**Atmospheric
Chemistry
and Physics
Discussions**

Interactive comment on "Process analysis of regional ozone formation over the Yangtze River Delta, China using the Community Multi-scale Air Quality modeling system" *by* L. Li et al.

Anonymous Referee #2

Review of L. Li et al.: Process analysis of regional ozone formation over the Yangtze River Delta, China using the Community Multi-scale Air Quality modeling system, Atmos. Chem. Phys. Discuss., 12, 15049–15082, 2012. Version Received: 20 April 2012 – Accepted: 25 May 2012 – Published: 13 June 2012.

The paper creates a conceptual model describing high ozone events over the Yangtze River Delta. The authors accomplish the task by using photochemical modeling by the Community Multi-scale Air Quality (CMAQ) model and observations from local monitors but their analysis and conclusions mostly rely on the CMAQ modeling and its options for Integrated Process Rates (IPR) analysis. The latter shows that regions switch between

ozone production and destruction based on emissions and that ozone transport from production regions aloft play a critical role in high concentrations versus time. Their conceptual model seems consistent with the analysis and observations but does have faults. (1) It does not employ quantitative measures when regions switch between production and destruction. The measure could have used the emission inputs or CMAQ predictions to determine when or where ozone chemistry switches between NOX and VOC limiting conditions. Alternatively, additional analysis could have used Integrated Reaction Rate (IRR) analysis to quantify what reactions and compounds dominate the photochemical sources and sinks of ozone. IRR is another analysis tool available in the CMAQ model. (2) IPR identifies horizontal transport as an important factor leading to high ozone over the delta. However, results do not discuss what amount of the transport comes from outside the smallest nested model domain. Figure 10 attempts to describe this amount but the figure is difficult to interpret based on the number and resolution of sub-figures. It may improve by reducing the number of sub-figures and increasing the sizes of the remainder. (3) The authors do not discuss uncertainties that may alter the conceptual model. For example, the modeling set-up used clear air conditions as the boundary conditions for the outer most nested domain. The condition introduces an uncertain because a strong potential exists long range transport of ozone and its precursors from outside the nested modeling domains such as Korea, Indo-China and Japan. Another example is that the index of agreement decreases from NO2 to NOX. The decrease infers a problem modeling partitioning between NO2 and NO either from emissions or the photochemical mechanism. The paper's conclusions may weaken because this partitioning plays in switching between ozone production via NO2 photolysis and destruction via NO titration. (4) The analysis uses the August 16th thru 17th period based on the SAES site but the authors need to give more information on whether the period covers typical conditions during ozone events such as the wind patterns, synoptic or emissions conditions. Such evidence will make their conclusions more robust. This reviewer believes that the paper merits final acceptance if the authors revise it to remove a majority of the above faults.

The below specific comments illustrate the above points or suggest additional ways to revise the paper.

Page 15053, line 26: The paper should replace Dennis et al. (1996) and Byun et al. (1998) with references that give information more relevant to the CMAQ version 4.6. The below examples give potential replacements.

Byun, D. and Schere, K.L.: Review of the governing equations, computational algorithms, and other components of the Models-3 Community Multiscale Air Quality (CMAQ) modeling system, Applied Mechanics Reviews, 59, 51–77, 2006.

www.cmascenter.org

www.cmaq-model.org

Note that the below additional example refers to CMAQ version 4.7 but the reference gives information better describing the photochemistry and deposition processes in CMAQ version 4.6.

Foley, K.M., Roselle, S.J., Appel, K.W., Bhave, P.V., Pleim, J.E., Otte, T.L., Mathur, R., Sarwar, G., Young, J.O., Gilliam, R.C., Nolte, C.G., Kelly, J.T., Gilliland, A.B., Bash, J.O.: Incremental testing of the community multiscale air quality (CMAQ) modeling system version, 4.7., Geosci. Model Dev. Discuss. 2, 1245-1297, 2009.

Page 15054, line 18: The methodology uses the clear air conditions for the outer most or largest modeling domain. This usage assumes that ozone and other pollutant have insignificant contributions transport from areas adjacent to the largest domain. Discuss whether and how the assumption can affect the paper's results.

Page 15057, lines 4-10: The paper does not make clear whether the selected episode characterizes typical condition during high ozone events. The beginning of the paper implies typical temperatures and relative humidity but states the measured ozone was extremely rare. Please clarify by discussing whether the August 16th thru 17th has other meteorological parameters typical in high ozone event such as wind patterns,

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weather fronts or dominant pressure systems.

Page 15058, line 19: The index of agreement noticeably decreases from NO2 to NOX. The change indicates problems simulate NO. Discuss how the error may affect accurately determining where ozone production and titration occurs over the domain. Page 15065, lines 9-22: The YRD appears to contain regions which are NOX or VOC limiting based on local sources and times. Could the author discuss ozone concentration based on the two limits?

Page 15056, lines 23-27: The paragraph implies that paper is a novel use of IPR within the CMAQ model system. It then recommends IPR for future use. A simple search shows IPR has been used in many publish journal article so IPR's utility has already been establish. The author should revise or delete the paragraph.

Interactive comment on Atmos. Chem. Phys. Discuss., 12, 15049, 2012.