## Bridging Existing Energy and Chemical Transport Models to Enhance Air Quality Policy Assessment

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#### Abstract

Connecting changes in emissions to air quality is critical for evaluating the effects of a specific policy. Here, we introduce a methodology to aid in assessing the air quality impacts of changes in the energy system. A set of widely varying scenarios that describe alternative potential evolutions of the US energy system is constructed using the TIMES energy system model. For each scenario, an R script is used to communicate future emissions changes to the CMAQ photochemical air quality model. Example results are shown, and the development of the TIMES scenarios is described for users who wish to adapt them to alternate geographies. Possible use cases include evaluating the air quality effects of specific emissions reduction measures or of broad changes to dominant technologies in major sectors such as transportation.



#### Keywords

air quality; scenario planning; grow-in-place; model integration

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#### **Highlights**

- Divergent scenarios enable robust modeling of the energy system under uncertainty
- Emissions changes from energy scenarios linked to modeling air quality impacts
- New features simplify robust and traceable energy-atmospheric modeling

Name of software or dataset	BRIDGE Basic Regional Interpolation to Distribute Growing Emissions	Divergent Scenarios	TIMES The Integrated MarkAI-EFOM System	EPA US9rT US nine region database for Times	CMAQ Community Multiscale Air Quality Model	<b>NEI</b> National Emissions Inventory
Developer and contact info	Kristen Brown; Kristen.Brown2 @utsa.edu	Kristen Brown; <u>Kristen.brown2</u> @utsa.edu	Gary Goldstein: <u>DecisionWare.</u> <u>NY@gmail.com</u>	US EPA ORD Kristen.Brown2 @utsa.edu	US EPA ORD https://epa.gov/ cmaq	US EPA https://gispub.e pa.gov/neirepor t/2017/
First available	2023	2020	2008	2020	2003	2020
Hardware required	Architecture independent	Architecture independent		Architecture independent	High- performance computing cluster	Architecture independent
Software required	R	TIMES	CPLEX, VEDA, Windows	TIMES	Linux; VERDI, netCDF,	
Availability	https://github.c om/Kris10Brow n/BRIDGE_TIM ES_to_CMAQ	https://github.c om/Kris10Brow n/TimesDiverg entScenarios	https://zenodo. org/record/466 0551		https://github.c om/USEPA/CM AQ	https://www.ep a.gov/air- emissions- inventories/201 7-national- emissions- inventory-nei- data
Cost	free	Free	Free* (requires purchase of solvers)	free	free/open source	free
Language	R		GAMS		Fortran	
Repository format & size		5Mb Excel		64Mb Excel		400 Mb zip

#### Software and data availability

#### 1. Introduction

While air quality has improved over recent decades in much of the world, air pollution remains an important public health problem, even in developed countries. Air quality management plans in the United States have historically considered only the near future (<10 years). This practice began when the most common mechanisms for emissions reductions were incremental changes in industrial processes or the adoption of end-of-pipe controls or other technologies that could be retrofitted onto existing infrastructure. Additionally, pressure is building globally to reduce emissions of greenhouse gases (GHGs). Transformative shifts toward cleaner forms of energy with net-zero GHG emissions would lead to significant reductions in air pollutant emissions, but will require decades to implement due to the significant expense and long lifetime of energy and transportation system infrastructure (Amann et al., 2011; NASEM, 2021). One challenge for long-term air quality planning is the complex and nonlinear relationship between the emissions associated with the built environment and energy system infrastructure and the resulting consequences for air pollution and human health.

The disconnect between emissions and ambient air concentrations is fundamental to environmental policy considerations. Emissions are the factor that society can control, but the resulting ambient concentrations of pollutants are what affect human health. Due to the complexities of atmospheric transport and the nonlinear chemical reactions associated with pollutant formation, there is often not a proportional relationship between emissions and concentrations, necessitating the use of computationally intensive simulations to assess the impact of potential control strategies. Several models are available to calculate future emissions and many models exist that predict air quality given emissions inputs, but these models have typically not been used in a linked fashion. Some of these models have focused on creating detailed representations of the emissions associated with specific scenarios or environmental regulations (Amann et al., 2011; Elobeid et al., 2013; Kaplan & Witt, 2019; Shi et al., 2017; Timilsina, 2018; Victor & Nichols, 2022, 2022; Zapata et al., 2018; Zhu et al., 2022). The Integrated MarkAI-EFOM System (TIMES) (Loulou et al., 2016) is one such model, and forms a part of the framework described here. Other analyses (Moghani & Archer, 2020; Pye et al., 2022) have used relatively crude representations of the effects of broadly applied emissions reductions with robust representations of pollutant formation and transport in the atmosphere. As emission reduction measures shift toward more long-term, capital-intensive strategies, it will become increasingly important to evaluate air quality projections on a longer time horizon, reducing the applicability of simplified emissions projections at a national or regional scale.

Previous attempts to unify the arenas of emissions projections and air quality impact assessments include reduced complexity models such as PCAPS (Baker et al., 2023), InMAP (Tessum et al., 2017), APEEP/AP3 (Muller & Mendelsohn, 2006), and EASIUR (Heo & Adams, 2015) among others (Eastham et al., 2023; Garcia-Menendez et al., 2015; Selin & Selin, 2023). These retain varying levels of complexity, but generally simplify the relationships from emissions to concentrations and reduce the temporal and sometimes spatial resolution to capture average changes in concentration with much lower computational cost. Other efforts to connect energy system and chemical transport models (Gonzalez-Abraham et al., 2015; Loughlin et al., 2011; Ran et al., 2015) have retained the computational complexity of using the Sparse Matrix Operator Kernel Emissions (SMOKE) model (CMAS, 2023) to generate speciated and spatially and temporally allocated emissions required for each future scenario analyzed, thereby incurring significant additional technical challenges.

In previous work, a scenario paradigm designed for the MARKAL model was used to produce plausible outcomes for future US emissions that differ significantly from one another (Brown et al., 2018). In this paper, the Brown et al. (2018) scenarios are implemented using TIMES to project emissions multiple decades into the future. These emissions projections are used to compute growth factors by sector, region, and species. The scale factors are used by the Community Multiscale Air Quality (CMAQ) model (US EPA, 2019) to directly modify an existing spatially and temporally resolved baseline emissions dataset. This methodology facilitates simulation of the air quality impacts of widely varying energy scenarios.

#### 2. Methods

This research demonstrates the linkage of a suite of existing models to facilitate examination of future air quality under widely varying scenarios. The TIMES model allows for

long-term projections of the broader energy-economic system, including simulating how existing and potential policies may shape the evolution of those systems through time. CMAQ represents atmospheric chemistry and physics with high spatial and temporal resolution. Combining the two models allows users to leverage the attributes of both modeling systems.

#### 2.1 TIMES

TIMES is an energy-economic optimization model that tracks fuels, feedstocks, and processes that convert between energy types and solves for the mix of technologies that meet energy service demands in each modeled region at the lowest total system cost (Loulou et al., 2016). TIMES users first create a reference scenario based on the technology and policy landscape as it currently exists, along with baseline assumptions about future demands, resource costs, and efficiency and other performance characteristics of available technologies decades into the future. A wide range of alternative scenarios can be generated by modifying assumptions about those future conditions. This work uses the United States nine region TIMES (US9rT) database and reference case (Lenox, 2019; Figure 1). The TIMES reference case uses year 2015 emissions as a baseline and represents specific policies that were in place as of 2019, including the Cross-State Air Pollution Rule (CSAPR), Tier 3 mobile emissions standards, corporate average fuel economy standards, and various new source performance standards. Approximations of state-level renewable portfolio standards are also included, aggregated to the regional level.



### Figure 1: Spatial aggregation in the US9rT model.

In addition to the reference case, this work uses a scenario paradigm (Brown et al., 2018) and narrative structure that were initially determined based on stakeholder input (Gamas et al., 2015). This work is adapted from the MARKAL framework to TIMES in a manner designed to be more flexible for creating a wide range of technological and policy scenarios, but the overall scenarios remain the same as in the MARKAL version (Brown et al., 2018). The scenarios consider two general factors driving decisions, the level of concern for the environment and the rate of technology development. While real-world conditions change through time, and thus base-year modeled conditions change as well, we believe our scenario background (i.e., technology vs. attitudes) remain highly relevant.

This general methodology was used with TIMES to produce five future emissions scenarios. By explicitly considering energy system dynamics, the resulting emission projections have greater regional, sectoral, and pollutant specificity than those typically used for projecting air quality. The scenarios (Figure 2) have been devised to illustrate combinations of traditional or new social paradigms around the environment alongside stagnant or innovative technologies. The *Low Tech, Eco* scenario represents a societal shift towards environmental protection in the absence of technological progress. The *High Tech, Eco* scenario includes this societal shift and an increased availability of transformative technologies. The *Comfort* scenario is characterized by stagnant social paradigms and a lack of technological advancements indicated by consumer preferences toward increasing comfort. *Other Priorities* exemplifies the effect of innovative technology when decisions are made without concern for the environment. Further discussion of these scenarios is available in Brown et al. (2018).



#### Figure 2 Scenario Descriptions

\* In Brown et al. (2018) the scenario names were: Status Quo = Business as Usual; Low Tech, Eco = Conservation; High tech, Eco = iSustainability; Other Priorities = Go Our Own Way; Comfort = Muddling Through

TIMES accounts for population growth and the associated increases in demand, technological characteristics such as costs, increases in energy efficiency, and improvements in emission control technology, as well as more stringent environmental regulations, all of which vary across scenarios. TIMES emissions outputs are calculated for each technology as a function of market share, specific energy use, conversion efficiency, and energy source, facilitating representation of the change in emissions and consequently the change in air quality. As an illustrative example, Figure 3 presents nitrogen oxide (NO<sub>x</sub>) emissions from light-duty vehicles (LDVs) by region and fuel type. Due to more stringent Tier 3 emission and fuel standards (Federal Register, 2014) and improvements in vehicle efficiency over the coming

decades, the total roadway emissions in 2045 are lower than the 2015 historical baseline in each scenario despite increasing vehicle mileage driven. In the *High-Tech, Eco* case, a much higher fraction of vehicles uses alternative fuels, which have different pollutant emission profiles. In *Other Priorities*, there is a large shift from gasoline to diesel LDVs, which have lower NO<sub>x</sub> but higher particulate matter (PM) emissions.



Figure 3 Modeled annual light-duty vehicle emissions of  $NO_x$  in 2045 compared to the model results calibrated to historical activity from the same sources.

#### 2.2 CMAQ

CMAQv5.3.1 is a three-dimensional, Eulerian air quality model (Appel et al., 2021; Byun & Schere, 2006) that includes gaseous, aqueous, and particle phase chemistry as well as atmospheric transport and aerosol dynamics to simulate interactions among pollutants and the environment. Meteorological inputs to CMAQ were generated using the Weather Research and Forecasting (WRF) model (Skamarock & Klemp, 2008). Both WRF and CMAQ were run with a 12 km horizontal resolution over a domain covering the contiguous US (CONUS) and portions of Mexico and Canada and extending vertically into the lower stratosphere.

CMAQ was run for a full year using 2016 meteorology and emissions from each of the six scenarios depicted in Figure 2. The Historical Baseline run is based on the National Emissions Inventory (NEI) 2017a emissions (US EPA, 2020). The five other model runs represent emissions projections in 2045 based on scaling factors determined by TIMES output.

Conventional approaches to generating perturbed emissions inputs for chemical transport modeling are time consuming, computationally intensive, and difficult to document. The current framework uses the new Detailed Emission Scaling, Isolation, and Diagnostic

(DESID) module (Murphy et al., 2021) within CMAQ to streamline the approach and create a structure that can be replicated for future work. DESID has many advantageous features, including that the emission rate modifications among scenarios are done online in CMAQ rather than the additional offline step to prepare them for each scenario, and that the emissions sector mapping between TIMES and CMAQ is simple and easily documented for traceability. By using DESID, we can separately scale emissions by pollutant, sector, and region.

#### 2.3 BRIDGING TIMES AND CMAQ

In addition to the new implementation of the MARKAL scenarios from Brown et al. (2018) in TIMES, the novel contribution of this paper is the bridge script that links the TIMES and CMAQ models. The model connection described here uses a grow-in-place methodology, by mapping the proportional change in regional emissions from TIMES to the same locations as current emissions. TIMES calculates emissions for each specific fuel-technology combination. CMAQ uses annual, county-level NEI data that are processed by the SMOKE model to create inputs that are chemically speciated and spatially and temporally allocated onto the modeling grid. A crosswalk was created to map the emissions from TIMES to the NEI via Source Classification Codes (SCC), following Loughlin et al. (2011). Table S1 (Supplemental Material) shows the mapping, with the use of wildcards (\*) to represent the multitude of included technologies of varying efficiencies and vintages.

Although TIMES allows for a robust differentiation of electricity generating unit (EGU) types, we restricted the categorization to just coal-fired and non-coal combustion for this growin-place methodology. In any situation where the range of technologies in the future differs significantly from the baseline, a determination must be made regarding the granularity of the emissions sectors to which the scaling factors are applied. Without aggregating non-coal combustion EGUs, the historically sparse distribution of combustion sources other than coal and natural gas would lead to unrealistic hot spots for scenarios with high adoption of biomass or waste-based combustion. Given that all EGUs provide the same service and we are not modeling a significant shift in relative distribution of population or electricity demand in any of the future scenarios, it is reasonable to apply the scaling factors to existing generators of electricity. All EGUs could have been lumped into a single scaling factor, but the underlying emissions profile of coal was sufficiently different to warrant treating it separately. Coal and natural gas, which are the two most widely used combustion generators in all cases, behave quite differently, with coal combustion decreasing and natural gas combustion increasing in almost all future scenarios. In addition to the EGUs, emissions were aggregated across light and heavy-duty vehicles by fuel types including diesel, gasoline, and other fuels. Other transportation emissions were grouped by modality, including air, rail, shipping, and non-road. Industrial emissions were grouped into sector as cement, chemical, food, metal, paper, refining, oil & gas extraction, or other industrial source.

The modeling time horizon and time steps used in TIMES simulations can be customized to the application, and we use a horizon of 2045 and 5-year time steps in this work. Emissions results are imported using code written in R, and the emissions of black carbon (BC), carbon monoxide (CO), ammonia (NH<sub>3</sub>), oxides of nitrogen (NO<sub>x</sub>), organic carbon (OC), PM in 10 (PM<sub>10</sub>) and 2.5 (PM<sub>2.5</sub>) micron size fractions, sulfur dioxide (SO<sub>2</sub>), and volatile organic

compounds (VOC) are extracted. A similar crosswalk shows the mapping between emitted species in TIMES and CMAQ.

Emitted Species	TIMES	CMAQ species
Black carbon	BC	PEC
Carbon monoxide	CO	СО
Ammonia	NH3	NH3
Oxides of nitrogen	NOx	NO, NO2
Particulate Organic carbon	OC	POC, PNCOM
Fine particulate matter	PM25	Fine
Coarse particulate matter	PM10	Coarse
Sulfur dioxide	SO2	SO2
Volatile organic compounds	VOC	TOL, XYLMN, BENZENE, NAPH, PAR, PRPA, MEOH, ETH, ETOH, OLE, ACET, FORM, KET, ETHY, ALD2, ETHA, IOLE, ALDX, ISOP, TERP

Table 1	Crosswalk	of	emissions	between	TIMES	and	<b>CMAQ</b>
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We used the region scaling feature in DESID, with regions corresponding to the Census divisions used in the US9r TIMES model. Emissions scaling factors to estimate future-year emissions for CMAQ are calculated by summing the annual emissions from TIMES separately for each pollutant, source category, and region for the base and future year, summand calculating the ratio of these future-year to base-year totals. Scaling factors are thus constant throughout the year. TIMES is calibrated to the year 2015, which we assume to be representative of the 2016 emissions processed by SMOKE. Emissions from sources external to the U.S. energy system, including anthropogenic sources outside the United States as well as natural emissions sources such as biogenic VOCs, wildland fires, windblown dust, and sea spray, are all unchanged from the present to focus the analysis on the impacts of changes in anthropogenic emissions.

#### 3. Results

The full suite of DESID input files with scaling factors from TIMES for each of the five future scenarios is available in the Supplement. The scaling factors for NO<sub>x</sub> emissions from LDVs are presented in Figure 4. Consistent with Figure 3, it is evident that the scaling factors are always less than 1 for gasoline vehicles in all future scenarios due to the fuel and emissions standards, increased use of alternative technologies, and improved fuel efficiency. However, since the fraction of LDVs operating on fuels other than gasoline is small in the historical baseline, the scaling factor for those emissions in the future can be quite large. There is significant variability among regions for diesel-fueled sources and other non-gasoline-fueled sources.



# Figure 4 Regional scaling factors for light duty vehicle $NO_x$ emissions by vehicle fuel type across all future scenarios. Other fuel includes compressed natural gas and ethanol. Note that each panel has a different y-axis.

Each unique combination of region (Figure 1), source (Table S1), and pollutant (Table 1) is represented by a scaling factor, so that each future scenario has over 1,500 scaling factors. As in the LDV NO<sub>x</sub> examples, these values range widely with minimum values of 0 in cases where a technology is no longer used in that region to many times the historical value. The range of scaling factors across regions and technologies (although omitting some pollutants for clarity) is shown in Figure 5. All scenarios also have at least some scaling factors that are greater than one, even when the concentrations overwhelmingly decrease in that region and scenario, e.g. for the *Low Tech, Eco* case in the Mid Atlantic region. This demonstrates the added value of incorporating air quality modeling into policy analyses, as dramatic air quality improvements may be obscured within complex changes in emission portfolios.



## *Figure 5 The range of technology-specific emissions scaling factors for four major pollutants plotted on a log scale.*

Annual average PM<sub>2.5</sub> concentrations at 12-km resolution are compared in Figure 6. The regional changes in concentrations can be linked to the scenario narratives. In *Other Priorities*, domestic fuels are preferred, leading to worse air quality near refineries and extraction sites

along the Gulf Coast and Intermountain West. In *Comfort*, air quality worsens across the country with larger changes near population centers, as people desire more energy-intensive goods and services. In the two eco-friendly scenarios there are large areas of improved air quality associated with a shift toward lower-emitting technologies. Even the *Status Quo* future has many areas with improved air quality associated with regulations that have already been enacted.



Figure 6 Annual average PM<sub>2.5</sub> concentrations modeled by CMAQ. The Historical Baseline plot shows concentrations in 2016, while the other panels show differences in 2045 from Historical Baseline.

The scenarios here do not represent specific policies and are intended to demonstrate variability in plausible prediction space. In *Other Priorities* case,  $PM_{2.5}$  concentrations are lower around many population centers, including Chicago, Los Angeles, and Pittsburgh. SO<sub>2</sub> is a major precursor to particulate formation and nearly all the future SO<sub>2</sub> emissions are lower in these scenarios. In *High Tech, Eco*, almost all coal-fired power plants in the West South Central region no longer operate, and simultaneously the oil and gas sector is much smaller; this leads to much lower  $PM_{2.5}$  concentrations in Texas, Oklahoma, and Arkansas. There are still hot spots in this region associated with increases in some industries such as mineral and chemical processing. In the Western Midwest, underground resource extraction increases in all scenarios, leading to a local increase in both  $PM_{2.5}$  and ozone concentrations (Figure 7).

There are situations where the emissions change may lead to air quality improving in some parts of a region while worsening in other parts. For example, PM<sub>2.5</sub> and ozone in the *Other Priorities* scenario show both increases and decreases in concentrations across many regions. The decreases noted above contrast with increases in northern Indiana, eastern Washington, and Scranton, PA. There is a high degree of variability in this scenario across the Midwest for PM<sub>2.5</sub> and across the east coast for ozone, with urban areas exhibiting decreases in both pollutants. The ozone changes in the West Coast region stand out (Figure 7), which is explained by the wide diversity of land use along the west coast, including highly populated urban areas, natural forests, and farmland. This highlights another benefit of examining the

CMAQ-simulated concentration fields in addition to the aggregated TIMES emissions. The CMAQ predictions provide a much richer interpretation of the spatially-dependent effects of each future emission scenario.



Figure 7 Summer season ozone concentrations for the Historical Baseline and differences from the Historical Baseline for each of the future scenarios.

One significant benefit of using a chemical transport model compared to analyzing emission changes alone is the ability to consider the impacts of air quality on human health or sensitive ecosystems. To assess these impacts, we calculated the change in population-weighted concentrations for each of the future scenarios using the concentration of ozone or  $PM_{2.5}$  and the population residing within the same grid cell (CIESIN, 2018). Then we calculate the average for each region and for the CONUS. These concentration changes are normalized by the population in each region (Figure 8):

$$X_R = \frac{\sum_i C_i P_i}{\sum_i P_i} - \frac{\sum_i H_i P_i}{\sum_i P_i}$$

where  $X_R$  is the population-weighted concentration change, *C* is the concentration of the pollutant, either annual average PM<sub>2.5</sub> or summer average maximum daily eight-hour average ozone (MDA8), *H* is the historical concentration of the same pollutant, P is the population in the same area in 2020, *i* refers to the 12-km grid cell, and *R* refers to the region. Population-weighted ozone decreases along the east and west coast for all future scenarios but increases for at least some interior regions in all scenarios except *Low Tech, Eco* and *Status Quo*. Exposure to PM is also reduced in all regions for *Status Quo* and *Low Tech, Eco* and nearly everywhere for *High Tech, Eco*. However, PM exposure in the *Comfort* scenario increases in every region. Comparing these values to the range of scaling factors in Figure 5, the benefit of the complete picture that includes ambient concentrations resulting from the emissions changes is in allowing the impacts of an intricate matrix of changing pollutant emissions on human exposure to be quantified.



Figure 8 Population-weighted concentration changes compared to historical values. The black dots indicate the average populated weighted change for the CONUS domain.

#### 4. Conclusion

The TIMES-CMAQ bridge tool facilitates analysis of the air quality impacts of future energy scenarios. Since TIMES and CMAQ are both models that are used in many nations, the bridge tool described here is broadly applicable. The mapping of the TIMES emissions technologies to CMAQ emissions sectors specified in the bridge tool must be developed for the TIMES database and emissions modeling platform used in any application.

One major benefit of bridging the TIMES and CMAQ models is an improved spatial picture of the changes in air quality. Both ozone and  $PM_{2.5}$  have adverse effects on human health. Improvements in air quality in densely populated areas will have greater impact on overall public health, so increased spatial resolution allows for additional insights into the exposure to pollutants. An example of this is the Houston, TX metro area, which has more than 7 million residents. In the *Other Priorities* scenario,  $PM_{2.5}$  concentrations are 0.5 to 2 µg/m<sup>3</sup> higher than the historical baseline, which would result in millions of people being exposed to increased pollutant levels. Conversely, in the *Low Tech, Eco* scenario, the largest increase is only 1.5 µg/m<sup>3</sup> and many parts of the metropolitan area have improved future air quality. In the *Other Priorities* case, increases and decreases in  $PM_{2.5}$  concentrations both occur in different parts of the South Atlantic and South Central regions. Many of the cities in these regions experience improved air quality. There are some locations with poorer air quality, potentially suggesting areas needing additional control measures to avoid worsening air pollutant concentrations and protect public health.

While the TIMES-CMAQ bridge method has many advantages, there are uncertainties remaining. The only emissions that were changed for the futures in this scenario are those associated with anthropogenic energy use within the United States. Therefore, changes in boundary conditions, energy-related emissions occurring in Canada and Mexico, emissions associated with agricultural activities, and emissions from wildfires were outside the scope of the study. Regulatory provisions adopted after 2019, such as the Inflation Reduction Act, were not considered in these scenarios, but could be added in subsequent refinements of this approach. Another uncertainty is that year 2016 meteorology was used for all simulations, but climate change may lead to changes in the future.

This method is an attempt to fill a gap in the modeling options available. The specificity is increased compared to a reduced complexity model or using either TIMES or CMAQ models alone. While this method uses a grow-in-place methodology to allocate future emissions, other procedures implement a more complex algorithm to attempt to predict the location of future large emissions sources such as EGUs (Wang et al., 2021). For situations where very large shifts in emissions are expected, these additional considerations may be warranted and have an important effect on the calculation. For instance, if the most common fuel source for motor vehicles changes from gasoline and diesel to compressed natural gas, the new emissions may differ enough that scaling doesn't accurately capture the chemistry. Another uncertainty not well captured in this approach is how the permitting process may affect the location of future emissions sources in areas in nonattainment of air quality regulations. There are also many future situations in which the geographic distribution of emissions, typically associated with population centers and transportation corridors, would likely be relatively consistent over time. The technique employed here suits these situations by providing detailed insight without overly burdensome calculations.

The TIMES-CMAQ bridge method can be used for a wide variety of future analyses. The TIMES scenario infrastructure is specifically designed to optimize the energy system with the addition of various policies or technologies while accounting for a wide range of uncertainties in possible future developments. The BRIDGE code then automates the process of creating the input file for CMAQ. The variety of scenarios considered provides a plausible estimate of the spread of future emissions and air quality, encompassing a wide range of potential outcomes and allowing the modeler to assess more robustly the impact of hypothetical policies or actions under a range of conditions and potentially avoid possible unintended consequences. The base year in CMAQ can be updated based on the most recently available NEI and the scenario files can be used with more recent updates to the TIMES database. This will allow for a simplified structure for many future investigations that will remain robust within the existing model architecture that is regularly maintained. The BRIDGE code as published is designed to work with the US9rT naming conventions, but as these are standard across TIMES databases, only minimal changes are needed to run CMAQ analyses based on other TIMES models. This work demonstrates how emission projections from energy system models such as TIMES can be linked to CMAQ to assess the air quality and health impacts of large-scale changes in the energy system.

#### 5. Acknowledgements

Author contributions: KB designed the research; KB, BM, and CN implemented the research; SN and KB analyzed the data; SN and KB wrote the paper; and BM and CN provided editing. We thank Dan Loughlin and Uma Shankar (EPA) for thoughtful comments on a draft of this manuscript. We also appreciate invaluable contributions from Kirk Baker (EPA) for providing the emissions inputs used by the CMAQ model.

#### Supplemental Info

Bridge code DESID input files

Table S1:

Crosswalk of emissions sources between models. Wildcards are used for the specific technologies in TIMES as there are additional age, control device, and efficiency specifications represented by these high-level technologies.

Description	Technology Names in US9rT	Source Sectors in NEI		
	(* =wildcard)			
Coal-fired power	ECOAL*, ECHPCOAL*, ECSTMR*,	Base Load/Load Following Units:		
plants	SECIGCC*, SECST* SEELCB*	Coal+Waste Coal		
Other Combustion	All E* except EXP* or those defined	Base Load/Load Following Units:		
power plants	for coal and SELF*, SEBSTM*,	Gas + Oil; Base Load/Load		
	SEELGWIE	Units		
Heavy duty vehicle	TBDSL*, TCDSL*, TH*B20*,	Heavy duty diesel		
(HDV) diesel	TH^DSL^ TMB20^, TMDSL^			
HDV gas	TBGSL*, TCGSL*, TH*GSL*, TM*GSL*	Heavy duty gasoline		
HDV other	TBCNG*, TCCNG*, TH*CNG*,	Heavy duty non-diesel non-		
	TH*LPG*, TMCNG*, TMLPG*	gasoline		
Light duty vehicle (LDV) diesel	TL*DSL	Light duty diesel		
LDV gas	TL*CONV* and TL*GSL	Light duty gasoline		
LDV other	TL*CNG, TL*LPG, TL*ELC, TL*ETH*, TL*E85*	Light duty non-diesel non-gasoline		
Airport	TA*	airports		
Non-road vehicles	TO*	Nonroad without agriculture		
Rail	TP* and TR*	Railyards, line haul rail		
Shipping	TS*	C1, C2, & C3 marine		
Residential	RSHWD*	Residential wood combustion		
Cement Industry	INC*	Cement Kilns NAICS 327		
Chemical industry	IC*	Chemicals NAICS 325		
Food Industry	IF*	NAICS 311		
Metal Industry	IM*	NAICS 331		

Non-metallic minerals	IN*	Nonmetallic minerals non-cement kilns NAICS 327
Paper industry	IP*	Pulp and Paper NAICS 322
Refineries	Technologies that output REF* commodities	NAICS 324
Other Industry	10*	Stationary non-EGU sources not in other tags
Oil & gas extraction	RSS*	Non-point oil & gas, Point oil & gas

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