TOAR Workshop 1.02
April 28-30, 2015
Agencia Estatal de Meteorología (AEMET), Madrid, Spain

Workshop Summary

Written and approved by the TOAR Steering Committee, June 25, 2015

TOAR Workshop 1.02 (second workshop of the first TOAR initiative) was held at Agencia Estatal de Meteorología (AEMET – Spanish Meteorological Agency) in Madrid, Spain, April 28-30, 2015. The workshop was funded by the World Meteorological Organization and AEMET, with logistical support provided by AEMET's Francisco Espejo. The workshop was coordinated by Owen Cooper (University of Colorado/NOAA ESRL, Boulder) and attended by 70 scientists from around the world (see attendance list at the end of this summary).

The workshop had several goals:

1) Develop a detailed outline of the assessment report
2) Select lead authors and co-authors for each chapter of the assessment report
3) Identify unique and high quality ozone time series around the world
4) Continue the development of the TOAR database
5) Identify the ozone metrics that will be calculated from the data uploaded to the database
6) Further develop the idea for a special issue and ancillary papers

Assessment Report Outline

During the workshop the outline of the assessment report was expanded and modified. Notably, the contents of Chapters 4 and 5 first described in the first TOAR Overview document (available on the TOAR webpage: http://www.igacproject.org/TOAR) were rearranged into three chapters to focus on the ozone metrics of most interest to the human health, vegetation and climate change research communities. The assessment report is targeted towards scientists from various Earth science disciplines. An Executive Summary will highlight the results relevant to policy makers. The report will be published as a series of stand-alone peer-reviewed papers linked by a special issue of an open-access journal. The assessment report will consist of eight chapters plus an executive summary and guide to the TOAR database. In addition, ancillary papers that either support TOAR goals or expand on TOAR chapters will also be included in the special issue. The TOAR Steering Committee will identify a journal to accommodate the needs of the TOAR special issue.

Following is the detailed outline of each chapter, including the list of authors. Both the outlines and the author list are permitted to be modified during the development of the report and the information listed below merely reflects the current state of thinking of the TOAR community. Future updates to the TOAR outline will be made on the TOAR wiki. Authors are listed with the lead author first, followed by the rest of the chapter writing team listed alphabetically.

Executive Summary: A summary (2 pages of text plus several figures) of the key findings from the report, with the goal of being policy-relevant and written in language that is understandable to policy-makers and the general public.
Authors: Chapter lead authors and the TOAR Steering Committee

Chapter 1: State of knowledge of tropospheric ozone sources, sinks and budgets

Chapter Writing Team: A. Archibald, Mhairi Coyle, R. Derwent, Y. Elshorbany, I. Galbally, G. Gerosa, A. Lefohn, M. Naja, J. Neu, A. Saiz-Lopez, P. Saxena, M. Schultz, I. Shahid, T. Wallington, H. Worden, P. Young

1. **The importance of ozone in the troposphere.**
   a.) Discussion of the role of ozone as a short-lived climate forcer, a toxic compound with human health effects, plant damage, source of OH and central role in the photochemistry of the troposphere.
   b.) Ordered the same as in chapter 4-6.
   c.) Discussion on what is tropospheric ozone – definition of the tropopause.
   d.) Key Figure: Zonal plot showing ozone as a greenhouse gas, ozone damage to plants and the ozone AQ issues, role of stratospheric ozone.
2. **The chemistry of ozone in the troposphere**
   a.) Our understanding has evolved with time as our knowledge of the processes has changed. Here we discuss the current status of knowledge on the sources and sinks of ozone in the troposphere. The Leighton understanding to the Atkinson era…
   b.) Link the processes to the distributions (i.e. time series) of ozone.
   c.) The role of different environments – very much as examples: Urban, free troposphere, free ocean, ice, forest. Discuss the sources and sinks and chemistry. Moving away from high NO_x and low NO_x.
   d.) Link the discussion to the areas covered in the plot
   e.) Discussion on the budget of ozone, difficulties in definition of tau-ozone?
   f.) Key Figure: Epic plot with example regimes and chemical reactions/processes.
3. **A historical perspective of our understanding of sources and sinks of tropospheric ozone**

a.) History of the role of the stratosphere as being thought to be the source of ozone and that only a small amount produced in situ. Reasons for the change of view, the emergence of HO_x catalyzed ozone production.
b.) Evolution of our understanding. Key FIGURE, the time line of sources, sinks, burden from models. This would include discussion on the role of changes in emission inventories, emissions themselves, kinetics etc. The evolution of our process understanding.

4. The known unknowns

a.) Based on the format of the figure, frame the discussion to focus on:
b.) Within the context of climate – major uncertainties include: for direct forcing, changes in circulation. Pre-industrial base lines. Feed backs from the biosphere, lightning.
c.) Within the context of AQ – the climate penalty, emissions policies.
d.) Within the context of the biosphere – land use change.
e.) Key figure – expert judgment (H,M,L) on the uncertainty around the key processes identified above and the impact of the process (H,M,L).

5. Future directions

a.) The use of DA
b.) New measurements to constrain the budget – can we measure ozone production?

Chapter 2: Tropospheric ozone observations

Chapter Writing Team: D. Tarasick, I. Galbally (co-lead), G. Ancellet, A. Boynard, M. Coyle, P. Cristofanelli, A. Ding, G. Dufour, Z. Fleming, G. Foret, A. Gaudel, B. Latter, X. Liu, G. Miles, M. Naja, J. Neu, D. Parrish, I. Petropavlovskikh, R. Seguel, M. Steinbacher, H. Tanimoto, A. Thompson, V. Thouret, R. Van Malderen, C. Vigouroux, T. Wallington, H. Worden, J. Ziemke

1. Historical observations 1850-1960

a.) What spatial and temporal information is available about surface ozone during the period from the mid-19th Century to 1960?
b.) Divide the world into 12 regions: 4 latitude bands, 3 longitude segments.
c.) What is the history of surface ozone measurements, concentrations, temporal concentration changes and associated uncertainties in each band?
d.) Are early aircraft and balloon based observations of free tropospheric ozone useful for detecting long term trends?

2. The transition period: 1960-1990

a.) What detail is known of tropospheric ozone for the period 1960–1990 from surface sampling, ozonesondes, aircraft and the first remote sensing?
b.) Which of these observations can be related to the current ozone standard?
c.) What knowledge about tropospheric ozone distributions and variability can be derived from them?

3. Quality observations: 1990-present

a.) What are the latitudinal, longitudinal and vertical distribution, annual cycle and the uncertainty and variability of these aspects of tropospheric ozone?
b.) What are the other pronounced variabilities observed in tropospheric ozone e.g. ENSO in the free troposphere and the diurnal variation of surface ozone?
c.) How representative is current sampling? Discuss issues with coverage in rural areas for the quantification of ecosystem effects; intercontinental inflow/outflow influences
d.) Observations of and applications of footprints (correlation lengths) of current observations

4. Observations of processes and rates

What are the uncertainties in current measurements of the following processes determining tropospheric ozone:

a.) stratosphere-troposphere exchange?
b.) in-situ ozone production?
c.) in-situ ozone destruction?
d.) surface deposition?
e.) radiative forcing?

5. The future

a.) New developments: new instruments and/or methods; near real time data provision; data assimilation; other emerging issues
b.) Recommendations for design of a future global observational program

Chapter 3: The Description of Global Ozone Metrics for Climate Change, Human Health, and Crop/Ecosystem Research

Chapter Writing Team: A. S. Lefohn, M. Coyle, Z. Feng, T. Haoye, M. Hazucha, K. Kobayashi, C. Malley, G. Mills, R. Musselman, V. Naik, E. Paoletti, M. Schaub, M. Schultz, P. Sicard, D. Simpson, L. Smith, X. Xu

1. Introduction

a.) What is an exposure/dose metric?
b.) Why are exposure/dose metrics important for describing global distribution and trends analyses?
c.) Why are exposure/dose metrics important for evaluating global change models?
d.) What is the relationship between a specific exposure/dose metric and hourly average ozone concentration distributions and why is this relationship important?

2. Distributions of hourly average concentrations

a.) Using empirical data, what are distribution and diurnal patterns for high- and low-elevation urban and rural ozone monitoring sites and how do these various patterns influence ozone metric values?

3. Description and scientific rationale of each exposure and dose metric and its anticipated application for assessing global distribution and trends for climate change, human health, and crop/ecosystem effects.

4. Description of statistical techniques used in the report and a critical discussion of the advantages and limitations of the use of each technique.

5. Additional sections as needed

6. Summary and Conclusions

Chapter 4: Present day ozone distribution and trends relevant to human health

Chapter Writing Team: To be determined (Preliminary list Z. Fleming, O. Cooper, X. Xu, Zhaozhong Feng)

1. The purpose of this chapter is to graphically display the present-day global distribution and trends of ozone using metrics of interest to researchers studying the impact of ozone on human health. Include reasons why the particular metrics used in this chapter were selected and refer to Chapter 3 for scientific rationale for the specific selections.

Chapter 5: Present day ozone distribution and trends relevant to vegetation

Chapter Writing Team: To be determined (Preliminary list O. Cooper, X. Xu, Zhaozhong Feng)

1. The purpose of this chapter is to graphically display the present-day global distribution and trends of ozone using metrics of interest to researchers studying the impact of ozone on vegetation. Include reasons why the particular metrics used in this chapter were selected and refer to Chapter 3 for scientific rationale for the specific selections.

Chapter 6: Present day ozone distribution and trends relevant to climate change

Chapter Writing Team: To be determined (Preliminary list A. Gaudel, O. Cooper, X. Xu)

1. The purpose of this chapter is to graphically display the present-day global distribution and trends of ozone using metrics of interest to researchers studying the impact of ozone on climate and tropospheric chemistry. Include reasons why the particular metrics used in this chapter were selected and refer to Chapter 3 for scientific rationale for the specific selections.

Chapter 7: Assessment of global-scale model performance for global and regional ozone distributions and trends

Chapter Writing Team: V. Naik (co-lead), P. Young (co-lead), J. Brandt, R. Doherty, M. Evans, A. Fiore, M. Hegglin, U. Im, B. Latter, R. Kumar, M. Lin, H. Liu, A. Luhar, G. Miles, D. Parrish, M. Prather, H. Rieder, J. Rodriguez, J. Schnell, M. Schultz, E. Sofen, S. Tilmes, O. Wild, M. Woodhouse, G. Zeng, L. Zhang

1. Introduction

a.) Motivation for evaluating models

b.) A brief history of global tropospheric ozone modeling. How does a model simulate tropospheric ozone and how has modeling evolved over time (2-D, 3-D CTMs to CCMs)? Plot - schematic of the evolution of models depicting the complexity of chemical/physical processes included in the models.

2. Techniques for evaluating global model-simulated surface and free troposphere ozone

a.) Methods adopted in the past. Most commonly used diagnostics/metrics in the published literature (e.g., monthly means). Highlight evaluations conducted within multi-model intercomparisons framework (ACCENT, HTAP-I, ACCMIP)

b.) Techniques that we may adopt in the future: benchmarking process-level details in models; examples of newer evaluation methods (e.g., spectral analysis)

3. Evaluate present-day global and regional O_3 distributions - focus on O_3 assessment metrics (not impact metrics)

a.) Review of processes responsible for model biases – what processes are missing or misrepresented in current generation models?

b.) Plots and tables:
Panel plot of maps of present-day annual mean mid-tropospheric ozone for all models (CMIP5, ACCMIP, others) compared with climatology derived from observations compiled in Chapter 2.
Climatological annual cycle of MDA8 ozone averaged over different regions of the world (or for selected representative stations) from existing model runs compared with observations compiled in the TOAR Database.

Table of present-day global tropospheric ozone burden (columns) from models and observations, and available modeled ozone budget.

4. **Model skill in simulating climatological extreme episodes**
    a.) based on the work of J. Schnell and others from literature

5. **How well do models capture observed variability at all time-scales?**
    a.) Discuss the drivers of variability – e.g, climate variability (ENSO, NAO, MJO…), shifts in emissions, meteorology…

6. **How well do models capture observed trends in annual and seasonal in ozone concentrations?**
    a.) Literature review of how the models perform for the preindustrial period
    b.) Drivers of long-term changes – e.g, strat-trop exchange, climate change, land-use change….
    c.) Plots
    Timeline plots of model monthly mean or MDA8 surface ozone vs. observed for the last 10-20 years averaged over the US, Europe, where we have better data coverage.
    Baseline surface ozone trends by season.
    Timeline of tropospheric ozone burden compiled in Chapter 2 vs. modeled burden (transient CMIP5 simulations + any other available).
    Plot similar to Figure 2.45 of BAMS, State of Climate (2014) report but also showing model values.

7. **Conclusions**
    a.) Key areas of model success and gaps
    b.) Recommendations on process-level understanding needed for models to realistically simulate ozone over the full range of spatial and temporal scales

Chapter 8: The Tropospheric Ozone Assessment Report (TOAR): Key findings and recommendations for future research

Chapter Writing Team: Owen Cooper et al.

Content: TBD

Guide to TOAR Ozone Metrics

a) How to access the data and code on the TOAR database.
b) Description of meta data for each site, archived on the TOAR database.

Ancillary Papers

During the workshop 10 possible ancillary papers were proposed. At this stage the papers are just ideas and are not commitments.

1) Focus on South Asia ozone distribution and trends (M. Naja and R. Kumar)
2) Ozone Correlation lengths, based on the work by E. Sofen and M. Evans
3) Analysis of IAGOS ozone and CO trends above Frankfurt
4) FTIR uncertainties (Corinne Vigouroux), in support of Chapter 2
5) Validation and application of new satellite retrievals that link the surface and the free troposphere (Gaelle Dufour), in support of Chapter 2.
6) PODy: measurements and modelled analysis (Mhairi Coyle)
7) Rural ozone trends across the UK (Mhairi Coyle)

8) Comparison between MOZAIC/IAGOS and ozonesondes above Brussels
9) AIRBASE ozone trend analysis across Europe plus NO_x analysis (Erika von Schneidemesser).
10) Comparison of Canadian ozonesondes to surface ozone observations

Statistics and Database Working Group

The Statistics and Database working group discussed statistical tests that will be applied to the database, the design of the database, and the exposure and dose metrics to be used in the TOAR analyses. For trending purposes, TOAR will use all hourly averaged ozone data that meet data capture criteria, treat each site separately for site-specific analyses, not combine data with another site's data when the data capture is poor for either site, and for regional comparisons, calculate the trend for each site individually and use statistical tests to compare the various regions. The non-parametric Mann-Kendall test will be used to identify significant trending and the Sen-Theil test to estimate the magnitude of trend. The parametric (e.g., linear/quadratic) test results will be compared with non-parametric results if statistical assumptions are met for the parametric tests. TOAR will assess trends over the entire time period, as well as different time periods for each site to investigate changes in trends over time.

The TOAR global database of (hourly) surface ozone observations is located at Forschungszentrum Jülich. A template of the data format for data uploads to the TOAR database is available at https://redmine.iek.fz-juelich.de/projects/toar/wiki/Join_database and includes a list of the metadata tags which are included in the database. The TOAR surface station database is operational and currently contains 6906 ozone data series from 6899 stations worldwide. Note, that some stations are double-counted if they belong to more than one network. Processing of readily available data from the larger networks will be completed in fall 2015, and Jülich will process additional datasets as they come in, although likely not before September 2015. Data access through JOIN will be available after August 2015. For data quality control, standardized reports with plots, as well as statistical assessments will be available. An outlier filter program will be implemented. Continuous discussion with data investigators will occur in order to assess the quality of the data. The database provides the capability to set the status of a data series and flag each individual data value (WMO standard flagging scheme). TOAR will use a suite of exposure and dose metrics for model evaluation, human health, and vegetation purposes. The Statistics and Database Working Group will characterize exposure and dose metrics at the surface. Specific data capture criteria unique to the individual metrics will be applied during the characterization process. The Group will not characterize metrics for the free troposphere, which will be characterized by the Free Troposphere and Satellite Working Group. A complete list of the draft exposure and dose metrics will be distributed in June for comment. This list can be found on the TOAR webpage: http://www.igacproject.org/TOAR. Among other applications, the surface ozone data will be compared to ACCMIP and/or CCMI model runs, which produce hourly surface ozone concentrations.

Additional Workshop Decisions and Outcomes

1) **Lists of regional working group members and surface ozone datasets**

   Member lists can be found on the TOAR wiki: https://redmine.iek.fz-juelich.de/projects/toar/wiki

   Available surface datasets will be easily accessible through the Jülich Open Web Interface (JOIN; http://join.iek.fz-juelich.de/) after August 2015.

2) **Free Troposphere and Satellite Working Group:** The primary product to be produced by this working group is a time series plot of the global/hemispheric/zonal tropospheric ozone burden using satellite retrievals (OMI/MLS, GOME/GOME2, IASI, OMPS), FTIR, IAGOS, ozonesondes and Umkehr instruments. A common unit will have to be decided upon. This plot will likely appear in Chapter 7. Model runs for CCMI will output their ozone data as monthly means for all grid cells, but output will be hourly at the surface. The Statistics and Database Working Group will only produce metrics at the surface and not the free troposphere, therefore the Free Troposphere and Satellite Working Group will have to produce several metrics (see the List of Exposure and Dose Metrics at http://www.igacproject.org/TOAR) in the free troposphere for comparison to the CCMI models.

3) **Coordinating lead authors still need to be determined for Chapters 4, 5 & 6.**

4) **The Steering Committee needs to identify a journal to host the TOAR special issue.**

5) **The Steering Committee needs to determine the location for Workshop 1.03, January, 2016.**

Timeline

June 5, 2015: The Statistics and Database Working Group will finalize the list of TOAR ozone metrics to be produced.

December, 2015: Additional data submitted to the TOAR database; produce first draft of assessment report

January, 2016: TOAR Workshop 1.03, location to be determined

December, 2016: Submit assessment report to a peer-reviewed journal and perform any necessary updates to the ozone metrics on the database

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