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Evaluating reduced-form modeling tools for simulating ozone and $PM_{2.5}$ monetized health impacts†

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Reduced-form modeling approaches are an increasingly popular way to rapidly estimate air quality and human health impacts related to changes in air pollutant emissions. These approaches reduce computation time by making simplifying assumptions about pollutant source characteristics, transport and chemistry. Two reduced form tools used by the Environmental Protection Agency in recent assessments are source apportionment-based benefit per ton (SA BPT) and source apportionment-based air quality surfaces (SABAQS). In this work, we apply these two reduced form tools to predict changes in ambient summer-season ozone, ambient annual $PM_{2.5}$ component species and monetized health benefits for multiple sector-specific emission control scenarios: on-road mobile, electricity generating units (EGUs), cement kilns, petroleum refineries, and pulp and paper facilities. We then compare results against photochemical grid and standard health model-based estimates. We additionally compare monetized $PM_{2.5}$ health benefits to values derived from three reduced form tools available in the literature: the Intervention Model for Air Pollution (InMAP), Air Pollution Emission Experiments and Policy Analysis (APEEP) version 2 (AP2) and Estimating Air pollution Social Impact Using Regression (EASIUR). Ozone and $PM_{2.5}$ changes derived from SABAQS for EGU scenarios were well-correlated with values obtained from photochemical modeling simulations with spatial correlation coefficients between 0.64 and 0.89 for ozone and between 0.75 and 0.94 for $PM_{2.5}$. SABAQS ambient ozone and $PM_{2.5}$ bias when compared to photochemical modeling predictions varied by emissions scenario: SABAQS $PM_{2.5}$ changes were overpredicted by up to 46% in one scenario and underpredicted by up to 19% in another scenario; SABAQS seasonal ozone changes were overpredicted by 34% to 83%. All tools predicted total $PM_{2.5}$ benefits within a factor of 2 of the full-form predictions consistent with intercomparisons of reduced form tools available in the literature. As reduced form tools evolve, it is important to continue periodic comparison with comprehensive models to identify systematic biases in estimating air pollution impacts and resulting monetized health benefits.

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Environmental significance

Reduced form modeling tools are being increasingly applied in the literature to analyze air quality impacts from policy scenarios as they are quicker and easier to implement than photochemical air quality models. Quantitative evaluation of these tools is necessary so that the scientific community can understand their limitations and uncertainties. We present a new reduced form modeling tool, the Source Apportionment-Based Air Quality Surfaces (SABAQS) method. SABAQS is one of the first reduced form models in the literature to include ozone in addition to $PM_{2.5}$ impacts. We compare SABAQS results against full-form modeling, EPA's latest source apportionment-based benefit per ton (SA BPT) values and 3 other publicly available reduced form tools for multiple emissions control scenarios.

Introduction

Exposure to ozone (O_3) and particulate matter less than 2.5 microns in aerodynamic diameter ($PM_{2.5}$) is known to have negative health impacts on humans.[1–3] O_3 in the troposphere is formed through chemical reactions of precursor pollutants such as nitrogen oxides ($NO_x = NO + NO_2$) and volatile organic

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compounds (VOCs) in the presence of sunlight and can also be transported thousands of miles downwind.[4] Thus, elevated O_3 levels in the US are generally found in locations with abundant precursor emissions and conducive meteorology but levels across the country can be impacted by emissions that occur in upwind regions. $PM_{2.5}$ can be directly emitted into the atmosphere or produced when emissions of precursors such as VOCs, NO_X and sulfur dioxide (SO_2) form $PM_{2.5}$ through chemical and physical processes.[4] The chemical constituents of $PM_{2.5}$ vary across the contiguous US regionally and by season due to seasonal and regional differences in emissions sources, atmospheric chemistry and meteorological conditions.[5–7]

The chemical and physical processes in the atmosphere that convert precursor gases to O_3 and $PM_{2.5}$ are complex.[4] Modeling systems that estimate the change in ambient O_3 and $PM_{2.5}$ due to changing emissions can vary greatly in terms of complexity. The most complex modeling systems are photochemical transport models that use a 3-dimensional Eulerian grid structure to represent emissions, transport, chemical conversion, and deposition.[8] Two photochemical models commonly used to support scientific and regulatory O_3 and $PM_{2.5}$ assessments are the Community Multiscale Air Quality (CMAQ) model[9] (**https://www.epa.gov/cmaq**) and Comprehensive Air Quality Model with Extensions (CAMx; **https://www.camx.com**). Both models have been shown to appropriately replicate the amount and relative proportions of O_3 and chemically speciated $PM_{2.5}$ when compared to ambient measurements.[10,11] Further, these tools have been used to assess O_3 and $PM_{2.5}$ impacts from single sources[12–15] and complex emission control programs including power plant trading programs[16] and motor-vehicle technology implementation.[17]

Since photochemical transport models have a detailed representation of chemistry and physical processes related to formation and transport of O_3 and particles, their application requires computing resources and technical expertise which may not be readily available to some who are interested in understanding how ambient O_3 and $PM_{2.5}$ may be influenced by a change in emissions. As a result, reduced form models have been developed to allow for quick and easy-to-use assessments of summer season O_3 and annual average $PM_{2.5}$ impacts from emission changes and subsequent monetized health impacts. Such models used recently in literature to estimate monetized health benefits of $PM_{2.5}$ include the Intervention Model for Air Pollution (InMAP),[18] Air Pollution Emission Experiments and Policy Analysis (APEEP) versions 2 (AP2),[19] and Estimating Air pollution Social Impact Using Regression (EASIUR).[20] In addition, the EPA has developed estimates of average dollar marginal health benefits for both O_3 and $PM_{2.5}$ per ton of abated emissions from different emissions source categories, known as source apportionment-based benefit-per-ton (SA BPT).[21,22] In this paper we describe a method for creating source apportionment-based air quality surfaces (SABAQS) that has been applied in benefits calculations for recent EPA rules addressing the power sector.[23–26] While the SA BPT and SABAQS methods both provide air quality benefits estimates derived from source apportionment tagging in photochemical modeling simulations, SABAQS produces spatially resolved air quality impacts while SA BPT produces only a national-level dollar value endpoint for emissions from each sector.

While many assessments include monetized health impacts estimated by one or more of these tools,[18,27,28] few compare predicted health impacts from emission control scenarios against photochemical model estimates.[29,30] A comparison of health impacts of specific facilities in Texas between reduced form models (APEEP and EASIUR) and full-form photochemical modeling paired with the Environmental Benefits Mapping and Analysis Program – Community Edition (BenMAP-CE)[31] demonstrated that the error that is introduced when representing how air quality responds to changes in different precursor emissions propagates through to the estimated health benefits.[30] The differences in air quality predictions can affect the size and distribution of the benefits attributed to air quality policies.

In this paper we start by comparing O_3 and $PM_{2.5}$ air quality changes estimated by SABAQS with changes derived from photochemical grid modeling simulations. We then compare O_3 and $PM_{2.5}$ monetized health damages derived from SABAQS to those derived from full-form models. Finally, we compare SABAQS results to O_3 and $PM_{2.5}$ monetized health damages estimated by the SA BPT, InMAP, AP2 and EASIUR. These comparisons were made using different emission control scenarios covering five economic sectors that range in geographic and technologic implementation complexity. The emissions scenarios developed for this assessment provide a framework for future comparisons and could be used to evaluate changes to future iterations of the tools included in this assessment. As reduced form tools evolve, it is important to continue periodic comparison with comprehensive models to identify systematic biases in estimating air pollution and resulting monetized health benefits.

Methods

Each emissions control scenario included a base year, a future year reference case and a future year control case (see Tables 1 and S-1†). The base-year represents emissions and meteorology from a year in the recent past for which ambient measurements are available for both meteorological parameters and air pollutant concentrations. Future year reference cases represent emissions that are expected to occur in the future assuming population growth, changes in energy demand and implementation of current on-the-books regulations but without the impacts of the control scenario evaluated. The future year control scenario (Table S-1†) represents a hypothetical or real policy that would result in emissions changes in one of 5 economic sectors: Electric Generating Units (EGUs) commonly referred to as power plants, mobile sources, cement, pulp & paper, or refineries.

Annual average $PM_{2.5}$ and summer season (May–Sep) average maximum daily 8 h (MDA8) O_3 were estimated for 12 km sized grid cells by CMAQ, CAMx and/or SABAQS for the seven future year reference and control scenarios. Each of these air quality surfaces were then input to BenMAP-CE to estimate

Table 1 Key elements of emissions scenarios including base and future years and reductions between the future reference case and the future control case by pollutant

	Scenario previously documented in Baker *et al.*[32]	Base year (meteorology & emissions)	Future year (base case and sensitivity emissions)	Annual total future-year emission reductions (thousand tons)				
				NO_x	SO_2	$PM_{2.5}$	VOC	NH_3
Mobile (tier 3)	Yes	2007	2030	348	13	9	181	—
EGU (clean power plan proposal)	Yes	2011	2025	424	427	63	10	3
EGU emissions sensitivity A	No	2011	2023	457	701	41	−5	−7
EGU emissions sensitivity B	No	2016	2023/2026	70	107	6	−0.1	−0.4
Pulp & paper	Yes	2011	2025	35	36	7	—	—
Cement kilns	Yes	2011	2025	97	55	13	—	—
Refineries	Yes	2011	2025	35	16	4	—	—

county-specific monetized health impacts. Air quality and health impacts for each scenario are determined as the difference between conditions modeled for the relevant projected future year control and future year reference scenarios. We note that we use both SABAQS and the full-form models to estimate changes in air pollution from hypothetical emissions perturbations. Given the hypothetical nature of these emissions perturbations it is not possible to validate models against measured resulting air pollution changes. While we use CAMx and CMAQ, which include complex representations of physical and chemical atmospheric processes, to ground-truth SABAQS estimates, we acknowledge that CMAQ and CAMx themselves have uncertainties.

Additionally, emissions changes associated with each scenario were used to quantify monetized health impacts associated with $PM_{2.5}$ changes and O_3 changes (where available) using InMAP, AP2, EASIUR and SA BPT. Inputs and outputs for these scenarios are summarized in Table 1 and inputs for 5 of these scenarios are also documented elsewhere.[32–34] Because the SABAQS method has currently only been developed for power sector emissions, the SABAQS estimates were only created for EGU control scenarios.

Description for full-form models

CMAQ and CAMx are both Eulerian photochemical grid models. These models ingest inputs of gridded initial conditions, hourly boundary conditions, gridded hourly meteorological fields and gridded hourly emissions of SO_2, NO_x, ammonia (NH_3), speciated VOCs, speciated $PM_{2.5}$ among other pollutants. The meteorological inputs were generated using the Weather Research and Forecasting (WRF) model.[35] Initial and boundary conditions were extracted from photochemical model simulations applied for larger domains and coarser grid scales.[36] The photochemical models themselves include modules to simulate emissions, atmospheric chemistry, atmospheric transport, particle dynamics and deposition and produce gridded hourly outputs of pollutant (*e.g.*, O_3 and speciated $PM_{2.5}$) concentrations and deposition.

Gridded seasonal or annual average concentrations generated by the photochemical models were used as an input to the BenMAP-CE program[31] for estimating associated health damages. BenMAP-CE applies epidemiologically derived concentration-response functions to estimate and value changes in the incidence of health impacts attributable to air quality, accounting for affected populations and baseline mortality and morbidity incidence within those populations, using the concentration-response function parameterized in eqn (1):

$$\Delta y = y_0(e^{\beta\Delta x} - 1)\text{pop} \quad (1)$$

y_0 is the baseline incidence rate for the health endpoint assessed; pop is the population affected by the change in air quality; Δx is the change in concentration for a specific air pollutant; and β is the effect coefficient linking exposure and health outcome, which is drawn from relevant epidemiological studies. Here, a single mortality concentration-response function[2] was used to estimate the number of premature deaths from annual mean changes in $PM_{2.5}$ with a β coefficient[22] of 0.007045846, and a second mortality concentration-response function[37] was used to estimate the number of premature deaths from summertime mean MDA8 O_3 with a β coefficient[22] of 0.007696104. The population and baseline incidence parameters were held constant across each scenario. Elemental carbon was used as a surrogate for all components of primary $PM_{2.5}$ and used to represent the full amount of primary $PM_{2.5}$ emissions. This was done to remove potential influence of secondarily formed organic aerosol on health damages reported for emission control scenarios modeled with photochemical grid models. Health impacts related to elemental carbon were linearly scaled proportionately to the total amount of primary $PM_{2.5}$ emissions to elemental carbon emissions. The estimated number and economic value of air pollution-attributable deaths and illnesses are subject to sources of uncertainty that we were unable to characterize quantitatively. Key sources of uncertainty include: the projected changes in the number and distribution of individuals exposed to air pollution in the future; the extent to which modeled air quality changes represent a reasonable surrogate for population exposure; the baseline rates of death and disease experienced by these populations; and, future

changes in income, which in turn affect individual willingness to pay to reduce the risk of premature death.

Description for reduced-form models

Developers of multiple reduced form tools provide county level marginal damages for annual $PM_{2.5}$ and provided each as part of an interactive internet site (**https://www.CACES.us/data**). Tools included as part of this repository include InMAP,[18] AP2,[19] and EASIUR.[20] EPA's SA BPT tool estimates benefits at the national scale expected to occur from reducing emissions from specific sectors. This tool accounts for the spatial nature of specific sectors and how emissions from those sectors interact with meteorology and chemistry in those locations. The SA BPT approach quantifies marginal $PM_{2.5}$ [21,38,39] and O_3 [38,40] health damages relative to a fixed amount of precursor emissions.

To develop SA BPT values, source apportionment was used to track the contribution of primarily emitted and precursors to O_3 and $PM_{2.5}$. The source apportionment capabilities within the CAMx model allows the user to tag sources or groups of sources by type and location.[41] The O_3 source apportionment technology (OSAT) within CAMx tracks the impacts of NO_x and VOC emissions through the model physical and chemical processes and outputs hourly gridded O_3 contributions from each user-defined emissions tag for each precursor pollutant. Similarly, the particulate matter source apportionment technology (PSAT) within CAMx tracks the impacts of SO_2, NO_x, and directly emitted PM (*i.e.*, primary PM) to PM species including sulfate, nitrate, organic carbon (OC), elemental carbon (EC), and crustal material. Gridded surfaces of sector-wide O_3 and $PM_{2.5}$ contributions were then applied to estimate total monetized health damages associated with each sector using BenMAP-CE. Finally, the marginal SA BPT health damages were calculated by dividing the sector-wide health damages by the sector-wide precursor emissions. These SA BPT values can then be used to provide estimates of monetized health effects for policy scenarios matching the spatial and temporal scale of the underlying emissions and health damages.[21] In this assessment we focus on the most recent SA BPT values for onroad sources (*e.g.* light-duty gasoline cars and motorcycles, heavy-duty diesel vehicles *etc.*),[39,40] industrial sectors[22] and EGUs.[22] Elemental carbon was used as a surrogate for all components of primary $PM_{2.5}$ and BPT values derived from elemental carbon were applied to total primary $PM_{2.5}$ emissions.

The method for creating SABAQS builds more control into the SA BPT methodology. Both tools leverage results from the source-apportionment instrumented capabilities within the CAMx model. However, while the SA BPT methodology only provides the user with marginal dollar per ton estimates based on total benefits calculated for each sector at a national or regional level, the SABAQS method allows the user to create intermediate air quality surfaces associated with a specified emissions scenario. To accomplish this, SABAQS makes the simplifying assumption that ozone and PM contributions can be linearly scaled based on emissions levels. OSAT separately tracks ozone formed under NO_x and VOC limited conditions (O3N and O3V) so each can be scaled to the relevant precursor. For $PM_{2.5}$, SABAQS makes the assumption that ammonium sulfate $PM_{2.5}$ can be scaled to SO_2 emissions, ammonium nitrate $PM_{2.5}$ can be scaled to NO_x emissions, and that primary OC, EC, and crustal material can all be scaled to total primary $PM_{2.5}$ emissions. SABAQS does not include capabilities for tracking $PM_{2.5}$ impacts from ammonia emissions.

The SABAQS method starts with "fused" surfaces of observed and modeled concentrations for ozone and $PM_{2.5}$ that are derived first by bias-correcting the base-year model predictions for each pollutant using enhanced Voronoi Neighbor Averaging (eVNA)[42–44] and then projecting the fused surfaces into the future by multiplying the base-year eVNA surface by gridded modeled relative response factors between base and future concentrations using EPA's Software for the Modeled Attainment Test – Community Edition (SMAT-CE).[45,46] The source apportionment contributions for each tag are then applied to adjust this future-year fused surface based on emissions changes associated with each tag using eqn (2):

$$C_{g,i} = \mathrm{eVNA_g} \times \left(\sum_{t=1}^{T} \frac{C_{g,t}\, S_{t,i}}{C_{g,\mathrm{Tot}}} + \right) \quad (2)$$

where:

- $C_{g,i}$ is the estimated fused model-observation concentration in grid-cell, "*g*", for emissions scenario, "*i*". For ozone, $C_{g,i}$ is calculated as the summer season average of MDA8 (ppb) while for $PM_{2.5}$, $C_{g,i}$ is the annual average concentration and is separately calculated for each $PM_{2.5}$ component species (*i.e.*, sulfate, nitrate, EC, *etc.*) ($\mu g\ m^{-3}$);
- $eVNA_g$ is the eVNA future year fused model obs concentration in grid-cell "g" in ppb and $\mu g\ m^{-3}$ for summer season ozone and annual average PM species concentrations respectively;
- $C_{g,\mathrm{Tot}}$ is the total modeled concentration in grid-cell "g" from all sources in the source apportionment modeling in ppb and $\mu g\ m^{-3}$ for summer season ozone and annual average PM species concentrations respectively;
- $C_{g,t}$ is the modeled source apportionment contribution in grid-cell, "g", from source apportionment tag, "*t*", in ppb and $\mu g\ m^{-3}$ for summer season ozone and annual average PM species concentrations respectively;
- $S_{t,i}$ is the EGU scaling ratio for emissions tag, "*t*" and scenario "*i*". For each pollutant, $S_{t,i}$ is calculated as the ratio of emissions associated with the tag, "*t*", in emissions scenario, "*i*", to emissions associated with tag, "*t*", in the modeled source apportionment case (*i.e.* 2023en and 2026fj cases from Table S-1†). Emissions used to calculate $S_{t,i}$ for each pollutant are provided in Table 2. $S_{t,i}$ is set to 1 for any source tags whose emissions are unchanged included the tag for from boundary condition contribution (*i.e.*, ozone or $PM_{2.5}$ transported into the modeling domain).

For ozone the $C_{g,i}$ values for O3N and O3V are added together to create a gridded surface of total summer-season MDA8 ozone associated with emissions scenario, *i*. For $PM_{2.5}$, the $C_{g,i}$ values for sulfate, nitrate, primary OC, EC and crustal material are added to unaltered bulk secondary organic aerosol (SOA)

Table 2 Description of emissions used for scaling ratio calculation for each pollutant

Pollutant	Emissions used to calculate $S_{t,i}$ (tons)
O3N	Ozone season (May–Sep) NO_x
O3V	Ozone season (May–Sep) VOC
Sulfate	Annual SO_2
Nitrate	Annual NO_x
Primary OC, EC and crustal PM	Annual primary $PM_{2.5}$

concentrations along with particulate ammonium and particulate water mass that are calculated based on degree of neutralization of nitrate in the base year and on nitrate and sulfate concentrations calculated for emissions scenario *i* using standard equations in SMAT-CE.[45,46]

Emissions scenarios

Five of the seven emissions scenarios used to support this assessment are described in more detail elsewhere.[32] Annual total nationally aggregated emission changes by pollutant for each scenario relative to the projected future year reference scenario are provided in Table 1.

One scenario from the Clean Power Plan Proposal (CPPP)[47] was used to represent a complex change in EGU emissions due to a trading program and changes to electricity dispatch. This scenario used the base year of 2011 and a future projection reference year of 2025.

Two additional EGU scenarios were created in order to further test the SABAQS method using the available EGU source tagging. Both EGU scenarios used a future reference year of 2023 projected from the 2016v2 emissions modeling platform.[34] In the first EGU "control" scenario, emissions perturbations in the sector were achieved by using an alternate older projection of 2023 emissions based on the 2011v3 emissions modeling platform[33] as the reference case and the newer 2023 EGU projection as the control case. This scenario will be referred to as EGU emissions sensitivity A. In the second ECU "control" scenario, emissions perturbations in the sector were achieved by swapping in projections of the EGU emissions out to 2026 reflecting impacts expected to occur in the sector over a 3 year period. This scenario will be referred to as EGU emissions sensitivity B.

Scenarios for four additional economic sectors were included to provide complex test cases with spatially and temporally heterogenous changes in multiple pollutants for the InMAP, AP2, EASIUR and SA BPT tools. The Tier 3 Motor Vehicle Emission and Fuel Standards Final Rule (Tier 3)[17] was selected as a mobile scenario. This scenario used a base year of 2007 and a future projection reference year of 2030. The cement kiln, refinery, and pulp & paper sector scenarios all used the base and future projection reference year from the CPPP cases. The control scenarios for these 3 sectors were generic hypothetical changes which applied across-the-board emissions reductions.[32]

Estimating air quality and monetized health benefits

Photochemical grid models were used to predict the change in annual average $PM_{2.5}$ and seasonal average MDA8 ozone for multiple complex emissions scenarios for EGUs, industrial sectors, and the onroad mobile sector. The base-year air quality surfaces for the photochemical model simulations of these emission control scenarios were modulated to match ambient data. Then, changes in air quality were derived from future year projections of emissions and separate simulations for alternative future year projected emissions that represented a change due to a specific emission control scenario. The difference between these annual photochemical model simulations represents the air quality impacts of the emission control scenario (Table S-1†). More details about photochemical model configuration and application are provided in the ESI Section.†

SABAQS was applied for the EGU emissions scenarios using state level changes in precursor emissions from EGU sources to estimate annual average $PM_{2.5}$ and seasonal average MDA8 ozone for the future year reference and control scenarios. In other words, impacts to ozone and $PM_{2.5}$ were separately tracked from EGU emissions in each state. Two different sets of state level EGU source apportionment were used with SABAQS. One was based on 2011 meteorology and projected 2023 EGU emissions ("2023en") and the other 2016 meteorology and projected 2026 EGU emissions ("2026fj"). More specifics about the SABAQS configuration and application are available in the ESI Section.†

BenMAP-CE was used to estimate monetized human health benefits for each air quality scenario simulated by the photochemical models and SABAQS. The difference between predicted future year reference and future year control simulations was used to represent the impact of the emissions control scenario.

National monetized health benefits for SA BPT were calculated by multiplying the aggregated emissions changes (Table 1) by sector and pollutant-specific BPT values. Health benefits were estimated using sector-specific BPT values for EGUs,[22] industrial sectors,[22] and mobile emissions.[39] $PM_{2.5}$ health benefits based on changes in emissions of NO_x, SO_2, and primary $PM_{2.5}$ were calculated for all sectors. Health benefits based on NO_x and VOC emissions for seasonal ozone were estimated only for industrial and EGU scenarios because ozone SA BPT values have not been developed for mobile sources.

We additionally predict health impacts of annual average $PM_{2.5}$ concentrations from three publicly reduced form models: InMAP,[18] EASIUR,[20,48] and AP2 (ref. 19) to provide context for SA BPT and SABAQS performance. Each of these tools were applied with county level precursor emissions changes applied to county specific marginal damages provided by the model developers. The data were obtained from the Center for Air, Climate, and Energy Solutions (**https://www.caces.us/data**) in february 2022 and reflect the version of those tools at that time. Health effects based on InMAP, EASIUR, and AP2 were selected for the American Cancer Society C-R function using a VSL of $11.3 M based on a 2025 future year (EGU and industrial sector scenarios) and of $11.6 M based on a 2030 future

year (mobile scenario) and a 2019 currency year.[22] The ground level values were used for the Tier 3 scenario and elevated stack values were used for the other scenarios.

Results & discussion

SABAQS air quality predictions

We start by comparing SABAQS predictions to full-form CAMx predictions of ozone and speciated $PM_{2.5}$ impacts for the CPPP case. For this comparison SABAQS used the 2023en source apportionment modeling dataset. Table 3 provides mean change in air quality concentrations averaged across all 12 km land-based contiguous US grid cells in CAMx and SABAQS. In addition, mean bias (MB), normalized mean bias (NMB), and spatial correlation (r) are calculated as described in ref. 11. Here a negative NMB indicates that SABAQS predicts a larger impact from CPPP than CAMx and a positive NMB indicates that SABAQS predicts a smaller impact from CPP than CAMx. For CAMx and SABAQS, primary PM is calculated as the sum of elemental carbon and crustal components. All statistics are calculated based on grid cells covering contiguous US land locations (*i.e.* excluding grid cells outsides of the US or over purely water grid cells).

First, we note that CAMx predicted domain-wide impacts of the CPPP scenario of around 0.3 ppb for seasonal MDA8 ozone and approximately 0.1 μg m^{-3} for annual average $PM_{2.5}$. Normalized mean bias for SABAQS is quite low for nitrate (7.0%) and primary $PM_{2.5}$ (9.2%). SABAQS NMB is higher for sulfate and ozone at −49.4% and −79.3% indicating that SABAQS shows a larger magnitude of impact from CPPP on these two pollutants than CAMx. As can be seen in the spatial correlation numbers between 0.55 and 0.97, SABAQS replicates the spatial patterns of ozone and $PM_{2.5}$ quite well. Spatial patterns predicted by CAMx and SABAQS and the differences between those surfaces are shown in Fig. 1–5 for each pollutant. Spatial patterns for secondary pollutants that form through chemical reactions in the atmosphere (*i.e.*, ozone, sulfate, and nitrate) are all above 0.85. Fig. 1 shows that ozone impacts from both CAMx and SABAQS are most pronounced in areas of the southern US, specifically emanating from modeled power plant locations in Texas, Arkansas, Mississippi, Alabama, Georgia and North Carolina. Fig. 2 shows that both CAMx and SABAQS predict nitrate reductions in the midwestern US and in the San Joaquin Valley of California, two areas of the country where ambient nitrate concentrations tend to be large. SABAQS somewhat underpredicts the magnitude impact of CPPP on nitrate compared to CAMx, especially in California. While we do not explicitly assess causes of SABAQS biases in this analysis, it is possible that some of the nitrate biases in San Joaquin Valley may result from the fact that SABAQS method does not include nonlinear chemistry impacts from ammonia emissions. Despite this limitation of scaling nitrate impacts linearly to NO_x emissions, national nitrate biases are relatively small. Fig. 4 shows that sulfate impacts from both CAMx and SABAQS also appear to be regional, covering much of the southern US from Texas eastward. The spatial correlation for primary PM is somewhat

Table 3 Comparison of ambient pollutant changes predicted by SABAQS and CAMx for the EGU control scenarios

Pollutant	Scenario	Mean impact: SABAQS (μg m^{-3} or ppb)	Mean impact: CAMx (μg m^{-3} or ppb)	MB[a] (μg m^{-3} or ppb)	NMB[a] (%)	r
Primary PM[b]	CPPP: 2023en	−0.010	−0.009	−0.001	−9.2%	0.54
	CPPP: 2026fj	−0.005	−0.009	0.004	43.7%	0.43
	EGU emissions sensitivity A	−0.005	−0.027	0.0219	80.9%	0.75
	EGU emissions sensitivity B	−0.001	−0.001	8.8×10^{-5}	12.3%	0.72
Nitrate	CPPP: 2023en	−0.006	−0.007	0.0005	7.0%	0.94
	CPPP: 2026fj	−0.007	−0.007	0.0001	1.5%	0.77
	EGU emissions sensitivity A	−0.006	−0.007	0.0006	9.2%	0.84
	EGU emissions sensitivity B	−0.001	−0.002	−0.0006	−45%	0.78
Sulfate	CPPP: 2023en	−0.099	−0.067	−0.0329	−49.4%	0.97
	CPPP: 2026fj	−0.101	−0.067	−0.0347	−52.0	0.88
	EGU emissions sensitivity A	−0.139	−0.121	−0.0185	−15.3%	0.96
	EGU emissions sensitivity B	−0.024	−0.022	−0.0019	−8.4%	0.96
Total PM[c]	CPPP: 2023en	−0.119	−0.0866	−0.0323	−37.3%	0.94
	CPPP: 2026fj	−0.127	−0.0866	−0.0399	−46.0%	0.86
	EGU emissions sensitivity A	−0.152	−0.159	0.0075	4.7%	0.94
	EGU emissions sensitivity B	−0.028	−0.023	−0.0046	−19.6%	0.75
Ozone	CPPP: 2023en	−0.557	−0.311	−0.246	−79.3%	0.88
	CPPP: 2026fj	−0.570	−0.311	−0.259	−83.2%	0.81
	EGU emissions sensitivity A	−0.502	−0.374	−0.128	−34.3%	0.89
	EGU emissions sensitivity B	−0.068	−0.047	−0.021	−44.6%	0.64

[a] For negative impacts (*i.e.*, decreases in ozone or $PM_{2.5}$ in the emissions scenario) negative bias and normalized mean bias values indicate that SABAQS predicts a larger magnitude impact than CAMx and positive bias and normalized mean bias values indicates that SABAQS predicts a smaller magnitude impact than CAMx. [b] Primary PM defined as elemental carbon + crustal material for the purpose of this comparison. [c] Total PM includes ammonium nitrate, ammonium sulfate, elemental carbon, crustal material and organic carbon. Organic carbon comparisons not made between SABAQS and CAMx because SABAQS organic carbon impacts only account for changes in primary organic carbon while CAMx organic carbon impacts account for changes in both primary and secondary organic carbon.

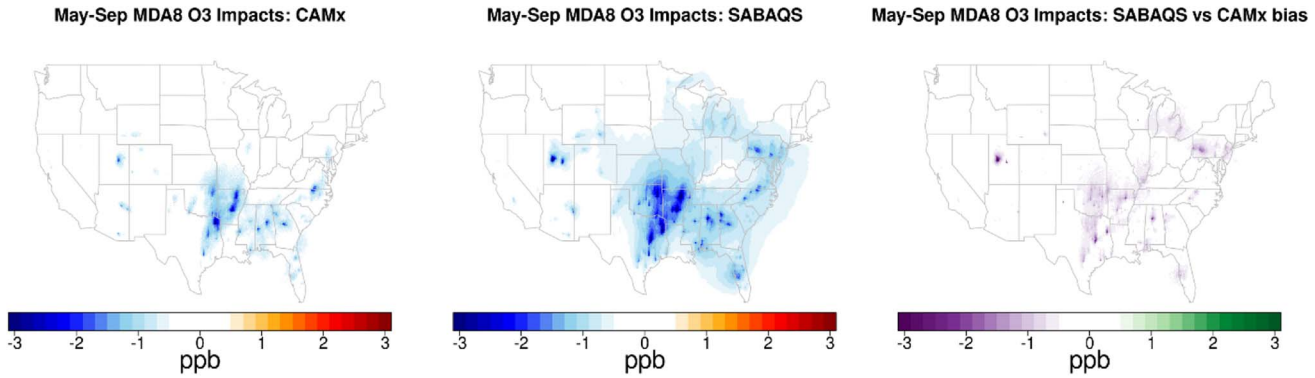

Fig. 1 Comparison of CAMx and 2023en-based SABAQS estimates of CPPP impacts on May–Sep MDA8 ozone. CAMx estimates shown on the left, SABAQS estimates shown in the middle and the difference between the two surfaces shown on the right with purple colors indicating a larger impact from SABAQS and green colors indicating a larger impact from CAMx.

lower due to the very local nature of primary PM impacts to the sources. Therefore, in states that are large in area and may include multiple sources throughout the state, full-form models can capture impacts of spatially heterogeneous primary PM emissions changes within the state while SABAQS is constrained to the spatial resolution of the underlying source apportionment tags (in this case state or multistate groupings). This is evident in Fig. 3 which shows CAMx and SABAQS estimates of primary PM impacts are concentrated in the same states (AZ, TX, AL, MS, GA and FL). However, within states like AZ, TX and GA it is evident that some individual EGU plant locations show larger impacts in CAMx while others show larger impacts in SABAQS. Presumably, a SABAQS simulation that tracked emissions from these EGU plants in separate tags would be able to better capture this within-state spatial impacts from primary PM. A sensitivity analysis that applied SABAQS using the 2026fj source apportionment dataset derived from a 2016 base year somewhat degraded agreement with the 2011-based CAMx modeling (Table 3 and Fig. S1–S5†). This analysis does not provide sufficient information to determine how much differing underlying meteorology *versus* emissions years between SABAQS and CAMx impacted these results.

Results from EGU emissions sensitivity A and EGU emissions sensitivity B are provided in Table 3 and Fig. S6–S15.† In contrast to the CPPP case, SABAQS produces sulfate and ozone surfaces with much lower magnitude of bias in the two EGU emissions sensitivities. Sulfate NMB was 15.3% and 8.4% for EGU emissions sensitivity A and EGU emissions sensitivity B respectively. Ozone NMB was 34.3% and 44.6% for EGU emissions sensitivity A and EGU emissions sensitivity B respectively. This shows that the overstatement of sulfate and O_3 response for the CPPP scenario is specific to that case and that the SABAQS methodology can match CAMx modeled sulfate and ozone surfaces more closely depending on the particular emissions scenario being estimated. For nitrate and primary $PM_{2.5}$ the two EGU emissions sensitivities have mixed results, with EGU emissions sensitivity A having relatively small nitrate bias (NMB = −9.2%) and relatively large primary $PM_{2.5}$ bias (NMB = −80.9%) and EGU emissions sensitivity B having relatively large nitrate bias (NMB = −45.0%) and relatively small primary $PM_{2.5}$ bias (NMB = −12.3%).

The four EGU scenarios provided here show that the SABAQS method reasonably captures the spatial patterns of changing ozone and $PM_{2.5}$ components in response to EGU emissions

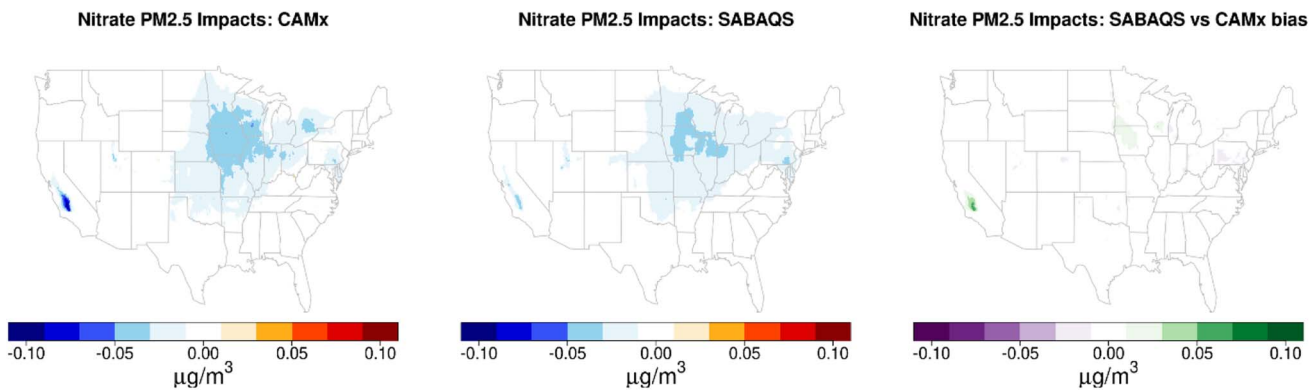

Fig. 2 Comparison of CAMx and 2023en-based SABAQS estimates of CPPP impacts on annual average $PM_{2.5}$ nitrate. CAMx estimates shown on the left, SABAQS estimates shown in the middle and the difference between the two surfaces shown on the right with purple colors indicating a larger impact from SABAQS and green colors indicating a larger impact from CAMx.

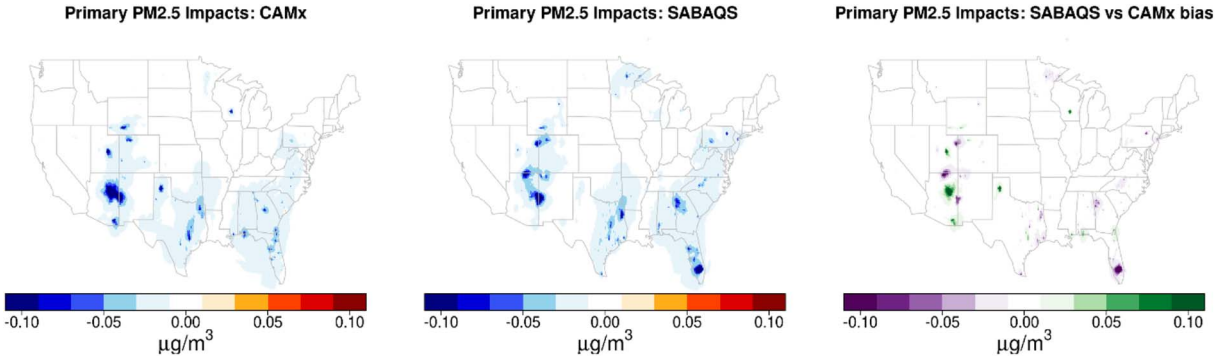

Fig. 3 Comparison of CAMx and 2023en-based SABAQS estimates of CPPP impacts on annual average primary $PM_{2.5}$ (EC and crustal material). CAMx estimates shown on the left, SABAQS estimates shown in the middle and the difference between the two surfaces shown on the right with purple colors indicating a larger impact from SABAQS and green colors indicating a larger impact from CAMx.

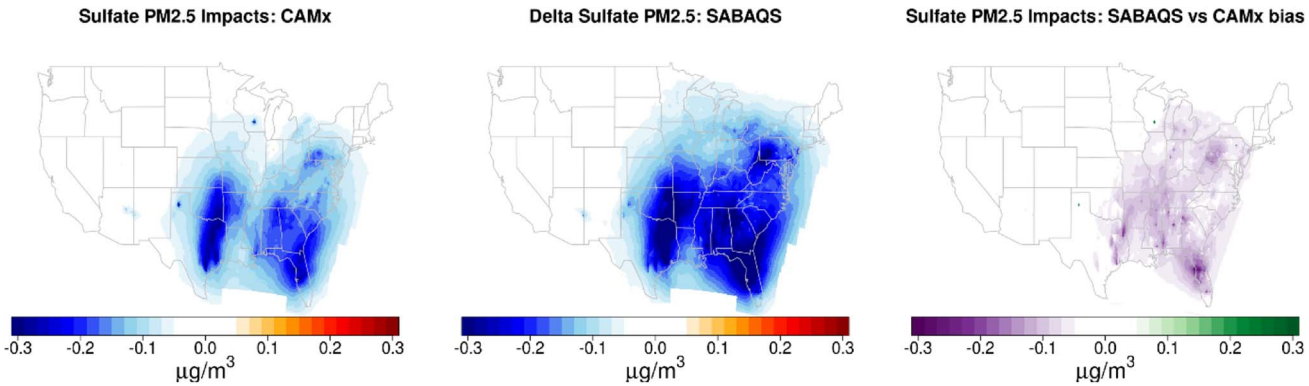

Fig. 4 Comparison of CAMx and 2023en-based SABAQS estimates of CPPP impacts on annual average $PM_{2.5}$ sulfate. CAMx estimates shown on the left, SABAQS estimates shown in the middle and the difference between the two surfaces shown on the right with purple colors indicating a larger impact from SABAQS and green colors indicating a larger impact from CAMx.

changes and provides a measure of the uncertainty of predictions for total annual $PM_{2.5}$ ranging from a 19.6% underestimate of the response to a 46% overestimate of the response and predictions of seasonal ozone ranging from a 34.3% to an 83.2% overestimate of the response.

Monetized health benefit comparison

The estimated economic value of air quality changes provides a common metric that may be used to compare the performance of each tool. Table 4 provides a comparison of ozone and speciated $PM_{2.5}$ health impacts derived from the SABAQS air quality surfaces in comparison to those derived from the full-form modeling tools using brute force emissions changes (Table S-1†). For the CPPP scenario, full-form $PM_{2.5}$ results were derived from two separate photochemical models: CMAQ and CAMx. The total $PM_{2.5}$ health benefits from the two full-form models were within 20% of each other with very similar predictions of nitrate and sulfate contributions but somewhat diverging predictions of primary $PM_{2.5}$ contributions. The underlying level of uncertainty in full-form models provides important context when comparing against reduced form estimates.

The comparison between monetized health benefits derived from SABAQS air quality to that derived from full-form air quality mirrors the performance of the underlying air quality predictions. SABAQS health benefits associated with $PM_{2.5}$ formed from NO_x emissions closely matches those derived from the full form models for all EGU scenarios. $PM_{2.5}$ health impacts from SO_2 emissions are substantially overpredicted by SABAQS for the CPPP scenario but match the full-form model derived estimates more closely for EGU sensitivity A and EGU sensitivity B. In contrast the health impacts associated with direct PM emissions for SABAQS fell between the estimates from the two full-from models for the CPP scenario but were underpredicted for EGU sensitivity A and EGU sensitivity B. Overall, SABAQ total $PM_{2.5}$ benefits for the CPPP scenarios were overpredicted by 44% or 70% depending on which full-form model was used and were overpredicted by 29% and 6% for EGU sensitivity A and EGU sensitivity B respectively. As described previously, SABAQS overpredicted the ozone air quality response to the EGU scenarios compared to the full-form models. When translated to benefits, SABAQS predicted higher ozone-related health benefits compared to the full-form approach by about 60% in EGU sensitivity A and B and by about a factor of 2 for the CPP proposal scenario.

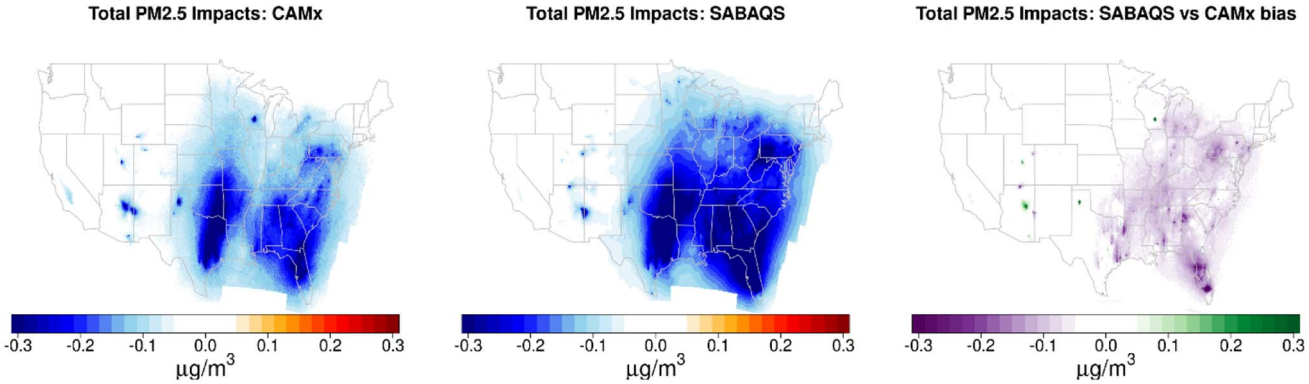

Fig. 5 Comparison of CAMx and 2023en-based SABAQS estimates of CPPP impacts on annual average total $PM_{2.5}$ (nitrate plus primary $PM_{2.5}$ plus sulfate). CAMx estimates shown on the left, SABAQS estimates shown in the middle and the difference between the two surfaces shown on the right with purple colors indicating a larger impact from SABAQS and green colors indicating a larger impact from CAMx.

Table 4 SABAQS-based monetized ozone and $PM_{2.5}$ health impacts (2019$ billion) for each EGU emissions scenario. $PM_{2.5}$ impacts are provided for speciated components of $PM_{2.5}$ (nitrate from NO_x, sulfate from SO_2, and primary $PM_{2.5}$) and the sum of speciated components (total $PM_{2.5}$). Benefits derived from full-form modeling simulations are shown in bold

			$PM_{2.5}$			
Scenario	Model	Ozone	NO_x	SO_2	Primary $PM_{2.5}$	Total $PM_{2.5}$
CPPP	**CMAQ/BenMAP**	—	**1.7**	**15.4**	**5.7**	**22.8**
	CAMx/BenMAP	**9.1**	**1.4**	**15.6**	**2.3**	**19.3**
	SABAQS/BenMAP[a]	18.3	1.7	27.5	3.7	32.9
EGU sensitivity A	**CAMx/BenMAP**	**11.4**	**1.7**	**32.3**	**4.2**	**41.0**
	SABAQS/BenMAP	18.2	1.8	39.5	1.2	43.3
EGU sensitivity B	**CAMx/BenMAP**	**1.2**	**0.3**	**5.0**	**0.2**	**5.2**
	SABAQS/BenMAP	1.9	0.5	5.9	0.1	6.7

[a] SABAQS results based on the CPPP: 2023en.

Next, we provide context for the SABAQS health impacts comparison by providing similar comparisons for the other four reduced form tools: SA BPT, InMAP, AP2, and EASIUR. Table S-2† and Fig. 6 show the monetized health impacts associated with $PM_{2.5}$ estimated by both photochemical grid models and reduced form tools for multiple emission control scenarios. For the EGU scenarios, the SABAQS estimates and the SA BPT estimates are based on the same underlying source apportionment modeling so differences between the two estimates are largely driven by the fact that SA BPT estimates are calculated by multiplying national emissions changes with a national SA BPT value for the EGU sector while the SABAQS estimates in this work account for state-level relationships between emissions and air quality impacts. Fidelity to the full-form predictions varied across tools, scenarios and $PM_{2.5}$ precursors. All tools predicted total $PM_{2.5}$ benefits within a factor of 2 of the full-form predictions consistent with intercomparison of reduced form tools presented elsewhere.[30,49] Many of the tools performed substantially better than a factor of 2 for some or all of the emissions scenarios. For instance, AP2, EASIUR and SABAQS all predicted total $PM_{2.5}$ benefits within ±50% of the full-form predictions for all scenarios, while InMAP and SA BPT predicted total $PM_{2.5}$ benefits within ±50% for 6 out of 7 scenarios and 4 out of 7 scenarios respectively. Performance for individual precursors was more variable. All reduced form tools predicted larger $PM_{2.5}$ nitrate impacts than the full-form approach but some tended to have less severe overpredictions (AP2 and SABAQS) while others tended to have more severe overpredictions (INMAP and EASIUR). SA BPT nitrate performance varied by emissions scenario. For $PM_{2.5}$ sulfate the direction of the bias in reduced form tool predictions varied by scenario for INMAP, AP2, EASIUR and SA BPT which all had underpredictions for some scenarios and overpredictions for others. In contrast, SABAQS tended to overpredict $PM_{2.5}$ sulfate benefits. For primary $PM_{2.5}$ the direction of the bias in reduced form tool predictions also varied by scenario for INMAP, EASIUR and SA BPT. In contrast, SABAQS tended to underpredict primary PM2.5 benefits.

Monetized health impacts related to changes in O_3 were only available for the full-form approach, SA BPT (EGUs and industrial sector scenarios) and SABAQS (EGU scenarios only). These comparisons are shown in Table S-3† and Fig. 7. The somewhat worse performance of SA BPT for EGU scenario ozone benefits compared to SABAQS is likely due to the national nature of the SA BPT calculation compared to the more spatially refined state-level information incorporated into the SABAQS calculations.

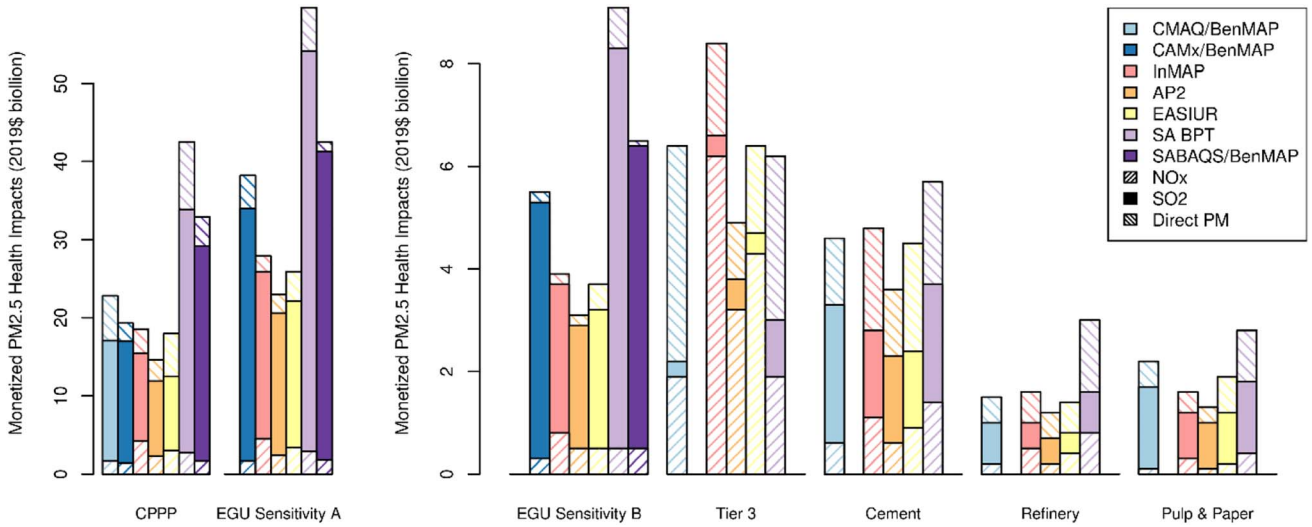

Fig. 6 Monetized $PM_{2.5}$ health impacts (2019$ billion) for each emissions scenario. Impacts are provided for speciated components of $PM_{2.5}$ (ammonium nitrate from NO_x, ammonium sulfate from SO_2, and directly emitted $PM_{2.5}$). SA BPT values for the Tier 3 scenario are based on the smallest eastern US BPT value (for Light duty class vehicles) from Table 2 of ref. 39.

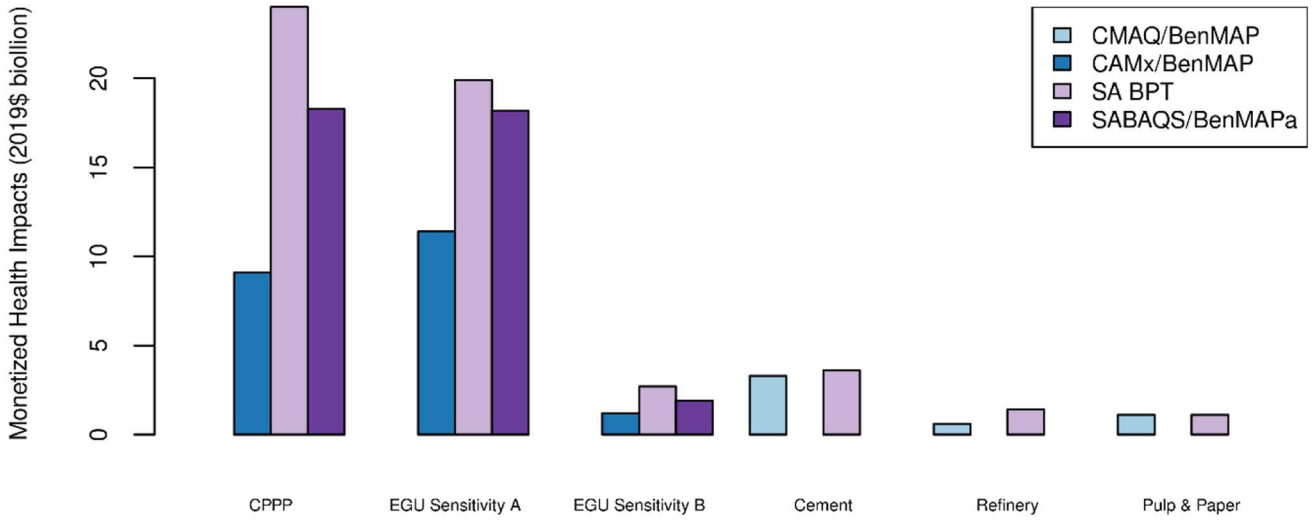

Fig. 7 Monetized ozone health impacts (2019$ billion) for each emissions scenario.

Predicted ozone-related health impacts from SA BPT were similar for the pulp and paper and cement kiln sector scenarios but different by more than a factor of 2 for the refinery sector scenario. The difference for the refinery sector was related to seasonal average MDA8 O_3 decreases in the Los Angeles area predicted by the photochemical grid model due to O_3 destruction reactions from NO_x outpacing O_3 formation reactions from NO_x compared to the benefit per ton approach that is based on source apportionment which was not designed to take this type of nonlinear O_3 response to emissions precursors into account. These processes were less impactful for the pulp and paper and cement kiln sectors because these facilities are usually located outside large urban areas where O_3 formation is usually limited by NO_x emissions rather than urban core areas that can be VOC limited.

Conclusions

Moneteized benefits derived from SABAQS and from SA BPT have a common set of limitations. First, the air quality changes and resulting health benefits are tied to the underlying representation of sources in the modeling. Therefore, these reduced form methodologies will more closely replicate full-form modeling estimates when the underlying representation of emissions sources are similar. Conversely, if the emissions inventories feeding the SABAQS or SA BPT values are outdated, then any changes in the spatial allocation of emissions sources and their proximity to population centers will impact the ability of these tools to predict benefits from emissions control scenarios. It is therefore important to periodically update the emissions used to derive both the SABAQS input dataset and the

SA BPT values as the magnitude and location of emissions sources evolve. Next, the set-up of the source apportionment tags is an important consideration when applying SABAQS or SA BPT to estimate impacts of any particular emissions scenario. In this work, the SABAQS EGU emissions scenarios relied on state-level tagging of EGU sources. SABAQS and SA BPT results that used tags with more or less specificity (in terms of source characteristics or spatial scales) would likely result in impacts that more or less closely resemble the estimates from a full-form model. Therefore, in applying these techniques it is important to design source apportionment simulations that appropriately group emissions sources for the scenario being evaluated. Anyone applying SABAQS to assess air quality benefits of local, regional, or national air quality policies needs to carefully design source apportionment tags to appropriately replicate the types of policies being assessed. Additionally, these methods rely on modeling that simulates air quality response under meteorological conditions that occurred in a single year. Since meteorology impacts how pollutants are dispersed as well as the chemical and physical processes that impact secondary pollutant formation, the methods rely on an annual simulation to adequately capture the typical range of meteorological conditions that influence air pollutant formation and transport. The meteorology in any particular year may differ from the meteorology originally modeled in the apportionment modeling, thus adding uncertainty to the generalization of the impacts estimated with these methods. A sensitivity analysis conducted in this work found that national SABAQS results were fairly robust even when using a different meteorological year from the underlying full-form modeling. Finally, both methodologies treat the relationship between emissions and air quality impacts as linear and additive. This approximation is a simplification of many complex atmospheric processes but does a reasonable job of creating a first-order approximation of air quality changes and associated benefits as shown by the results in this comparison.

Here we have compared air quality and health estimates derived from various reduced form tools to that of full-form photochemical air quality models, to determine how comparable results are and which tools may be best used for regulatory analyses that do not permit full-form analyses. Specifically, we evaluated ambient summer-season ozone, ambient annual $PM_{2.5}$ and its components, and monetized health benefit estimates from several reduced form tools for a variety of sector-specific emission control scenarios. Performance of reduced-form models varied by tool, pollutant, and emissions scenario. The SA BPT tool is generally suitable for use in applications examining impacts of emissions reductions that are similar in magnitude and geographic scope to those used to derive the SA BPT relationships. We caution that SA BPT cannot capture ozone disbenefits in locations that are highly VOC limited so should not be used to replicate ozone impacts of NO_x emissions changes for sources predominantly located in locations known to be VOC limited. The SABAQS method was able to replicate spatial patterns of ozone and PM impacts from EGU emissions scenarios with correlation coefficients ranging from 0.64–0.89 for ozone and 0.75–0.94 for total $PM_{2.5}$. SABAQS overpredicted ozone health benefits but more closely captured $PM_{2.5}$ health benefits from the EGU scenarios. We conclude that SABAQS is a reliable reduced form tool to use in EGU or other similar stationary source regulatory analyses in which full-form analyses are not feasible. Overall, both SA BPT and SABAQS predict monetized health impacts similarly to other reduced form models available in the literature.

Disclaimer

The views expressed in this article are those of the authors and do not necessarily represent the views or policies of the US Environmental Protection Agency.

Author contributions

Conceptualization: GM, HR, HS, KRB, MZ, NF, SLP; data curation: EC, GM, HR, JB, KRB, MA, MZ, SLP; formal analysis: HR, HS, JB, JS, KRB, MA, SLP; funding acquisition: CJ; investigation: CJ, GM, HR, HS, JB, KRB, MA, NF, SLP; methodology: CJ, EC, HR, HS, JB, KRB, MA, SLP; project administration: CJ, EC, HR; software: CJ, HR, KRB, NF; supervision: HR, MA, SLP; validation: CJ, HR, HS, JB, JS, MA, SLP; visualization: CJ, HS, JS, KRB, MA; writing – original draft: EC, HS, KRB; writing – review & editing: EC, HS, JS, KRB, MZ, NF, SLP.

Conflicts of interest

There are no conflicts to declare.

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