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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Understanding high wintertime ozone pollution events in an oil and natural gas producing region of the western US" *by* R. Ahmadov et al.

Anonymous Referee #2

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This paper deals with a WRF/CHEM modeling study to simulate and explain wintertime ozone events in the Uintah Basin (UB), Utah. When I first saw the paper, I was excited and was curious to see how a 3D model would contribute to better understanding of these O3 events, but eventually my disappointment grew as I came across several obscure parts and inconsistencies, which need substantial explanation (for specific details see below).

General comment: The authors make a reference to Baker et al. (2011). This paper actually mentions that the occurrence of a cold pool is a frequent observation in the western US, including urban areas such as Salt Lake City. Salt Lake City is not too

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far away from the UB and has quite similar climatological conditions. The authors should explain, why the occurrence of wintertime ozone events is confined to oil and gas producing regions.

There is no doubt that Figure 3b clearly shows enhanced O3 levels in 2013 compared to 2012. Also, the observations of ozone show a gradual increase from day to day in those episodes the authors define (29 Jan - 8 Feb; 12-17 Feb; 19-21 Feb). It looks to me that in the observations the ozone background in the UB continuously increases from about 40 ppbv to about 80 ppbv in the first period (similar in the other periods). Daily increases are superimposed and are about 40 ppbv - 50 ppbv. This feature is different from O3 events in the Upper Green River Basin (UGRB), where daily increases of about 100 ppb can be observed, while the background values remain about the same level (Carter and Seinfeld, 2012; Rappengluck et al., 2014; Oltmans et al., 2014). The authors show that using the top-down emission scenario the model is able to capture the peak O3 values. However the model fails to replicate the nighttime ozone levels. The authors mention that this is caused by stronger katabatic winds at night in the model, which advect cleaner background air from outside the UB. This raises a few questions:

Chemistry:

1) It looks like the model simulates larger daytime O3 increases than are observed. For instance, on 6 Feb it seems there is an O3 increase of 70 ppbv in the model, while the observations show an increase of about 30 ppbv over the background values. A similar feature can be seen in Figure 6. Does the model overestimate chemical processes vs meteorological processes?

2) It is unclear whether the authors used a chemical mechanism, which is adjusted to colder temperatures similar to the approach by Carter and Seinfeld (2012). In case they did not adopt this approach, the authors should explain the reasoning for their different approach.

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3) On page 20306 the authors state that the top-down oil/gas emission estimates are based on regression slopes of individual compounds with CH4 observed between 10-16 MST. How did the authors account for the different photochemical decay of these compounds in the calculation of the regression slopes?

4) Tables 3a and b show almost the same NOx levels in 2012 and 2013, while hydrocarbon levels in 2013 are significantly enhanced. Why is this case?

5) While tables 3a and b provide a general overview of the model performance for a range of compounds for daytime hours of the time frames shown in Figures 3a and b, it would be good to see specific time series of some selected other compounds than O3, e.g. NOx, methane, toluene, HCHO, HNO3. In particular toluene would be nice, as the different emission inventories are shown in Figure 2.

Meteorology:

1) Recirculation processes might be of importance as shown by Rappengluck et al for the UGRB. At some point (page 20315) the authors mention recirculation processes in the west-east direction. However, I have some problems finding this feature in the data shown. Figure S2d shows little diurnal variation in the wind direction (mainly ranging from SE to SW) and would actually indicate some persistent transport in the south-north direction. Unfortunately, Figure 5 only shows horizontal wind vectors and no upslope/downslope vectors, which could otherwise help to understand, whether there would be circulation processes in the vertical in the basin.

2) In table S2 the authors mention that 18 layers within the lowest 500 m were used in WRF-CHEM. A recent WRF/CHEM study employing various PBL schemes (Cuchiara et al., 2014) showed ambiguous results for the different PBL schemes. How do the modeled vertical profiles of meteorological parameters agree with observations in the UB?

3) The PBL height is a very critical quantity. Figure S3 shows a very poor relation-

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ship between observed and modeled daytime PBL height, even when averaged over 3 hours. Different PBL schemes may yield different results (see Cuchiara et al., 2014); this is most likely more challenging in snow-covered areas. What was the reasoning to pick MYNN level 2.5? Have you employed other PBL schemes and what were the results? It would be helpful to see a time series of modeled vs observed PBL heights to see whether the model performance is different on individual days and/or hours of the day.

4) On page 20312 the authors mention that biases in the model meteorological fields could be affecting either year's statistics for observed and simulated chemical species (i.e. table 3a and b). In order to support this statement it would helpful to include a table similar to tables 3a and b for meteorological parameters

Additional remarks:

p 20299, lines 13-14: It should be shortly described, what the differences between the VOC mixture from oil and NG production operations vs vehicle emissions are, as there are also similarities.

p 20299, line 25: It is not correct to mention that in both years, 2005 and 2008, very high O3 values were measured. Schnell et al (2009) report O3 values of above 140 ppbv for the year 2008, only. In 2005 O3 values were much lower (above 75 ppbv) according to Schnell et al (2009).

p 20299, line 27-28: Rappengluck et al (2014) report O3 values well above 160 ppbv, not $\sim$160 ppbv.

p 20299, line 28 and following lines: It would be good to mention the altitudes of the UB and the UGRB, as this might also have an impact on photolysis rates. Also, it is worth to mention that the UGRB is considered a non-attainment area by the EPA with regard to the 8 hr O3 standard.

p 20300, line 9: 160 ppbv of O3 were not reported by Schnell et al (2009). However,

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values of more than 160 ppbv for the 2011 UGRB field study are reported by Carter and Seinfeld (2012) and Rappengluck et al (2014). The latter publication also shows O3 sonde data with more than 170 ppbv in the boundary layer.

p 20301, lines 11-13: It should also be mentioned that PBL heights may have been quite different in these specific studies.

p 20301, lines 24-28: Tethersonde data for the UB are not presented in Oltmans et al. (2014).

p 20302, lines 27-28: The statement that valley cold pools are caused by an approaching upper-level trough and midlevel cooling is not correct and is not presented this way in Reeves and Stensrud (2009).

p 20303, lines 2-4: The original reference should be cited, which is Zhong et al (2001) and not Baker et al (2011), who are citing Zhong et al.

p 20306, line 7: It is not clear what the authors mean, when they say "when the boundary layer is active".

p 20306, lines 27-28: The authors should justify why they assume that the VOC speciation is the same for both oil and NG wells.

p 20309, lines 11-13: The chemical species for which idealized vertical profiles were used should be explicitly mentioned. This can also be done in table S2. How were initial and boundary conditions for O3 represented?

p 20309, line 18: What albedo values were used for 2012?

p 20313, lines 6-7: It would be good to mention the value for the HNO3 deposition velocity explicitly here. From the statements on page 20308, lines 19-25, I had the impression that apart from O3, also dry deposition for other species were adjusted to wintertime conditions with snow cover. What were the "other species"?

p 20313, lines 8-9: It should be stated that HNO3 dry deposition velocity to snow is not

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only low at cold temperatures, but increases with increasing temperature (Johansson and Granat, 1986), and also depends on atmospheric stability (Bjorkman et al., 2013), which means it displays a diurnal variation, with a maximum during daytime, when also ambient HNO3 tends to have maximum values.

p 20314, lines 14-15: Only horizontal vectors are shown in Figure 5, but no downslope (or upslope) flows.

p 20314, lines 15-17: Figure S2d predominantly shows SE winds during the morning hours which cannot lead to a transport from west to east.

p 20317, lines 16-18: I assume enhanced photolysis rates were also important for NOx sensitive regimes studied by Carter and Seinfeld (2012).

p 20319, line 26: I assume the authors mean "...less than or equal to 5 carbon atoms" instead of "...greater than or equal to 5 carbon atoms".

p 20319, lines 27-29: It should be added that the magnitude of the disproportionate impact of the oil/gas sector aromatics also depends on the amount of HONO found in ambient air according to Carter and Seinfeld (2012) and thus may be variable.

p 20324, line 19: I would suggest to add "...in snowy conditions in the UB"

Tables:

Table 1: Abbreviations used in table S2 should be included (MYNN, NAM, RRTMG).

Table 2a: Metric units should be used.

Table 3a/b: The root mean square error should be presented.

Table S1: The table caption should mention that regressions with CH4 were performed. NOy is not a VOC. I would suggest to replace VOC in the header row by a more appropriate term.

Table S2: I would suggest to include the following information: initial and boundary

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chemistry conditions, information about advection schemes, photolysis and dry deposition treatment. Would be good to include a map which shows the domains.

Figures:

Figure 2: Letters for the measurement sites are extremely tiny.

Figure 5: The authors state in table S2 that 18 layers within the lowest 500 m were used. However, wind vectors are shown for less layers.

Figure 6: Information about the measured and modeled PBL height should be included. Also, wind vectors should be included

References:

The Edwards et al (2014) paper has been submitted. It is up to the editor, but personally I feel it is not helpful, since the reader has no access to this literature:

Literature:

Bjorkman et al. (2013): Nitrate dry deposition in Svalbord, Tellus B, 65, 1-18.

Cuchiara et al. (2014): Intercomparison of planetary boundary layer parameterization and its impacts on surface ozone formation in the WRF/Chem model for a case study in Houston/Texas, Atmos. Env., 96, 175-185

Zhong et al. (2001): Meteorological processes affecting the evolution of a wintertime cold air pool in the Columbia Basin, Mon. Weather Rev., 129, 2600-2613

Interactive comment on Atmos. Chem. Phys. Discuss., 14, 20295, 2014.