TOAR Workshop 1.01
December 10-11, 2014
NOAA Earth System Research Laboratory, Boulder

Workshop Conclusions and Assessment Report Outline

Compiled and approved by the workshop participants, January 16, 2015

Summary

Tropospheric Ozone Assessment Report (TOAR): Global metrics for climate change, human health and crop/ecosystem research, is a new Activity of the International Global Atmospheric Chemistry Project (IGAC), approved by the IGAC Scientific Steering Committee on March 13, 2014 (www.igacproject.org). TOAR's mission is to provide the research community with an up-to-date global assessment of tropospheric ozone's distribution and trends from the surface to the tropopause. In fulfilling this mission, TOAR has two primary goals: 1) Produce the first tropospheric ozone assessment report based on the peer-reviewed literature and new analyses conducted by TOAR; 2) At hundreds of measurement sites around the world (urban and non-urban), generate freely accessible ozone metrics for global-scale impact studies of ozone on human health and crop/ecosystem productivity, and generate diagnostics relevant to climate forcing by tropospheric ozone.

On December 10-11, 2014, TOAR Workshop 1.01 (the first workshop of the first assessment report) was held at the National Oceanic and Atmospheric Administration's (NOAA) Earth System Research Laboratory (ESRL) in Boulder, Colorado, with funding from NOAA ESRL's Chemical Sciences Division and IGAC. The workshop was attended by ten internationally recognized scientists with expertise in the observation and analysis of tropospheric ozone, with remote participation from six additional experts. During the workshop participants formed an initial steering committee of five members and produced a detailed outline of the report with defined working groups. In addition, participants discussed ozone metrics that will be calculated and outlined the structure of the database that will store the metrics. Finally, the goals of TOAR Workshop 1.02 were established, which will be hosted by the Agencia Estatal de Meteorología (AEMET – Spanish meteorological service) and co-sponsored by the World Meteorological Organization in Madrid, during the last week of April, 2015.

Introduction

Tropospheric Ozone Assessment Report (TOAR): Global metrics for climate change, human health and crop/ecosystem research, is a new Activity of the International Global Atmospheric Chemistry Project (IGAC), approved by the IGAC Scientific Steering Committee on March 13, 2014 (www.igacproject.org).

Mission:

To provide the research community with an up-to-date global assessment of tropospheric ozone's distribution and trends from the surface to the tropopause.

Goals:

1) Produce the first tropospheric ozone assessment report based on the peer-reviewed literature and new analyses.

2) Generate ozone metrics at hundreds of measurement sites around the world (urban and non-urban), freely accessible for research on the global-scale impact of ozone on climate, human health and crop/ecosystem productivity.

Organization:

TOAR is a science-led effort initiated by IGAC, and developed by an international team of scientists. TOAR receives financial and logistical support from IGAC, the US National Oceanic and Atmospheric Administration, and The World Meteorological Organization (an agency of the United Nations).

Steering Committee (formed December 11, 2014):

Owen Cooper (Chair), CIRES, University of Colorado/NOAA ESRL, USA, owen.r.cooper@noaa.gov

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Additional Steering Committee members have been identified and will be contacted. The initial steering committee will oversee TOAR activities until the second workshop, when the full steering committee will be implemented.

Brief History:

During the time period when TOAR became an official IGAC Activity and the 13th IGAC Science Conference in Natal, Brazil (September 22-26, 2014), Owen Cooper (TOAR Chair) discussed the goals of TOAR with scientists in the atmospheric sciences community, as well as with scientists who perform research on the impacts of ozone pollution on human health and vegetation. Following these conversations, Owen Cooper invited ten internationally recognized scientists to TOAR Workshop 1.01 (the first workshop of the first assessment report) held at the National Oceanic and Atmospheric Administration's (NOAA) Earth System Research Laboratory (ESRL) in Boulder, Colorado, December 10-11, 2014. With funding and support from the NOAA ESRL Chemical Sciences Division and IGAC, this workshop brought together these scientists with expertise in the observation and analysis of tropospheric ozone, with remote participation from six additional experts. The workshop participants were charged with completing four tasks:

1) Produce a detailed outline of the report with defined working groups.
2) Identify the primary ozone metrics to be calculated and outline the structure of the database which will archive the metrics.
3) Form a steering committee.
4) Define the goals of TOAR Workshop 1.02 to be hosted in Madrid during the last week of April, 2015, by the Agencia Estatal de Meteorología (AEMET – Spanish meteorological service), and co-sponsored by the World Meteorological Organization.

The workshop conclusions pertaining to each task are described in detail in the remainder of this workshop synopsis. Figure 1 provides a graphic description of the workflow of the assessment report.

1) Detailed assessment report outline with defined working groups

Purpose of the assessment report: To provide the scientific community with an up-to-date and comprehensive peer-reviewed, open-access reference that:

i) Displays the present-day observed ozone distribution and trends for the surface (urban and non-urban), the free troposphere, and the tropospheric column
ii) Reviews the ability of global-scale models to replicate the global/regional ozone distribution and trends and identifies future needs for ozone observations
iii) Describes the open-access database containing the global ozone metrics produced and archived for the report. Metrics will be calculated from observations that extend through the end of 2013.

Audience: The report is targeted towards scientists, with an Executive Summary relevant to policy makers.

Sources of data and references: Data used in the calculation of ozone metrics and new analyses in the assessment report will consist of hourly observations from established quality-controlled monitoring networks or from research-grade experimental sites (a definition for such sites is required). TOAR will organize several working groups to identify the ozone data sets in various regions of the world that are most appropriate for accomplishing the goals of TOAR. Besides the regional working groups, a separate working group will be established to identify the statistical tests that will be applied to the database, as well as the code used to calculate ozone exposure and dose metrics and statistics. The function of each working group is described in a separate section below.

All supporting documents mentioned in the report will be limited to peer-reviewed journals and peer-reviewed reports such as IPCC AR5 or publications by the LRTAP Convention, including the Task Force on Hemispheric Transport of Air Pollution, EMEP and the ICP Vegetation.

Report Format: From the six chapters of the assessment report and the Guide to TOAR Ozone Metrics, seven peer-reviewed, stand-alone publications will be produced. All chapters, the Guide to TOAR Ozone Metrics, and the Executive Summary will appear in the same journal and issue and will be clearly linked. A potential journal is Elementa (http://www.elementascience.org/). However, discussions will be held with a journal to determine if a workable format is available. The Steering Committee may also decide to submit a brief synthesis of the assessment report to a high profile journal.

Report Authorship: Each chapter will be written by a team of experts. An author contributing to a chapter must be an expert in the subject matter covered by that chapter, and must have a record of publishing articles in that area in the peer-reviewed literature. Each chapter will have a coordinating lead author who will be listed as the first author. All other scientists contributing to the writing of the chapter will be listed as co-authors. Each chapter will have at least one TOAR Steering Committee member as a co-author. All authors must approve of the content of the chapter before it is submitted for peer-review. In the case of disagreements among authors, alternative views will be represented in the materials; the TOAR Steering Committee will also seek to resolve authorship conflicts should they arise. In addition, a majority of the TOAR Steering Committee must approve the content of each chapter prior to submission.

REPORT CONTENT

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.

Chapter 1: A review of our understanding of tropospheric ozone sources and chemistry

a) Why ozone is important
b) Initial stratospheric attribution
c) Discovery of photochemical ozone in Los Angeles, and ozone production on urban, regional and hemispheric scales
d) Evolution of our chemical understanding, including deposition to water, surfaces and vegetation, and biogenic/anthropogenic emissions that regulate ozone production
e) History of the debate over the relative contributions of the stratosphere and photochemistry to the tropospheric ozone budget and processes, and the emergence of global chemistry-transport modeling. Consideration should also be given to the influence of ozone depleting substances and greenhouse gases on the quantity of ozone in the stratosphere and stratospheric dynamics, which subsequently affect the transport of ozone from the stratosphere to the troposphere.
f) A cartoon illustrating important ozone chemical and transport processes

Chapter 2: History of Tropospheric Ozone observations

a) Describe 19th century semi-quantitative Schönbein observations and reliability

b) Quantitative ozone observations from the late 19th century (Montsouris) and early 20th century (European high-elevation sites). How representative are these data?
c) Expansion of baseline ozone observations in the 1950s (International Geophysical Year) through the 1970s
d) Global surface coverage, urban and non-urban
e) Vertical profiling with ozonesondes and lidar. Tropospheric column ozone from ground based FTIR
f) Aircraft and satellite programs, present and future
g) Uncertainties of observational techniques and potential inconsistencies in long time series.

Chapter 3: Present-day ozone distribution (period TBD): Global/regional maps of various ozone metrics

a) Human health, vegetation and climate
b) Surface, free troposphere, tropospheric column
c) Temporal variations: diurnal, seasonal
d) Frequency distributions based on different metrics (i.e., 1-h, 8-hr, etc.) and time periods (i.e., monthly, seasonal, annual)
e) Emphasize the importance of seasonal cycles, as well as other systematic temporal cycles, for defining metrics that can provide tests of model simulations.
f) Highlight current regions with extreme ozone and compare to Los Angeles during the 1960s/1970s.

Chapter 4: Observed global ozone trends and variability: Global/regional maps of various ozone metrics

a) Long-term trends (i.e., using all data in a time series) and changing trending patterns (i.e., running 15-year and second derivative)
b) Human health, vegetation and climate
c) Surface, free troposphere, tropospheric column
d) Seasonal differences; interannual variability
e) Regionally representative time series constructed from site-by-site analysis

Chapter 5: Assessment of global-scale model performance in replicating global and regional scale ozone distributions and trends

a) This chapter will assess results from the peer-reviewed literature. No new modelling studies will be conducted for TOAR, but links will be made to CCMI and TF HTAP. The purpose is to provide an overview of the regions of the world where model estimates of ozone are most accurate and where errors and biases are greatest, covering the surface, free troposphere and tropospheric ozone burden.
b) Use power series expansion of historical ozone data for defining metrics that can provide tests of model simulations. Explore other new metrics for model evaluation.

Chapter 6: TOAR summary, recommendations and outlook

A range of topics including: addressing data gaps, preferred measurement techniques, and targeting regions for enhanced observations where ozone changes are expected to be rapid, etc.

Guide to TOAR ozone metrics (a stand-alone peer-reviewed paper)

a) Description and scientific rationale of each exposure and dose metric and its anticipated application.

b) Description of statistical techniques used in the report and a critical discussion of the limitations of the use of each technique.
c) How to access the data and code on the TOAR database.
d) Description of meta data for each site, archived on the TOAR database.

Working Groups: The eight working groups associated with identifying the most appropriate data for meeting TOAR's goals will be comprised of scientists with extensive knowledge of ozone data quality and metrics issues in their geospatial region of expertise. The working group associated with identifying the appropriate statistical techniques and database approaches will be comprised of scientists with extensive knowledge in these areas. The responsibility of a regional working group ends when the group delivers its data to the Statistics and Database Working Group (Figure 1).

a) *Asia Working Group*: Covers the region east of the Ural Mountains to the International Dateline, from the North Pole to the Equator, but excluding South Asia and the Middle East.
b) *South Asia Working Group*: India, Pakistan, Nepal, Sri Lanka, Bangladesh, Arabian Sea and Bay of Bengal.
c) *Africa and Middle East Working Group*: including Cape Verde Islands, Madagascar and La Reunion.
d) *North America Working Group*: USA, Canada, Greenland, Bermuda, Hawaii
e) *Central and South America Working Group*: includes Mexico and Caribbean Sea.
f) *Europe Working Group*: includes Iceland, Svalbard, the Mediterranean Sea and extends eastward to the Ural Mountains. Excludes the Middle East.
g) *Southern Hemisphere Working Group*: Australia, New Zealand, Antarctica and any island sites not allocated to other working groups. Excludes Africa and South America.
h) *Free Troposphere and Satellite Working Group*: Global coverage focusing on the following platforms: ozonesondes, aircraft, lidar, FTIR, satellite-detected tropospheric column ozone.
i) *Statistics and Database Working Group*: Charged with identifying statistical tests to be applied to the database, and the code that will be used to calculate exposure and dose ozone metrics and statistical tests. The code must be developed and documented such that future updates to the metrics database can be easily conducted by new users. This group will also design the database and will upload the final ozone metrics to the database.

Potential for parallel ozone precursor reports:

The Workshop participants considered the suggestions of several colleagues that TOAR also include ozone precursor gases. The participants overwhelmingly decided that the first TOAR should focus only on ozone due to the considerable amount of effort required to develop and produce the report and ozone metrics database. The participants agreed that in the event of a second TOAR, ozone precursors could be included if resources allow. In the meantime, should interested scientists wish to produce ozone precursor assessments in parallel with TOAR, the TOAR steering committee is willing to coordinate workshops, share ideas and make the TOAR database available for archiving ozone precursor metrics. The publication schedule of the first TOAR will proceed independently of the schedules associated with any ozone precursor assessment reports. However, the Steering Committee will seek arrangements with TOAR's publishing journal to link the ozone precursor publications to the TOAR special issue.

2) Description of metrics, logistical needs, database development and personnel

A major goal of TOAR is to calculate several exposure and dose ozone metrics relevant to studies of tropospheric chemistry and climate, human health impacts and crop/ecosystem impacts. These metrics will be calculated for hundreds of surface sites around the world, with appropriate metrics calculated for relatively infrequent free-tropospheric observations (e.g. monthly means rather than 1-h or 8-h averages). A database (to be hosted at Forschungszentrum Jülich in collaboration with the data centers of various global and regional networks) will be developed to make the metrics and associated statistical analyses (e.g. trends) publicly available. Following is a minimum list of metrics that will be calculated; additional metrics may be added with the approval of the Steering Committee.

Model-measurement comparison metrics

a) Monthly median, 5^{th}, 25^{th}, 75^{th} and 95^{th} percentiles: relevant for chemistry-climate model evaluation. The focus will be on daytime values to avoid comparison problems between nighttime values influenced by shallow boundary layers and coarse model grid cells. However some mountain-top sites, such as Mauna Loa, are representative of broad areas if the focus is on nighttime values. The statistical working group will determine the best daytime and nighttime hours to use.
b) Meteorologically filtered metrics: For comparison to chemistry-climate models, ozone metrics at selected sites will be filtered according to meteorological conditions such as wind direction.
c) Spatially averaged metrics: metrics will be produced on a 1°x1° grid, averaging all sites of a particular category (e.g. rural) within the grid cell.
d) Free tropospheric metrics: Due to infrequent sampling these metrics will be limited to monthly means for sites with 3 or more profiles per week, and seasonal means for sites with 1 profile per week. However, the daily MOZAIC/IAGOS profiles at Frankfurt will allow for monthly 5^{th}, 25^{th}, 50^{th}, 75^{th} and 95^{th} percentiles. Output will be on pressure surfaces, every 25 hPa.
e) Tropospheric column ozone (TCO) metrics: At present, OMI/MLS TCO gridded monthly means are produced by NASA at 1°x1.25° resolution. Products from other satellites should be made available on the same grid for direct comparison.
f) Trajectory mapped ozone: a gridded product that uses global wind fields to distribute ozonesonde observations several days upwind and downwind, as described by *Liu, G., Liu, J., Tarasick, D. W et al., (2013), A global tropospheric ozone climatology from trajectory-mapped ozone soundings, Atmos. Chem. Phys., 13*.
g) Polynomial fits (i.e., power series expansions) at selected baseline sites: polynomial "shape factors" that describe long-term trends will be calculated for selected baseline sites and made available in table form, as described by *Parrish et al. (2014), J. Geophys. Res. Atmos., 119, 5719–5736, doi:10.1002/2013JD021435*.
h) Fourier series expansion of seasonal cycles at selected baseline sites: a very few harmonic terms adequately describe seasonal cycles; these will be calculated for select baseline sites and made available in table form.

Human health metrics

a) Average Concentration Index: 4^{th} Highest 8-h Average Concentration for Each Year. Twenty-four running 8-h averages are used to identify the daily maximum 8-h value.

b) Average Concentration Index: 4th Highest 8-h Average Concentration for Each Year. However, each day a daily maximum 8-h value is determined using the running 8-h values between 0700 and 2300 h as per the recommendation of the U.S. EPA's November 25, 2014 Proposed Ozone Standard. The last 8-h period of the day begins at 2300 h and ends at 0700 h the next day. (U.S. EPA Proposed Revision to the 8-h standard).
c) Average Concentration Index: Maximum daily 8-h average.
d) Average Concentration Index: Maximum daily 1-h average.
e) Average Concentration Index: Running mean of the 3-month average of the daily 1-h maxima.
f) Cumulative Threshold Index: SOMO35 (sum of excess of daily maximum 8-h means over the cut-off of 70 μg/m^3 (35 ppbv) calculated for all days in a year). Similarly, SOMO10 and SOM00 will be calculated.
g) Cumulative Exposure Index: 4th highest W90 5-h Experimental Exposure Index as described in *Lefohn et al. (2010), Inhalation Toxicology, 22(12): 999‑1011*.
h) Percentiles: Annual and seasonal percentiles (median, 5th, 25th, 75th and 95th) of hourly average concentrations over 24-h period.

Vegetation metrics

a) Cumulative Exposure Index: W126 (7-month, 24-h-April-October in NH/reverse in SH)
b) Cumulative Exposure Index: W126 (3-month, 24-h-June-August in NH/reverse in SH)
c) Cumulative Exposure Index: W126 (7-month, 12-h-April-October in NH/reverse in SH)
d) Cumulative Exposure Index: W126 (3-month, 12-h-June-August in NH/reverse in SH)
e) Cumulative Exposure Index: AOT40, 6-months April-Sept (further discussion is required to determine the specific type of AOT40 to calculate)
f) Cumulative Exposure Index: AOT40, 3-months April-June
g) Average Concentration Index: Maximum daily 12-h average or daylight mean average
h) Flux-Based Index: PODyIAM (requires observations or model estimates of light, VPD and temperature. Does not require soil moisture or phenology). Is the threshold value the same for all regions and vegetation types? Need to determine the source of the additional parameters: observations and/or models? Can also include POD3IAM for application to crops and POD1IAM for application to trees.
i) Flux-Based Index: PODy (requires all modifying factors; more complex to calculate; needs soil moisture inputs and phenology paramaterization). Need to determine the source of the additional parameters: observations and/or models?
j) Annual and seasonal percentiles (median, 5th, 25th, 75th and 95th) of hourly average concentrations over 24-h period

3) Formation and charge of Steering Committee

The Steering Committee is charged with leading and coordinating TOAR activities to ensure that the first assessment report is published and that the TOAR database is populated with the exposure and dose metrics covered by the report. The Steering Committee target membership by the time of the Madrid Workshop is nine members, however additional members can be added with a majority vote. Steering Committee members have equal voting rights and the Committee must have an odd number of members to allow for tie-breaking votes. Members commit to serving on the Steering Committee until the first assessment report is published and the ozone metrics covered by the report are made available on the database.

During the workshop five participants (listed below) volunteered to serve on the initial Steering Committee. The workshop participants agreed that the Steering Committee should be expanded

to include representation from nations beyond North America and Europe. Representation from China and India is desirable due to existing and potentially increasing ozone pollution problems in these nations.

Present Steering Committee members (to be expanded to at least nine members prior to the Madrid Workshop):
Owen Cooper, Chair
David Tarasick
Allen Lefohn
Martin Schultz
Mathew Evans
Anne Thompson

4) TOAR timeline, and goals of Workshop 1.02 in Madrid

a) Early January 2015: announce Madrid workshop and make a general appeal for participants. Advertise the need for chapter leads and co-authors, as well as working group members. Based on the response, the Steering Committee will designate chapter and working group facilitators to lead breakout groups at the Madrid workshop. Also, communicate with scientists interested in parallel ozone precursor assessment reports and coordinate efforts.

b) January 22, 2015 – Finalize Steering Committee membership.

c) January 30, 2015 – Telecon to discuss collaboration tools and their status.

d) January 31, 2015 - Solicit proposals for statistical tests and upload documents to wiki.

e) February 28, 2015 - Formally initiate the regional working groups and statistical/database working groups based on the response from the Madrid workshop solicitation. Additional members can join at the Madrid workshop.

f) *April 28-30, 2015 – TOAR Workshop 1.02, Madrid, Spain*

The first day of the workshop (April 28) will be a working meeting of the Statistical Working Group, which will outline the appropriate statistical analyses to be applied to the data in the ozone database. These results will be proposed at the full workshop. The main workshop for all participants will occur on April 29-30. Goals of the workshop are: complete the identification of all ozone datasets for analysis; for each chapter produce outlines and compile reference lists; determine coordinating lead authors and co-authors for each chapter; determine membership of the working groups, including working group leads; produce a detailed timeline for the writing of the report, depositing data in the database and the calculation of exposure and dose ozone metrics and statistics.

g) Activities following the Madrid Workshop will be scheduled during the workshop. However the tentative schedule discussed at the workshop is as follows:

May – December 2015: Collect ozone observations and populate TOAR database, begin work on calculating ozone metrics around the world

December 2015: Produce first draft of assessment report

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

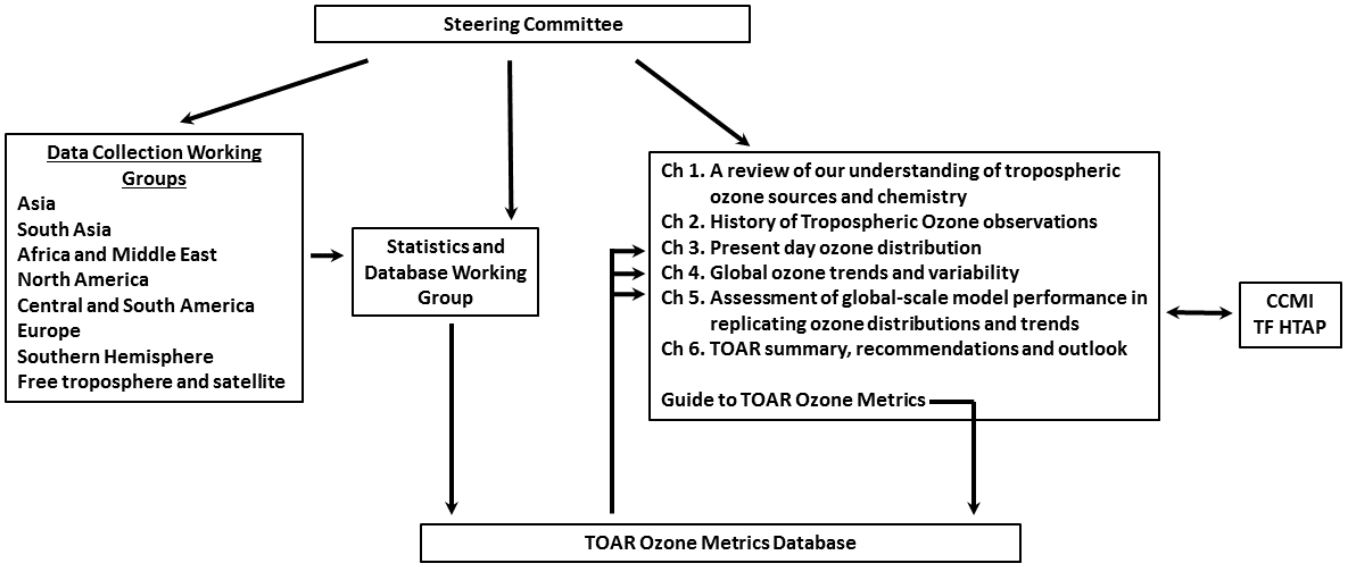

Figure 1. Work flow diagram of the assessment report.

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The following researchers were not physically present, but either joined the workshop via webinar or contributed material:

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