and other variables for a longer period (for example, June, July, and August) to see whether the meteorological conditions of the simulation period is adequately representative over the study area.

We have added a paragraph to show time series of the observational temperature, relative humidity, wind speed and direction at Xianyang meteorological station during the summertime of 2013 on Page 7: "Figures 3a-d show the temporal variations of the temperature, relative humidity, wind speed and direction at Xianyang meteorological station (Figure 1c) during the summer of 2013. In general, the Guanzhong basin is hot and humid in the summer, with an

average temperature of 26.7°C and relative humidity of 67.2% recorded at the Xianyang station. The winds are not strong in the basin; the average wind speed is around 3 m s⁻¹ at the Xianyang station. During the simulation period, the observed average temperature, relative humidity, and wind speed at Xianyang station are 27.9°C, 63.4%, and 3.4 m s⁻¹, respectively, representing typical summertime meteorological conditions."

2. It is also recommended to show longer period of observed ozone and $PM_{2.5}$ concentrations in Xi'an and surrounding areas, not only to justify the choice of the short simulation period, but also provide useful realistic observations for future studies.

We have added a paragraph to show longer period of observed O₃ and PM_{2.5} concentrations in Xi'an and surrounding areas on Pages 7-8: "The profiles of summertime hourly O_3 and $PM_{2.5}$ concentrations averaged over 13 sites in Xi'an are also shown in Figures 3e and 3f, respectively, to provide an overview of the air quality in the summer of 2013. The observed average $PM_{2.5}$ and peak O_3 concentrations frequently exceed 75 and 160 µg m⁻³, respectively, showing bad air quality in Xi'an. The simulation period corresponds to a heavy pollution episode with fairly high O_3 and $PM_{2.5}$ concentrations, which often occurs during summertime. Figure 4 further presents the monthly minimum, 5th percentile, median, 95th percentile, and maximum observations of near-surface O_3 concentrations in the afternoon averaged over 13 sites in Xi'an during the period from April 2013 to March 2014. The seasonal cycle of O₃ levels in Xi'an shows high summertime O_3 concentrations, which is consistent with that in North China Plain (Cooper et al., 2014). In the study of Cooper et al. (2014), the midday O_3 mixing ratio in North China Plain peaks in June and then decreases in July and August due to the southerly monsoon flow. However, during the summer of 2013, the median O_3 concentration in the afternoon in Xi'an increases progressively from about 90 µg m⁻³ in June to 120 µg m⁻³ in August, with the maximum increasing from about 170 µg m⁻³ in June to 210 µg m⁻³ in August, which is possibly caused by the inland location of Xi'an with less monsoon precipitation during summertime."

3. In Section 3.1.1, the authors tried to explain the possible causes for the biases of simulated wind speeds and wind directions. It would be more convincing if any evidence could be found from previous studies with similar comparisons.

We have included two previous studies on the biases of simulated wind speeds and directions in the WRF model on Page 9: "(Chen et al., 2011; Lee et al., 2011)".

4. It would be helpful if the authors could briefly introduce the air quality standards in China as many readers might not be familiar with them.

We have added a paragraph and a table to provide a brief introduction of the air quality standard in China on Page 7: "The Chinese air quality standard released in 2012 is categorized into six levels based on the observed hourly and daily pollutants concentrations. During summertime, O_3 and $PM_{2.5}$ are the major atmospheric pollutants. A brief summary of the air quality standard based on the hourly O_3 and $PM_{2.5}$ concentrations is presented in Table 1."

Table 1 Air quality standards, individual air quality indices (IAQI) and their corresponding hourly O₃ and PM_{2.5} concentration limits

Air quality standards	IAQI	Hourly O ₃ concentration (μg m ⁻³)	Hourly PM _{2.5} concentration (μg m ⁻³)
Excellent	50	160	35
Good	100	200	75
Lightly polluted	150	300	115
Moderately polluted	200	400	150
Heavily polluted	300	800	250
Severely polluted	300 ⁺	800^{+}	250 ⁺

5. It would be helpful to show a map of biogenic emissions (similar to Figure 2b) so that the readers can have a sense of the relative magnitudes of biogenic VOC emissions versus anthropogenic emissions.

We have added the map of biogenic emissions (isoprene) in Figure 2 on Page 36 along with anthropogenic emissions.

6. The paper would be more influential if the authors could stress more on the PM_{2.5} and ozone concentrations in north China (Page 30582, line 16 to Page 30583 line 13). For example, the authors could discuss more about the similarities and differences of the ozone formation regimes in Xi'an versus other mega-cities in north China. Does the dilemma of O₃ control strategy also exist in other cities?

We have added a paragraph to discuss the similarities and differences of the ozone formation regimes in Xi'an versus other mega-cities in north China on Page 21: "Studies in North China show that the BTH area is under a VOC-sensitive regime (Wang et al., 2006; Tang et al., 2012).

Xue et al. (2014) also reports that O_3 production is VOC-limited in both Shanghai and Guangzhou, but NO_x -limited in Lanzhou."

We have compared the summertime O₃ and PM_{2.5} concentrations in Xi'an to those in the main cities of BTH, YRD, and PRD, and included a paragraph on Page 8: "Table 2 shows the comparison of summertime O₃ and PM_{2.5} concentrations (averaged in the afternoon) in Xi'an to the main cities of BTH, YRD, and PRD in China during 2013. The O₃ and PM_{2.5} concentrations in cities of BTH are much higher than those in Xi'an, showing the heavy air pollution in BTH. Due to the impact of frequent precipitation in South China, the PM_{2.5} concentrations in the cities of YRD and PRD are lower than those in Xi'an, but the O₃ concentrations in Shanghai and Hangzhou are still higher than those in Xi'an. Generally, the air quality in Xi'an is better than that in the cities of BTH, but worse than that in Guangzhou of PRD."

Table 2 Summertime O₃ and PM_{2.5} concentrations (averaged in the afternoon) in the main cities of Guanzhong basin, BTH, YRD, and PRD in China during 2013.

Region	City	$O_3 (\mu g m^{-3})$	$PM_{2.5} (\mu g m^{-3})$
Guanzhong	Xi'an	104.6	48.5
ВТН	Beijing	133.9	74.7
	Tianjin	116.9	78.1
	Shijiazhuang	140.4	86.6
YRD	Shanghai	122.9	47.1
	Hangzhou	110.5	35.0
	Nanjing	96.6	41.2
PRD	Guangzhou	94.9	29.4

We have also included a paragraph to discuss the possible dilemma of O₃ control strategy on Page 22: "Since the release of "Atmospheric Pollution Prevention and Control Action Plan" in 2013 (http://www.gov.cn/zwgk/2013-09/12/content_2486773.htm), the stringent PM_{2.5} control strategy has been implemented in China. The summertime PM_{2.5} concentration in the afternoon in Xi'an has decreased from 48.5 μg m⁻³ in 2013 to 38.8 μg m⁻³ in 2014; however, the O₃ concentration has increased from 104.6 μg m⁻³ in 2013 to 114.7 μg m⁻³ in 2014. The same trend is also found in the cities of BTH: the PM_{2.5} concentration has decreased from 71.5 μg m⁻³ in 2013 to 57.4 μg m⁻³ in 2014, while the O₃ concentration has increased from 125.8 μg m⁻³ in 2013 to 139.1 μg m⁻³ in 2014. Therefore, the decrease of the PM_{2.5} level might enhance O₃ production, which is consistent with the results in the present study."

Technical corrections:

1. Page 30564, line 18 Please spell out VOC.

We have spelled out the abbreviation VOC on Page 1: "VOC (Volatile Organic Compounds)-sensitive".

2. Page 30570 line 12 and Page 30581 line 1 The RMSE of surface temperature is 1.0 °C while in Table 1 it is 1.1 °C.

We have updated the RMSE of surface temperature on Page 9 according to the table (Table 3 now): "1.1 °C".

3. Page 30572 line 6 "the plume formed in the urban region of Xi'an is pushed to the north of Xi'an and surrounding areas in the afternoon...", which seems to be inconsistent with Figure 6f. As shown by Figure 6f, the convergence zone is located in the south of Xi'an and surrounding areas.

We have corrected the sentence on Pages 10-11: "On August 24, the plume formed in the urban region of Xi'an was pushed to the south of Xi'an and surrounding areas in the afternoon and the simulated O_3 concentrations were less than 200 μ g m⁻³ in the urban area of Xi'an, generally consistent with the observations."

4. Page 30583, line 20 Please specify the base year.

We have specified the base year (2010) on Page 22: "since the base year (2010)".

5. There are some grammatical errors throughout the manuscript and I suggest the authors go through the manuscript carefully. Here are some examples. 1). Page 30566, line 18 "at the nine districts" -> "in the nine districts". 2). Page 30570, line 1 "results in" -> "results from" 3). Page 30574, line 10 "closed" -> "close" 4). Page 30576, line 14-16 The sentence "which is determined ... in the presence of sunlight" sounds a little weird. 5). Page 30582, line 10 "whether" is not used correctly. Line 17 "having experiencing" -> "experiencing". 6). Page 30583, line 1

Delete "within"?

We have corrected the grammatical errors in Comments (1), (2), (3), (5), and (6) on Pages 3, 8, 13, 21, and 22, respectively. The sentence in Comment (4) is revised on Page 15: " O_3 formation in the atmosphere is a complicated photochemical process, which is determined by its precursors from various sources and transformation in the presence of sunlight." And the sentence in Comment (5) is revised on Page 21: "...but neither individual anthropogenic emission nor biogenic emissions play a dominant role in the O_3 formation ..."

6. There are some places in the manuscript that need appropriate references. For example, page 30574, line 11 after "...under humid conditions". Page 30583, line 10 "With the implementation of stringent air quality standards for PM_{2.5} in China since 2014 (need ref.), O₃ has been frequently reported to be the major pollutant during summertime in the Beijing-Tianjin-Hebei area with the decrease of the PM_{2.5} level (need ref.), which is consistent with the results in the present study."

We have added a reference after "...under humid conditions" on Page 13: "(Wang et al., 2014)".

We have updated the sentences and included measurements from China MEP on Page 22: "Since the release of "Atmospheric Pollution Prevention and Control Action Plan" in 2013 (http://www.gov.cn/zwgk/2013-09/12/content_2486773.htm), the stringent $PM_{2.5}$ control strategy has been implemented in China. The summertime $PM_{2.5}$ concentration in the afternoon in Xi'an has decreased from 48.5 μ g m⁻³ in 2013 to 38.8 μ g m⁻³ in 2014; however, the O_3 concentration has increased from 104.6 μ g m⁻³ in 2013 to 114.7 μ g m⁻³ in 2014. The same trend is also found in the cities of BTH: the $PM_{2.5}$ concentration has decreased from 71.5 μ g m⁻³ in 2013 to 57.4 μ g m⁻³ in 2014, while the O_3 concentration has increased from 125.8 μ g m⁻³ in 2013 to 139.1 μ g m⁻³ in 2014. Therefore, the decrease of the $PM_{2.5}$ level might enhance O_3 production, which is consistent with the results in the present study."

Tables and Figures:

1. Table 2 needs appropriate citation for the data presented.

The data source has been specified below the table (Table 4 at present): "The original data are from China MEP." We have added a paragraph to describe the observations of O_3 , NO_2 , and $PM_{2.5}$ used in the study on Page 6: "The real-time hourly measurements of O_3 , NO_2 , and $PM_{2.5}$

used in this study are released by China MEP and can be accessed from the website http://106.37.208.233:20035/. The historical profile of the observed ambient pollutants can be accessed at http://www.aqistudy.cn/. The O_3 , NO_2 , and $PM_{2.5}$ concentrations are measured by using Model 49i Ozone Analyzer, Model 42i (NO-NO₂-NO₃) Analyzer, and Model 5030 SHARP Monitor from Thermo Fisher Scientific, USA, respectively. All the instruments are maintained and routinely calibrated by China MEP to assure data quality."

2. Figure 2. It is recommended to add "anthropogenic" before emissions in the title. Also please specify the meaning of the black lines in the plots.

We have modified the figure caption for Figure 2 and the meaning of the black lines in the plots has been specified in the figure caption on Page 29: "Geographic distributions of anthropogenic emissions of (a) nitrogen oxide, (b) volatile organic compounds, and (c) biogenic isoprene emission in the simulation domain. The black lines present provincial boundaries in China."

3. Figure 9 "scattering plot" -> "scatter plot".

We have corrected the figure caption (Figure 11 now) on Page 29: "(a) scatter plot of measured daily aerosol constituents ..."

4. Figure 13. There are no explanations for how Y-axis is defined. According to Page 30577, line 2 and line 10, the changes of J[NO₂] and O₃ concentrations are defined as (SEN-REF), i.e. results from sensitivity simulation minus results from reference simulation. However, the changes of J[NO₂] and O₃ concentrations in Figure 13 are both negative, which are calculated as (REF-SEN). This inconsistency caused confusion when I first read the text and looked at the figure.

We have changed the definition according to the figure (Figure 15 at present) on Pages 15-16: "Aerosols significantly decrease $J[NO_2]$ by 30-70% (defined as (REF-SEN)/SEN)" and "in Xi'an and surrounding areas, the reduction in O_3 concentration (defined as (REF-SEN))".

5. Figure 15 Please add the unit for plot (a) and (b) beside the legend. "a 50% reduction" is duplicated in the title.

We have added the unit in the figure (Figure 17 at present) and the duplication is removed on Page 30.