AIR QUALITY EXPERT GROUP

Modelling of future $PM_{2.5}$ in support of the Defra air quality target setting process.

Summary of the $PM_{2.5}$ modelling workshop and advice on key issues to consider.

15th March 2021

Introduction.

Atmospheric models are central to providing estimates of atmospheric concentrations of air pollution. The use of models is very diverse in air pollution management – for example they allow for the prediction of air pollution where it is not measured, they provide short-term forecasts of air quality for public information (analogous to weather forecasts) and can provide estimates of the atmospheric impacts arising from changes in emissions. For this last application they are an essential part of the toolkit used to inform the policy development process, and for evaluating progress in meeting air quality targets.

The use of atmospheric models for the estimation of air pollution in the future, looking out on multi-year timescales, is particularly challenging. In general, the further ahead in years a model aims to predict, the more uncertain that prediction becomes. The forecasting of likely changes arising from emission reductions over decadal timescales is exceptionally difficult. The complete modelling of the behaviour of atmospheric particles (which in the atmospheric community are often referred to as aerosol particles, or simply 'aerosols' and the mass of which is commonly referred to as particulate matter) remains a major fundamental challenge in atmospheric science. It is worth noting that the single largest uncertainty in model-based prediction of future climate change also arises from the uncertainty in estimating the climate effects of aerosol particles; the technical challenge therefore impacts on issues well beyond air pollution policy development.

As part of the target setting process for the *Environment Bill*, AQEG (details in Annex A) have been asked to provide scientific advice relating to some recent modelling work on $PM_{2.5}$ (particulate matter less than 2.5 µm in diameter) that has been commissioned by Defra and to subsequently provide:

i) Commentary on the key processes and uncertainties that may affect model predictions of UK concentrations of $PM_{2.5}$ on the timescale of ~2030-2050,

and,

ii) Provide recommendations that Defra may wish to consider in its future commissioning of modelling work in support of target development.

AQEG has considered of a range of scientific and technical evidence. This includes material submitted to Defra *via* a public call for evidence (see: https://www.gov.uk/government/news/call-for-evidence-on-fine-particulate-matter-air-quality-targets), discussions held an expert workshop on $PM_{2.5}$ modelling on 1st Feb 2021 (see Annex B), and a series of reports provided by Imperial College based on modelling using the UK Integrated Assessment Model (UKIAM), referred to here as ApSimon, H. *et al*., Imperial College.

This short report is not intended to replace independent and more detailed peer-review of the reports and model estimates provided to Defra by Imperial College under contract. This report draws together the presentations and discussion related to the modelling workshop.

Overview of key issues in modelling future $PM_{2.5}$

$PM_{2.5}$ comprises primary (that is, directly emitted particulate matter) and secondary particulate matter that forms from chemical reactions between pollutants in our atmosphere. Atmospheric models of $PM_{2.5}$ attempt to represent concentrations through the inclusion of emissions (both primary PM and chemical precursors of PM), the transformation of those emissions through chemical and physical processes, and the transport and dilution of pollution by dynamical processes (weather). Each of these has uncertainties associated with it, and all models must make compromises along the way. For example models must define a spatial resolution at which they operate, the level of chemical detail in the underlying emissions (which themselves are uncertain), the time steps between calculations or the complexity of the chemistry and physics they simulate. The various trade-offs in modelling were highlighted in the workshop by numerous presenters, e.g. Evans, M. *et al*., University of York, Carruthers, D. *et al*., CERC.

Some models may aim to model the chemistry of PM processes explicitly, that is reaction by reaction. There are parameterised chemical schemes for secondary aerosols in models such as CMAQ (Beevers, S. *et al*., Imperial College); EMEP4UK (Nemitz, E. et al., UKCEH) and GEOS-Chem (Evans, M. *et al*., University of York). Other models represent secondary inorganic aerosol (SIA) based predominately or exclusively on empirical relationships informed, for example, by knowledge of land-use type (*e.g*. PCM, Stedman, J. *et al.,* Ricardo; ADMS, Carruthers, D. *et al.,* CERC). It is important to stress that different models are typically optimised for particular tasks, and there is no single 'best' model. This was exemplified at the workshop with models that had capabilities that spanned predictions from a few metres at the roadside (Carruthers, D. *et al.,* CERC) through to the representation of PM within multidecadal climate simulations (Dacre H. *et al*., University of Reading).

In this short report some of the key scientific issues will be explored in outline in order that the outputs from modelling studies commissioned by Defra can be accompanied by a suitable narrative that sets out i) areas of broad agreement on future PM, as predicted by models, ii) areas of uncertainty in modelling future $PM_{2.5}$ iii) how uncertainties might be addressed and handled in future work.

Points of broad agreement

In an ideal world modelling would be able to provide an accurate picture of $PM_{2.5}$ concentrations in 5 or 10 years from now for a range of different policy scenarios and related emissions reductions. In practice, models can provide only an informed guide to the likely direction and scale of change, where that change may occur geographically and when. Inevitably models have to neglect potential effects for which they do not have a simulation or scenario, and make choices around which future pathway for emissions they apply. Choices must be made over boundary conditions to impose on model domains, *i.e*. for concentrations, meteorology, climate and the base year to use as a starting point for future projections and on the meteorology on which to base the model prediction. Despite this range of factors, evidence presented at the workshop showed a number of areas of broad agreement on future $PM_{2.5}$ that it is valuable to capture. Evidence from a diverse range of model types was presented and there was no prescribed emissions dataset or meteorology applied to the Defra call for evidence or in the modelling workshop.

- For those models that made predictions of future $PM_{2.5}$ there was broad agreement regarding a trajectory of continued reductions in annual average $PM_{2.5}$ concentrations out to 2030. (e.g Beevers, S. *et al*., Imperial College, Nemitz, E. *et al.,* UKCEH, ApSimon, H. *et al*., Imperial College.)

- Irrespective of model, reductions in $PM_{2.5}$ occurred right across the UK, with the large majority of the UK land area likely to be below 10 μg m^{-3} by 2030. There was consistency between models in showing that locations in central London were those most at risk of concentrations exceeding an annual average concentration of 10 μg m^{-3} in 2030, although the extent of this was very sensitive to the emissions scenarios and also the base year used. (Beevers, S. *et al*., Imperial College, Nemitz, E. *et al*., UKCEH, ApSimon, H. *et al*., Imperial College.)
- There was consistency between models in predicting that large areas of central and south eastern England would experience annual average concentrations in the range 6-8 μg m^{-3} by 2030. The remainder of the UK showed concentrations typically below 6 μg m^{-3}. There was general agreement between models that secondary inorganic and organic components in combination would comprise the largest sub-component of $PM_{2.5}$ looking across the UK as whole. Beevers, S. *et al.,* Imperial College, Nemitz, E. *et al*., UKCEH, ApSimon, H. *et al*., Imperial College, Evans, M. *et al*. University of York, Stedman *et al*., Ricardo.
- However, primary emissions of PM in urban areas remain an important factor in determining population exposure and there is considerable uncertainty in their future emissions trajectories. Changes in urban primary PM emissions would have significant impacts on the attainment of 10 μg m^{-3} limit value in cities. (ApSimon, H. *et al*., Imperial College, Beevers *et al*. Imperial College) The local impact of these primary emissions on concentrations is highly sensitive to the model resolution, with higher resolution models predicting higher localised concentrations.
- There was consistency across models in identifying a role for transboundary processes and that a substantial fraction of $PM_{2.5}$ in 2030 in the south east of England would, on an annual average basis, be derived from continental sources. (Beevers, S. *et al.,* Imperial College, Nemitz, E. *et al*., UKCEH, ApSimon, H. *et al*., Imperial College, Evans, M. *et al*., University of York, PCM, Stedman, J. *et al.,* Ricardo, Colette *et al*., INERIS.)
- There was a range of evidence presented showing the sensitivity of $PM_{2.5}$ calculations to meteorological and natural factors, for example the choice of base year used for model calculations had a substantial effect on predictions, and the effects of changing biogenic/natural emissions. Beevers, S. *et al.,* Imperial College, Colette, A. *et al.*, INERIS; Dacre H., *et al.,* University of Reading.
- Models all kinds rely on ambient monitoring data to help calibrate their responses and cross-check their performance. The availability and quality of this data was shown to have significant impact on modelling outputs produced and conclusions drawn (Carruthers *et al*., CERC, Beevers *et al.,* Imperial College, ApSimon *et al*., Imperial College). $PM_{2.5}$ is notable as being subject to larger measurement uncertainties than some other gaseous pollutants. Models of present-day concentrations of $PM_{2.5}$ will therefore be affected by uncertainties in that measurement data, as will future predictions. A specific example of differences between different $PM_{2.5}$ instrument types were discussed most recently at AQEG meeting 53 (3rd Feb 2021); these kinds of practical monitoring issues have potentially under-recognised impacts on modelling also.
- Related to the above, the challenges and uncertainties in measuring $PM_{2.5}$ are becoming more important as concentrations in general continue to fall over the UK, and particularly for present-day and future background/rural measurements of $PM_{2.5}$. The linkage between observations in the AURN (and other networks) and $PM_{2.5}$ modelling need to be continually reviewed as instrument technologies change over time.

- There was agreement between participants on four broad key factors that could lead to deviations in the future trajectory of $PM_{2.5}$ in models. These are summarised as:

  i) Incomplete or inaccurate representation of all relevant emissions, both primary PM and precursors, ii) the simulation of secondary $PM_{2.5}$ processes and potential non-linearities in the chemical processes in future atmospheres iii) the sensitivity of future UK $PM_{2.5}$ to transboundary effects and international trends in emissions, including shipping and iv) unpredictable natural factors including those arising from climate change.

Uncertainties in modelling future concentrations

Different models presented at the workshop showed some clear areas of agreement, for example in the geographic location of future $PM_{2.5}$ reductions, general trends over time and the likely dominant chemical components in 2030. This was not in any sense a formal model intercomparison and given the different set ups for models it is important to avoid artificial precision being inferred from these different model projections. Many models compared performance against past data to provide confidence in future predictions, but recognised that these observational datasets were often limited in number and subject to uncertainties themselves. Recognising both model and measurement uncertainty is of particular significance for $PM_{2.5}$ given targets for the future may include an integer annual-average concentration value.

Some of the potential confounders of model forecasts are themselves highly uncertain and it is unlikely to be feasible for Defra-commissioned modelling to estimate quantitatively the scale or sometimes even the direction of the effect. Climate change impacts on atmospheric circulation is an example of an externality that may affect future $PM_{2.5}$ significantly, but this is very difficult to represent in the target-setting work being undertaken now. In cases such as this, a narrative description of the possible effect is required so that interpretation of model predictions, and ultimately decision-making, is suitably informed and contextualised.

Some uncertainties arise from the range of possible future changes in emissions that may occur, or how the chemistry of the atmosphere may respond to those emissions. For some of these issues recommendations can be made to help Defra develop an appropriate range of model scenarios that capture a reasonable breadth of likely futures. In the next sections some of the areas of uncertainty discussed at the workshop will be expanded on.

i) Representation of emissions

Emissions are the starting point for atmospheric modelling of $PM_{2.5}$ and Defra is commissioning a range of scenarios of future emissions from key sectors, in consultation with user and industry groups. Projections of emissions are inherently uncertain since they require judgements to be made about societal trends, economic factors and behaviours, technology and the evolution of emission controls. Although AQEG have not reviewed the final emission scenarios to be used in modelling of future $PM_{2.5}$, relatively robust predictions are likely to be available for some sectors. For example, future emissions from fossil fuel power generation, or ICE vehicle tailpipe emissions are likely to be forecast out to 2030 with some skill. Emissions estimates beyond 2030 become increasingly uncertain.

There are however some significant emissions sectors that will contribute to future $PM_{2.5}$ that are known to be poorly captured in existing emissions inventories, often because there is no requirement to report those emissions as part of the National Emissions Ceiling Directive (NECD). Evidence presented at the workshop highlighted that emissions of PM, such as those arising from cooking and intermediate volatility organic compounds (IVOCs), are not currently included in the National Atmospheric Emissions Inventory (NAEI), and therefore subject to large modelling uncertainties (Beevers, S., Imperial College, ApSimon, H., et al., Imperial College, Allan, J. University of Manchester). Non-exhaust particulates from vehicles, wood-burning and other domestic emissions are likely to remain a critical source of primary emissions for 2030 that play an influential role in determining urban exposure and attainment of limit values. There remain important differences in the methods and estimates of some emissions in different inventories, for example NAEI vs London AEI for woodsmoke. The choice of emission scenarios has a significant influence on the attainment of a 10 $\mu g\ m^{-3}$ annual limit value in some urban centres. (ApSimon, H., *et al.,* Imperial College, Beevers, S. *et al.,* Imperial College).

For sub-sectors where there are large emission uncertainties, model runs should aim to capture a suitable range of plausible estimates of emissions, and the sensitivity of the overall $PM_{2.5}$ outcomes to that sector quantified. It is of course possible for errors in different source sectors to cancel one another out, nonetheless the possible sensitivity of overall $PM_{2.5}$ projections to individual sectors needs to be visible to decision-makers.

ii) Secondary $PM_{2.5}$ processes

A common theme raised during the workshop, and more broadly in the call for evidence, is the challenge of representing secondary particles. There is uncertainty not just in the emissions scenarios that will be followed for precursor species such as SO_2, NO_x and NH_3, but how a given mixture of those (and other) precursors may translate chemically into $PM_{2.5}$ concentrations. All models showed the importance of secondary PM as a contributor to overall UK $PM_{2.5}$ mass. The contribution is dependent to a degree on geography, but they are likely to play a key role in defining background and urban concentrations over much of the UK in 2030. This arises in large part because of further anticipated reductions in primary emissions of PM. The development of chemical and physical model schemes that represent secondary inorganic aerosols (SIA) are considered to be more advanced than those for secondary organic aerosols (SOA).

At present models are typically evaluated against measurements and then adjustments made to those models in their representation of PM and associated response to changes in precursor emissions. Through adjustment of model schemes, it is possible to achieve satisfactory agreement between models and present-day measurements, and this has been recently completed with the UKIAM following previous AQEG feedback. There is however uncertainty in the reliability of extrapolating present-day 'tuned' relationships between precursors (such as NH_3, NO_x and SO_2) and secondary SIA to future conditions. The response of SIA is known to be complex and non-linear and can be subject to multiple chemical pathways, and models tested on past observations may not perform as well for as yet unseen atmospheric conditions.

Secondary organic aerosols are an area of particular uncertainty and whilst they are included in most models the representation of their formation is rudimentary and sometimes highly parameterised. In general, there is a tendency for observations of PM in the UK to show larger contributions from SOA than are mechanistically estimated in models (Nemitz *et al.*, UKCEH, Colette *et al*. INERIS) although the measurement datasets with which to make comparisons are very limited. Some compensatory approaches are included in models, for example by the introduction of a SOA background concentration (Nemitz *et al.*, UKCEH). Since SOA arise from both natural and anthropogenic precursor emissions and can be sensitive to other co-pollutants, there is no clear consensus on whether as a sub-class of PM they would be expected to fall over the period to 2030. A cautious approach to SOA would be prudent in the modelling of $PM_{2.5}$.

It is important that current models are evaluated against observations to ensure that current SOA contributions to $PM_{2.5}$ are adequately reflected. Since the future emissions of IVOCs and

BVOCs are uncertain, and VOC emissions are predicted to fall only by small amounts, a conservative approach would be to maintain the concentrations of this sub-component of $PM_{2.5}$ as constant to 2030.

iii) Transboundary effects,

An area of consensus across models was the role that transboundary transport of pollutants can play in determining background concentrations over the UK, and in turn placing limits on the attainability of $PM_{2.5}$ targets in UK cities. This is also in line with previous conclusions that AQEG has made, see for example *Fine Particulate Matter ($PM_{2.5}$) in the United Kingdom* report. Modelling presented by ApSimon *et al.*, provided an assessment of the sensitivity of $PM_{2.5}$ to a range of different European emission reductions, either NECD, or some fractional attainment thereof. A more extreme example was presented by Evans *et al*., where *in extremis* should all UK anthropogenic emissions be eliminated, large areas of southern England would still likely experience annual average concentrations of the order 6-7 $\mu g\ m^{-3}$ due to transboundary transport. Whilst brute force emissions changes often do not fully capture how local and regional emissions interact with one another, it is still illustrative of the potential scale of influence from non-UK sources for some parts of the UK. All models presented included some component on transboundary PM in their appointment of sources.

Since transboundary effects have notable effects it may be worthwhile to explore the sensitivity of future UK $PM_{2.5}$ to a wider range of possible scenarios for example adjusting NECD attainment of different emissions individually, and by nation, particularly for near-neighbour / North Sea countries. It may be helpful to identify whether there may be specific international emissions reductions, by sector, country or chemical, that would deliver enhanced benefits to the UK, should those emissions be reduced beyond NECD limits for 2030. ApSimon *et al.* presented the impacts of international and coastal shipping emissions on UK $PM_{2.5}$, a source that makes an important contribution to SIA over the UK, and particularly in southern and southeast England. Quantifying the possible impacts of future international agreements to further reduce shipping emissions on the UK air quality would be valuable.

Although addressed in more detail in the next section, an important factor determining transboundary contributions to the UK are the prevailing meteorological conditions. A shift in the airmass trajectories arriving in the UK can potentially lead to changes in transboundary impacts on the UK even for constant overall European emissions (*e.g* for dust, Colette *et al*., INERIS). It is well-recognised that slack flows of air from the low countries in springtime, and when fertiliser use is high, is a meteorological condition that can lead to high PM in the UK. Changes in circulatory patterns could have the effect of amplifying, or indeed reducing, the frequency of those events.

iv) Natural factors and climate change.

$PM_{2.5}$ concentrations are complex to predict because they are determined not only by anthropogenic emissions, but also by contributions from persistent natural sources such as seasalt and SOA arising from biogenic VOC emissions. Added to this are other intermittently large natural sources such as wildfires and Saharan dust. A complex set of interactions exist between all these components, many of which are also highly sensitive to meteorology. This makes $PM_{2.5}$ concentrations sensitive to a broad range of natural factors that are frequently not within national controls and that can be hard to predict both in an operational forecasting sense, and for long-term policy evaluation.

Dacre *et al.* highlighted the sensitivity of UK $PM_{2.5}$ to changes in atmospheric circulation patterns in Western Europe, showing that under future climate change scenarios in 2050 Rossby wave breaking over northern Europe may shift eastwards leading to a reduced frequency in stagnation events for the UK, and an increase in precipitation (which scavenges pollution). The effects are complex to evaluate in a UK context; fewer stagnation events would likely reduce the worst 24-hour periods for high $PM_{2.5}$, but this shift in weather pattern may also increase the overall period of time where air flows from continental Europe to the UK, with increases in $PM_{2.5}$ on an annual average basis. Dacre *et al.,* highlighted the large uncertainties in climate modelling at this scale, although the sensitivity of those concentrations to those climate-related uncertainties is likely to be lower than the sensitivity to emissions.

It would not be practicable for Defra to try to model a range of future climate change dynamical scenarios on $PM_{2.5}$ but the possible positive or negative effects of climate change on circulation as an influence need articulating in any accompanying narrative on future $PM_{2.5}$ feasibly. The capability to model changing meteorological effects in city environments, and how these may influence dilution and ultimately concentrations and exposure, remains challenging. Whilst considerable advance has been made in the street scale modelling of traffic emissions, in future the effects of urban emissions from other sources (*e.g*, from buildings, biogenic sources etc) will need to be properly captured, and this may be superimposed on altered meteorological patterns due to climate change.

Natural factors also play a key role in emissions of some primary $PM_{2.5}$ and PM precursors. As identified earlier, biogenic emissions of BVOCs contribute to the mass of SOA in air, and this factor is sensitive to conditions such as temperature, cloud cover and rainfall, as well as of course depending on land-use practices. In general higher temperatures lead to higher BVOC emissions and by extension more SOA, so on balance increases in SOA from biogenic emissions across Europe might be anticipated due to climate change (Colette *et al.*, INERIS). Some further exploration through modelling of the possible scale of impacts of increased BVOC emissions across Europe as a consequence of climate change and the resultant effects on transboundary SOA would be useful to complete.

Other acknowledged contributors to UK $PM_{2.5}$ arise from natural, or semi-natural emissions from biomass burning and from wind-blown dust. Whilst biomass burning (*e.g*. forest fires, moorland and peat fires) are not generally considered to be a significant factor for $PM_{2.5}$ on an annual basis in the UK, changes in rainfall and land-use may alter this. As has been seen from some recent moorland and peat fires the effects locally on $PM_{2.5}$ can be significant. Climate change may change the frequency of these events not just in the UK but more widely in Europe, which may feed-back on the UK $PM_{2.5}$ background. Evaluating from literature and available data the current impact of wildfires on $PM_{2.5}$ would be valuable in providing additional context to modelling.

Sporadic long-range transport of mineral dust to the UK is a fairly common occurrence and can perturb $PM_{2.5}$ over periods of days to a week or more. The frequency of wind-blown dust events is sensitive to meteorological patterns (*e.g.* the frequency of airmasses arriving in the UK from North Africa), and rainfall pattens that may lead to desertification. As with BVOC emissions it is very difficult to predict the likely direction of any change on a 2030 timescale and indeed perhaps no change may be a likely outcome, but the scale of effect makes it worth considering in narrative descriptions of external effects (Colette *et al*., INERIS).

One final potential perturbation to future $PM_{2.5}$ from natural sources would be from remote volcanic emissions either of PM directly or via SO_2 emission. Whilst such an event would be random and likely short-lived, rather than a long-term systemic alteration of $PM_{2.5}$ such as those arising from climate change, it is nonetheless a highly unpredictable natural factor that may change annual average concentrations and hence compliance with a limit value in a given year.

Exposure reduction and tracking policy progress

Discussions at the workshop, and model data presented, focused on ambient concentrations and $PM_{2.5}$ in the context of attainment of limit values. Within the Environment Bill framework, a $PM_{2.5}$ population exposure reduction target is also possible. This brings additional challenges for both measurement and models. Put simply, the skill of models to predict exposure reduction of $PM_{2.5}$ may not be uniform across the UK. There is limited data on the ability of models to accurately predict rates of change. Exposure reduction metrics will challenge models to provide predictions in locations where the concentration of $PM_{2.5}$ is already relatively low, for example in the range 4-8 mg m^{-3} and where changes year on year may only be small, and potentially less than the measurement uncertainty. Spatial variability in contributing sources; for example the balance between local emissions and transboundary contributions, may lead to different uncertainties in model predictions of exposure reduction for different locations. At this time there is limited data to evaluate model to model variability in their estimates of exposure reduction outcomes.

$PM_{2.5}$ modelling is likely be important to predict and evaluate progress towards meeting interim and long-term air quality objectives. Progress in reducing $PM_{2.5}$ is unlikely to follow simple linear trends over time and may vary by location. This may be due to a multitude of factors including variability in year-to-year meteorology, non-linear aspects to the chemistry, or the timing of new emissions controls. Models are likely to be critical to support the diagnostic interpretation of ambient monitoring data. This will require capability to adequately predict overall $PM_{2.5}$ concentrations and to correctly deconvolute the contributing factors that have given rise to observed trends.

Tracking changes in concentrations also provides challenges for measurement, especially in locations where concentrations are low, and where the likely rate of change is small. Modelling to evaluate progress must be informed by chemically-speciated aerosol particle measurements to connect emissions, model sub-processes and ambient $PM_{2.5}$ concentrations. $PM_{2.5}$ is an operationally defined metric. This means that different measurement approaches produce different results, within a defined uncertainty envelope. It is therefore critical that consistent measurement techniques and quality assurance are deployed to track change and exposure reduction over a decade or more. Instruments and techniques may also differ in their sensitivity to the various components of the aerosol particle mixture, affecting their ability to track changes as the particle source mix changes over time.

Table 1 provides a summary of the uncertainties in modelling future $PM_{2.5}$ concentrations and recommendations on how these could be evaluated in the work planned by Defra.

Table 1. Summary of modelling uncertainties and recommendations

Type of Uncertainty	Description	Scale of potential impact on 2030 predictions?	Direction of effect on future $PM_{2.5}$	Recommendation for future modelling
Emissions projections	The projection of emissions across the diverse range of sources that contribute to $PM_{2.5}$ is inherently uncertain, and these grow the further into the future from the present day. Some emission sectors are poorly represented in models even for present-day emissions.	Impact of errors or uncertainties in any one emission sector are potentially modest, but in combination could lead to large errors in the estimation of future $PM_{2.5}$.	Unclear, either direction of effect is possible, or neutral if uncertainties in different emission sectors lead to error compensation.	Ensure a suitable range of UK emissions trajectories are included (accepted that this is already a work in progress in Defra). Ensure that poorly described emission sectors are included with scenarios that capture the full range of plausible emission rates for example from cooking, vehicle non-exhaust, domestic emissions.
Chemical processes in pollution models	A substantial fraction of $PM_{2.5}$, now and in the future, is secondary in nature. Models must be capable of suitably representing the chemical and physical processes that generate secondary inorganic aerosols (SIA) as contributors to UK $PM_{2.5}$. Model parametrisations of SIA 'tuned' to the conditions of today may not represent the atmosphere under future chemical conditions.	The impact of secondary PM, relative to primary $PM_{2.5}$ will grow over the next decade so uncertainties or errors in models are likely to become more significant the further models project in the future	Unclear, although on balance may lead to higher $PM_{2.5}$ than anticipated based on previous model / measurement comparison which tend towards non-linearities and dampened PM reductions as precursor concentrations decline.	Recent use of model-measurement comparisons to improve the parametrization of SIA formation in UKIAM has been beneficial. Future model simulations should consider what impact a less responsive $PM_{2.5}$ (SIA) relationship to precursor reductions would have on future $PM_{2.5}$ estimates.
	Measurements indicate that secondary organic aerosols (SOA) are a significant component of UK $PM_{2.5}$ but they are not well represented in models. There is evidence existing models used for feasibility studies underestimate their mass contribution when modelled mechanistically and require background adjustments to match observations	SOA are likely to grow in relative significance as a fraction of $PM_{2.5}$ as primary emissions reduce.	Unclear, due to very large modelling uncertainties in the response of $PM_{2.5}$ to future POA and VOC/IVOC reductions. Also unclear SOA response from biogenic precursors.	Evaluate model performance against UK observations to confirm whether SOA contributions are being broadly correctly reflected as a fraction of $PM_{2.5}$ mass. Given large uncertainties in contributing sources take a conservative approach to assumed future emissions including no reduction by 2030. Include also possible impact of increased biogenic SOA by 2030.
Transboundary impacts	Transboundary contributions play an important part in defining UK $PM_{2.5}$ baseline, and particularly so in the SE England. Future $PM_{2.5}$ is therefore significantly dependent on emissions reductions in the rest of Europe and from shipping.	Should European nations substantially over or under achieve on emissions reduction commitments the impacts on the UK, and particularly in London and SE England would be significant. Unanticipated changes in shipping emissions could have substantial impacts in some UK regions	Depends on whether emissions under or over perform against baseline assumptions. Some notable concerns regarding likelihood of meeting obligations on NH_3, leading to an increase in $PM_{2.5}$ relative to feasibility scenarios	Modelling has included an assumption of met NECD targets, and some assessments assuming a *pro rata* underperformance against NECD. Consider a sector by sector and /or pollutant by pollutant evaluation of the impacts of different levels of attainment, and also the impacts on the UK of an overachievement against European NECD, or from individual near-neighbours.
	Changes in transboundary import of natural $PM_{2.5}$, notably mineral dust, biogenic aerosols, seasalt, all impact on UK $PM_{2.5}$. Any change in the input of these natural emissions will impact on $PM_{2.5}$.	Likely modest, although dust events may have larger short-term episodic impacts.	Could lead to increases in $PM_{2.5}$ although possibly smaller than anthropogenic transboundary impacts	Use modelling and measurements to evaluate the scale of the impact of these natural factors and develop a suitable narrative to place the possible unpredictable, and uncontrollable, nature of transboundary natural emissions changes on $PM_{2.5}$ in a suitable context. Provide an estimate of the plausible range of impacts on future $PM_{2.5}$.

Natural factors, meteorology and climate change	An increase in the frequency of biomass burning events, such as moorland and forest fires due to climate change or land management practices by impact on UK $PM_{2.5}$.	This may become significant at a regional scale towards end of decade, although some potential for mitigation through land-use management may be possible (e.g. uplands, peat drainage practices etc).	Likely increase $PM_{2.5}$ relative to feasibility scenarios, possibly significant regionally.	Identify whether biomass burning is represented in the models being used. Evaluate the possible scale of the contribution and the impact of a change in annual emissions of the order of doubling from present day.
	$PM_{2.5}$ is sensitive to meteorological conditions, which influence circulation patterns, transboundary pollution and other processes such as photochemistry and wet/dry deposition. These may change due to climate change: change in frequency and location of blocking highs, changes in precipitation etc.	Possibly significant on an episodic basis towards end of decade	Unclear direction of effects, significant uncertainty in climate forecasts	Likely not possible to simulate climate changes effects on future $PM_{2.5}$, but the possible impact of climate change on the attainment of $PM_{2.5}$ targets in the future should be captured in narrative form. The scale of influence of meteorological variability should be captured through the use of multiple different meteorological years for model simulations. The ability to model the effects of changing meteorology on urban dispersion and boundary layer processes remains an important modelling capability.
Exposure reduction	Estimating future exposure reduction requires the simulation of trends in $PM_{2.5}$ across the UK, including locations where $PM_{2.5}$ is already low. The skill of models to predict exposure reduction may vary depending on the contributing sources at any given location.	Modelling exposure reduction is likely to be more robust in locations experiencing higher concentrations due to high primary contributions and larger fractional reductions occurring. Estimating exposure reduction in low concentration regions or the rural environment may come with significant uncertainties.	Unclear direction of effect.	Limited number of models have thus far focused on exposure reduction as a $PM_{2.5}$ target, and there is limited data available with which to compare predictions between different models. Increased confidence in exposure reduction projections would be gained from the use of a wider range of models.
Monitoring data	Models are heavily dependent on ambient monitoring data to provide calibration and to enable assessment of model performance, The measurement of $PM_{2.5}$ is subject to uncertainties, and there are technological challenges in maintain comparability between instruments over time. As $PM_{2.5}$ concentrations decline the measurement uncertainty is becoming a more significant issue.	The reliance on historical $PM_{2.5}$ monitoring data to help tune models leaves them vulnerable to uncertainties in that data. Changes in the types of instruments used to measure $PM_{2.5}$ over the next decade may lead to a re-calibration of models and therefore changed predictions.	Unclear direction of effect, but technical changes in the AURN and other networks may lead to revisions of model forecasts.	The effect on model predictions arising from uncertainty in $PM_{2.5}$ measurements used for model calibration and training requires further investigation. It is likely not possible to fully resolve this issue quickly, but an understanding of the scale of potential impact on projected $PM_{2.5}$ concentrations is required.

Annex A

About the Air Quality Expert Group

AQEG is an expert committee of Defra and considers current knowledge on air pollution and provides advice on such things as the concentrations, emission sources and characteristics of air pollutants in the United Kingdom. AQEG reports to Defra's Chief Scientific Adviser, Defra Ministers, Scottish Ministers, the Welsh Government and the Department of the Environment in Northern Ireland (the government and devolved administrations). Members of the group are drawn from those with a proven track record in the fields of air pollution research and practice.

Terms of Reference

The Air Quality Expert Group (AQEG) is an expert committee of the Department for Environment, Food and Rural Affairs (Defra) and considers current knowledge on air pollution and provides advice on such things as the levels, sources and characteristics of air pollutants in the UK. AQEG reports to Defra's Chief Scientific Adviser, Defra Ministers, Scottish Ministers, the Welsh Government and the Department of Agriculture, Environment and Rural Affairs in Northern Ireland (the Government and devolved administrations). Members of the Group are drawn from those with a proven track record in the fields of air pollution research and practice.

AQEG's functions are to:

- Provide advice to, and work collaboratively with, officials and key office holders in Defra and the devolved administrations, other delivery partners and public bodies, and EU and international technical expert groups;
- Report to Defra's Chief Scientific Adviser (CSA): Chairs of expert committees will meet annually with the CSA, and will provide an annual summary of the work of the Committee to the Science Advisory Council (SAC) for Defra's Annual Report. In exception, matters can be escalated to Ministers;
- Support the CSA as appropriate during emergencies;
- Contribute to developing the air quality evidence base by analysing, interpreting and synthesising evidence;
- Provide judgements on the quality and relevance of the evidence base;
- Suggest priority areas for future work, and advise on Defra's implementation of the air quality evidence plan (or equivalent);
- Give advice on current and future levels, trends, sources and characteristics of air pollutants in the UK;
- Provide independent advice and operate in line with the Government's Principles for Scientific Advice and the Code of Practice for Scientific Advisory Committees (CoPSAC).

Expert Committee Members are independent appointments made through open competition, in line with the Office of the Commissioner for Public Appointments (OCPA) guidelines on best practice for making public appointments. Members are expected to act in accord with the principles of public life.

Further information on AQEG can be found on the Group's website at:
https://www.gov.uk/government/policy-advisory-groups/air-quality-expert-group

Membership

Chair

Professor Alastair Lewis
National Centre for Atmospheric Science, University of York

Members

Dr James Allan
National Centre for Atmospheric Science, University of Manchester

Dr David Carruthers
Cambridge Environmental Research Consultants

Dr David Carslaw
Ricardo Energy and Environment and University of York

Dr Gary Fuller
King's College London

Professor Roy Harrison OBE
University of Birmingham

Professor Mat Heal
University of Edinburgh

Dr Eiko Nemitz
UK Centre for Ecology & Hydrology

Professor Claire Reeves
University of East Anglia

Ad hoc members

Professor David Fowler CBE
Formerly the Centre for Ecology and Hydrology

Dr Ben Marner
Air Quality Consultants

Dr Andrew Williams
University of Chester

Professor Nicola Carslaw
University of York

Ex officio members

Dr Sarah Moller

National Centre for Atmospheric Science, University of York and Senior Research Fellow, Department for Environment, Food and Rural Affairs Systems Research Programme

Central Management and Control Unit of the automatic urban and rural networks: **Dr Richard Maggs**, Bureau Veritas

National Atmospheric Emissions Inventory: **Dr Tim Murrells**, Ricardo Energy and Environment

Non-automatic hydrocarbon monitoring networks and metals monitoring network: **Dr Paul Quincey**, National Physical Laboratory

Quality Assurance and Quality Control of the automatic urban network and the non-automatic monitoring networks: **Dr Paul Willis**, Ricardo Energy and Environment

Assessors and observers

Roger Herbert
Welsh Government

Barry McCauley
Department of Agriculture, Environment and Rural Affairs in Northern Ireland

Andrew Taylor
Scottish Government

Alison Gowers
Public Health England

Secretariat

Shaun Brace
Department for Environment, Food and Rural Affairs

Dr Mohamed Ghalaieny
Department for Environment, Food and Rural Affairs

Michelle Brailey-Balster
Department for Environment, Food and Rural Affairs

Annex B

AQEG Modelling Workshop

Online, 1st February 2021 13:00 – 16:30

Workshop objectives

The workshop will inform the work being carried out by Defra to develop new air quality targets for England. The Air Quality Expert Group (AQEG) is advising Defra on technical aspects of this work including the air quality modelling planned to inform the development. They launched a call for evidence (CfE) to seek input from the wider research community to aid them in providing this advice. This workshop will enable AQEG to gather further information from selected respondents and discuss the overall findings from the CfE and what this means for their advice to Defra.

The workshop attendees will discuss issues relevant to the modelling planned to feed into the targets work in order to ensure (a) the modelling commissioned is as robust as possible under the time/resource constraints and (b) there is a clear understanding of the limitations and uncertainties of modelling so that the outputs are used appropriately.

Workshop attendees: AQEG members, guest researchers selected by AQEG from those who responded to the CfE and Defra and Devolved Administration observers.

Agenda

13:00	Welcome and housekeeping	Ally Lewis, AQEG Chair
13:10	Introduction to the targets and purpose of the workshop, includes summary of the CfE and responses received	Dan Waterman, Defra
13:25	UKIAM – recent changes, comparisons with other models and monitoring, key uncertainties and modelling plans	Helen ApSimon, Imperial College London
13:45	Questions	All
14:00	BREAK	
14:10	CMAQ (10 mins plus 5 mins questions)	Sean Beevers, Imperial College London
14:25	EMEP4UK (10 mins plus 5 mins questions)	Eiko Nemitz, UKCEH
14:40	PCM (10 mins plus 5 mins questions)	John Stedman, Ricardo
14:55	ADMS Urban (10 mins plus 5 mins questions)	David Carruthers, CERC
15:10	BREAK	
15:20	HADGEM3 – impact of climate change on future air quality (10 mins plus 5 mins questions)	Helen Dacre, University of Reading
15:35	CHIMERE (10 mins plus 5 mins questions)	Augustin Colette, INERIS France
15:50	GEOS-Chem (10 mins plus 5 mins questions)	Mat Evans, University of York
16:05	Discussion – (a) the main limitations and uncertainties of AQ modelling, (b) recommendations for Defra’s target work	All
16:25	Summary and next steps	Ally Lewis, AQEG Chair
16:30	CLOSE	