Commentary
Modelling of ozone over South Africa: Needs and challenges

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With a large range of precursor emission sources, both anthropogenic and natural, surface ozone levels in South Africa have a potential to be high enough to impact human health and plant life. It is also noted that with the increase in anthropogenic emissions due to development on a national scale, these surface ozone levels are likely to increase, making air quality management a necessary priority in securing improved human health.

Numerous monitoring campaigns, as well as continuous measurements via monitoring networks, indicate that elevated surface ozone levels exist within and outside of urban conurbations. However, analyses of measurement data indicate that in some areas, the levels of ozone are not increasing (Balashov et al., 2014). The spatially complex interactions of precursor gases, and thus ozone formation, owe much to the distribution of regional emission sources. The Highveld region, for example, is dominated by coal-fired power generation and the petrochemical industry, but also occurrences of biomass burning. Cities are heavily influenced by emissions from domestic fuel burning and traffic. In terms of ozone and its long spatial range transport and formation, both the rural (also rural-industrial) and urban regions interact, creating exceedances of the national standard in areas far removed from the precursor emission source regions. This not only makes it difficult to describe the spatial and temporal distribution of surface ozone, such that meaningful impact assessments can be made, but also to manage the potential precursor emission sources as ozone formation becomes a regional issue. The current suite of measurements that have occurred and are continuing to occur around the country provide merely a glimpse into ozone and its chemistry over South Africa. Furthermore, even with better measurements, an understanding of the dominant processes that drive ozone formation (and in general the oxidative capacity of the regional atmosphere) is still elusive, at least in its ability to be spatially and temporally comprehensive. While it is still acknowledged that further measurements will indeed aid in adding pieces to the puzzle, a more involved investigation through informed and appropriate numerical modelling must be considered.

Air quality modelling, in the context of investigating ozone formation, will seek to describe regional atmospheric chemistry. These models are utilized as tools with which specific questions may be answered. Broadly speaking, in terms of ozone, these questions centre around:

1 - “How much ozone is being formed?” The answer to this question can feed directly into impact assessments, either for human health or ecosystems.

2 - “What precursor emission sources contribute to ozone formation?” The answer to this question firstly enables better management of ambient air quality through focused emissions interventions, and then also more generally allows an understanding of a region’s chemistry (i.e., is the region NO_x or VOC limited?) such that larger, strategic emissions mitigation strategies may be developed.

An air quality model must be able to adequately simulate pollutant transport and transformation to answer these questions. What is required then is a scientifically up-to-date model, and inputs that are realistic and appropriate for the model’s needs. Inputs often associated with air quality models are listed below:

- Meteorological data (for air quality (AQ) models not coupled to meteorological models): This data drives transport of pollutants within the model and provides moisture, temperature and pressure estimates for chemical processing.

- Emissions inventory: Since the air quality model simulates transport and transformation of emitted pollutants, the emissions inventory forms the most important input to the model. In modelling ozone, and thus atmospheric chemistry, all precursor emissions need to be accounted for at a fine temporal and speciated scale (for VOC and PM). These range from industrial to biogenic sources. The temporal detail ensures that diurnal and seasonal cycles, particularly important for biogenic and domestic fuel burning sources, are captured and the response from ozone formation is simulated. Additionally, since ozone formation depends on various chemical reactions involving NO_x and the many VOC compounds (each with their own reaction rates), it is necessary to disaggregate total VOC emission estimates into the constituents being considered by the chemical processing modules in the model.

- Photolysis rates (for AQ models not coupled to a radiative transfer simulation): Photolysis rates are assigned to individual photochemical reactions according to how much solar radiation is available, and is dependent on solar angle, column ozone, column clouds and column moisture in general. Initial rates may be determined externally to the air quality model by use of data regarding the optical state of the atmosphere (moisture, aerosol and ozone), a radiative transfer model, and a database to cross reference the impact of radiation on standard, photochemical reaction rates. These may be further modified within the air quality model based on simulated aerosol optical depth.

- Initial and boundary conditions: This data allows the model to contextualize a simulation within an appropriate representation of reality. The initial conditions serve only to initialize the model by providing ambient concentrations at the beginning of a model run, and are thus only important for a short time. The boundary conditions are, however, much more important as they indicate to the model at each time-step the amount of pollutants entering the model domain from the lateral (east/south/west/north) and upper (highest model level) boundary. This then will depend on the size of the model domain chosen; and is a necessity of limited-area models (as opposed to global models). The domain boundary is best located in areas that exhibit near uniform (or at least easily determined) pollutant concentrations, such as those that primarily experience air quality at background pollutant levels. Thus, background station monitoring data can be used. If the domain boundaries fall within areas of significant emissions or pollutant transport, then these will have to be represented at each boundary. This is a complex task, effectively having to model further pollutant emissions and transport outside of the model domain. This often necessitates an additional simulation, but on a larger and coarser grid that feeds into the finer grid. However it should be noted that even the larger grid would need boundary input. It is thus advisable to create the domain large enough to include all significant emission sources, as well as those that significantly impact the simulation area of concern. One approach to simplifying lateral boundary estimation (if one cannot increase domain size any further) is to use global chemistry transport model (e.g. MOZART and GEOS-CHEM) outputs to specify boundary conditions. If a national domain is selected, monitoring data from the Cape Point GAW station can be used as initial as well as boundary conditions, together with any measurements along the north and east boundaries, (e.g. stations at Kruger National Park).

In addition to the preparation of input data, numerous model options need to be selected, which can include time-step considerations, topography handling, type of chemical processors and mechanisms (generally simplification by grouping discrete species and reactions) for description. The choice of chemical mechanism to be used is an important one and performance trade-offs (since a more accurate chemical mechanism might contain more explicit species and thus be more computationally expensive), specific non-standard reaction inclusions (e.g. inclusion of mercury chemistry) and ability to provide emission input for the mechanism need to be considered.

Once a model is run it is necessary to assess performance through comparison with measurements. The continuous ozone monitoring occurring nationally is essential to this required evaluation, and consistent quality control is vital. It should also be noted that while ozone measurements within cities or close to large precursor emission sources are useful, those in rural regions are also important. Model performance for an ozone simulation is generally assessed on the ability of the model to predict the magnitude and timing of peak ozone events. Thus both ozone as well as precursor measurements are needed to assess the build-up of precursors during an episode and the resultant ozone formation. A particularly useful measurement to compare to model outputs would be that of VOC species, such as ethane (or ethene) or formaldehyde, on a continuous (or at least for a year) basis. This can provide direct insight into the model's chemistry simulation and emissions characterization used therein.

From the above, one may appraise the capacity in South Africa to develop model platforms for the simulation of ozone by considering each of the aspects required to run an air quality model. Capacity to generate meteorological data through numerical simulation is present within South Africa through the South African Weather Service (SAWS) and the various regional climate modelling groups. In fact, private consultants may even offer this service for a fee. Air quality monitoring (for use in performance assessment and boundary conditions) activity in South Africa is also relatively high; with academic and professional organisations conducting much research into methodologies and application. However, on this aspect there is still room for growth as the appetite for measurements of more than just the criteria pollutants increases due to greater complexity in air quality issues being tackled.

Currently, the most limiting factor in producing simulations of ozone in South Africa is the lack of accurate, credible and peer-reviewed emissions data of a high temporal and spatial resolution. Ideally, such information should also be vetted by national or provincial government (together with stakeholders) so that agreement is reached before modelling can be done as results can then be deemed "official" and then considered legally applicable. As it stands, there is no official national emissions inventory for any of the source classes of precursor emissions. The current piece-meal approach, focused on single sources or source categories, to constructing an emissions inventory cannot be used for simulating ozone, as the non-linear response introduced by chemical transformations only intensifies any impact from biases/incompleteness in an inventory. Only when all relevant sources of precursor gas emissions are captured in acceptable detail (i.e. spatial, temporal and species) can more accurate predictions of ozone be sought.

Even so, it should be noted that the air quality models used may be termed "research models" since the science behind many of the processes included are constantly changing as the research community resolve atmospheric chemical dynamics in more detail. There will thus also need to be a bridge to close the gap between policy and decision makers with the research community. A primary driver is an increase in computational resources, allowing these models to reduce the performance trade-offs often used. That is not to say that valuable conclusions cannot be attained from the current set of models, but rather an open scientific process needs to be followed in building and working with these models, such that expectations are maintained and results are correctly interpreted. In the local context, much of the research required will still fall upon emissions estimation before we can even begin to question the accuracy of air quality models due to their own inherent abilities.

References

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