Linking Electricity and Air Quality Models by Downscaling: Weather-Informed Hourly Dispatch of Generation Accounting for Renewable and Load Temporal Variability Scenarios

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Abstract

National models of the electric sector typically consider a handful of generator operating periods per year, while pollutant fate and transport models have an hourly resolution. We bridge that scale gap by introducing a novel fundamentals-based temporal downscaling method (TDM) for translating national or regional energy scenarios to hourly emissions. Optimization-based generator dispatch is used to account for variations in emissions stemming from weather-sensitive power demands and wind and solar generation. TDM is demonstrated by downscaling emissions from the electricity market module in the National Energy Model System (NEMS). As a case study, we implement the TDM in the Virginia-Carolinas region and compare its results with traditional statistical downscaling used in the Sparse Matrix Operator Kernel Emissions (SMOKE) processing model. We find that the TDM emissions profiles respond to weather, and that nitrogen oxide emissions are positively correlated with conditions conducive to ozone formation. In contrast, SMOKE emissions time series, which are rooted in historical operating patterns, exhibit insensitivity to weather conditions and potential biases, particularly with high renewable penetration and climate change. Relying on SMOKE profiles can also obscure variations in emission patterns across different policy scenarios, potentially downplaying their impacts on power system operations and emissions.

Synopsis

This research proposes a novel downscaling methodology to link macro-energy system models and air quality models accounting for projecting power emissions changes due to renewable technology innovation, weather-informed system operation changes and load variability.

Keywords: power systems, power emission, energy transitions, emission projection

1. Introduction

An oft-stated objective of policies and strategies to combat climate change is the achievement of a net-zero emission economy by the mid-21st century. To limit global warming to 1.5°C, the Paris Agreement set targets for greenhouse gas emissions to decline 45% at least before 2030 and to reach net-zero by 2050

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worldwide [1],[2]. In the US, President Biden has set an ambitious national goal of achieving a carbon pollution-free power sector by 2035 and a net zero emissions economy before 2050 [3]. Because the energy sector is responsible for 73% of greenhouse gas emissions globally, decarbonizing the energy system is the emphasis of policy [4],[5]. Various clean energy transition "pathways" and "roadmaps" have been proposed and widely discussed by government, academia, and industry [4],[6]–[8]. Decarbonizing the electricity sector is often the focus of these plans, not only because power production is responsible for 25% of worldwide emissions [9], but also because electrifying the transport and building sectors is viewed as key to their decarbonization.

Recently, the social impacts of the energy transition have gained the attention of the public, policy makers, and researchers, with a focus on effects such as air quality, public health, energy equity, environmental justice, and labor markets [10-16]. Analyzing these impacts requires the integration of different modeling tools from various disciplines, such as long-term macro-energy system models/integrated assessment models [16],[17], air quality models [18],[19], dose-response models for health impacts [21], and aggregated sectoral micro-economic models (i.e., power, transportation, and building) [22-24], among others. However, it is often difficult to coordinate the inputs and outputs of these models to provide an integrated look at the multiple impacts of policy as those models are usually implemented on different spatial and temporal scales. In the temporal dimension, for instance, most macro-energy systems or climate models reduce computational complexity by decreasing the temporal resolution of the data used. Instead of 8760 hours/yr, the National Energy Modeling System (NEMS) model uses nine time-block periods per year for its load inputs and electricity outputs, while the Regional Energy Deployment System (ReEDS) model applies an aggregated seventeen time-blocks to represent the within-year distribution of loads [10, 11]. Thus, the rough output of such a model cannot be directly used by air quality models that require highly resolved temporal data (i.e., an hourly time step) as inputs. Therefore, (temporal) downscaling techniques are needed to link aggregated system models with air quality models.

A downscaling method usually takes an aggregate spatial or temporal forecast of climate, economic, or other variables as an input (or "predictor"), and produces a more detailed and disaggregated scenario of those variables or other variables that are affected by those inputs. Current downscaling methods can be categorized into statistical [26-32], dynamic [33-36], and fundamentals-based [37, 39] approaches. We review the existing literature associated with each approach in Support Information (SI) Section 1, focusing on applications to electricity demand, generation, and emissions downscaling.

However, existing downscaling methods have limitations in capturing the effects of long-term (beyond 10-15 years) changes in power generation mixes or climate (e.g., average temperatures). Such factors, which can significantly impact the amount and timing of power emissions during energy transitions, are not well represented or ignored. In the case of statistical approaches, the assumption that the statistical relationship built using historical or current system data will still be valid for the future system could fundamentally limit downscaling projections to just the next handful of years rather than the decades covered by energy transition scenarios. Meanwhile, the precision of temporal downscaling is restricted by the physical model used. For instance, the temporal resolution of GCM (General Circulation Model) results downscaled using RCMs (Regional Circulation Models) is often in 6-hour time steps, which is not detailed enough to represent the diurnal operation of a power system and its associated emissions [33]. In addition, a fundamentals-based method was used by Loughlin et al. [39], who proposed an SCC-mapped[1] grow-in-place (GIP) method to link MARKAL and SMOKE-CMAQ (Sparse Matrix Operator Kernel Emissions - Community Multi-scale Air Quality) modeling frameworks to project and simulate both the location and time series of energy sector emissions. A combined GIP and SMOKE (GIP-SMOKE) model does temporal downscaling by converting annual emissions into hourly emissions through its default allocation factors/temporal profiles, which may consider the pattern differences between day and night, weekdays and weekends, and months or seasons, but have the shortcoming of being assumed to not change in future years.

Therefore, better downscaling methods are desirable to generate more accurate emission profiles that can represent how temporal emissions patterns evolve over future years in response to renewable investment, changed power system operations, and variable weather conditions. Firstly, an improved downscaling approach should be able to capture changing net-load patterns (gross load less renewable generation, e.g., the so-called Duck Curve of the California power system[2]) and timing of demand peaks. These variations are expected to create a greater need for more flexible ramping of fossil-fueled thermal plants to maintain system reliability, inevitably altering the corresponding amount and timing of power sector emissions. Second, the new approach should account for climate change which might affect future power system reliability by magnifying the impacts of weather on demand variability [42], [43]. Climate change can also reduce or increase the generation of renewable energy, and warming reduces the effective capacity and Carnot efficiency of thermal plants [42, 44-46]. These shifts deserve careful attention when assessing the impacts of power emissions on air quality and public health, as the effectiveness of power emission reduction can be significantly influenced by changes in emissions distribution over the year and their correlations with synoptic conditions [47]. For instance, elevated NO_x emissions during high temperature/high demand days may coincide with conditions favorable for ozone formation [40]. However, the temporal profiles in SMOKE generally do not capture these correlations because those profiles are designed to represent historical

[1]The Source Classification/Category Codes (SCCs) system was developed by US EPA to classify different types of activities that generate emissions [41]. Each SCC is given to a unique source category-specific process or function that emits air pollutants.

[2] The duck curve is a graph shows the difference between electricity demand and solar energy production over a day. It was devised by the CAISO to illustrate an aspect of challenges that renewable energy poses to system flexibility.

average conditions and do not represent their day-to-day random variability. As a result, SMOKE may underestimate peak generation emissions while overpredicting emissions during other time periods [48]. . The latter are often focused instead on projecting long-term changes in siting patterns due to large-scale fossil retirements and renewable investments, and require national downscaling of results from NEMS and other national models.

In this paper, we focus on developing temporal downscaling methods for electricity systems that can more precisely represent impacts of renewable energy growth and other system changes on the level and variability of power emissions accounting for economic, technical, and climate drivers. The proposed method is intended to combine the advantages of both statistical downscaling and dynamic downscaling. Some simple drivers like temperature, wind speed, and solar radiation are processed and downscaled by statistical methods. Our method then applies optimization to simulate electric generator operations on an hourly times scale using those statistically downscaled meteorological variables, based on the locations of existing and new power plant projected using a site-and-grow (SAG) [49] spatial downscaling method. SAG is designed to model the spatial distribution of changes in generator locations based on modeling of generator retirements and new plant construction. SAG constrains overall future installed capacity mixes using future scenarios from national or regional energy models, and chooses where to site new facilities based either on statistical methods reflecting past siting patterns [40] or optimization methods that account for transmission, water, land availability, and other factors affecting siting, especially the amount and distribution of wind and solar resources in the case of renewable generators [49]. The advantage of optimization-based SAG models is that they can account for siting costs and requirements for new generation technologies that can differ significantly from drivers of siting decisions for traditional thermal generators.

The resulting temporally downscaled emissions are expected to anticipate how changes in technology, policy, and climate drivers affect when and how facilities are operated on an hourly scale. Using this new method, we are able to address the following research questions: 1) *How do hourly emission distributions from thermal plants vary and correlate with meteorological conditions in the context of climate change, and how do they compare to traditional methods that don't account for meteorological variability?*, and 2) *How do hourly distributions of power sector emissions compare under alternative policy and technology scenarios, accounting for the response of emissions to the penetration of wind and solar energy and its contributions to net-load variations?* The proposed hybrid statistical-SAG-temporal optimization-based method for temporal and spatial emissions downscaling is a novel approach in that this is the first time that a downscaling method considers hourly operations of a power system in response to renewable energy penetration and climate drivers over a multi-decadal time scale.

The rest of the paper is organized as follows. Section 2 introduces the proposed temporal downscaling methodology and case study assumptions. Section 3 shows the numerical case study for the SERC

Virginia/Carolina (SRVC) region in the year 2050[1] under several energy transition scenarios. Section 4 discusses implications of these results and recommends future research directions.

2 Methods

2.1 Temporal Downscaling Model

The proposed temporal downscaling model (TDM) disaggregates energy outputs from a scale of multi-hour time blocks (several blocks per year) yielded by a national or regional aggregated electricity model to an hourly scale while accounting for how power systems will be operated in the future under significant renewable penetration as well as varying meteorological conditions under climate change and an assumed policy scenario. Specifically, the TDM is designed to link the NEMS model and the SMOKE-CMAQ model but is not limited to these two particular models. It can be extended to downscale emissions from the electric power component of any other macro-energy system model, integrated assessment model, or other time-aggregated models of power system operations for use in any pollutant fate and transport model.

Here, we describe the specific steps of TDM, assuming that the locations and sizes of electric generators for some future scenario have been provided by the NEMS-SAG method [49]. The TDM comprises two major steps as shown in Figure 1, each being explained in detail in SI Sections 2.1-2.2, respectively. (Note that in our application, the execution of NEMS and SMOKE was done by collaborators on other research teams, while our contributions are the SAG-TDM downscaling components of the overall process). The first step addresses net-load adjustments which will affect hourly MW demands (loads) and potential MW generation by renewables (solar, wind). It is made up of three substeps (SI Sections 2.1.1-2.1.3, respectively). The first substep is the development of hourly load and meteorological scenarios simulated from external models (Step 1a. ReEDS and WRF model, Fig. 1). The second substep consists of load adjustments (Step 1b, Fig. 1), and the third step is a simulation of potential renewable profiles (Step 1c, Fig 1). The last two substeps predict and simulate future hourly load and renewable production profiles consistent with patterns of statistically downscaled meteorological variables. These profiles are then used as inputs in the second step of TDM (Step 2, Fig. 1).

[1] The year 2050 scenario is selected as a long-term transition case study, which is furthest forecasting year under the used NEMS version. The proposed framework can be also used for the other short and intermediate years such as 2030 and 2040, and even longer term 2100 if meteorological data and energy projection information are available.

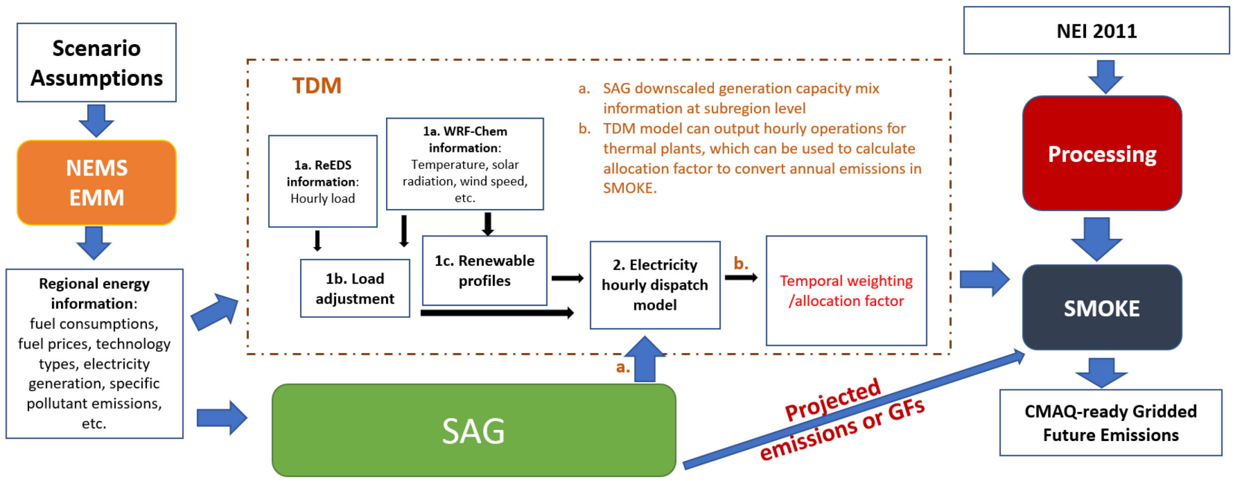


Figure 1. Schematic of methodology linkages within the two-step TDM framework

The core of the second step is an optimization-based hourly electricity dispatch model that determines hourly generation from each generation type in each subregion (and ultimately power plant) in the model, while matching the aggregate temporal profile of such generation from the national or regional aggregate model (here, NEMS). The detailed notation and formulations of the model can be found in SI Section 2.2. The power flows among NEMS' EMM regions by load block are solved by the NEMS model and are therefore used in the TDM as "boundary conditions" for its downscaling procedure. Within each EMM region, the transmission lines and subregions are represented as pipe-and-bubbles. Security constraints among subregions, which account for the need to limit flows to less than some multiple of the thermal capacity of transmission lines because of possible line outage contingencies are represented by a derated transmission capacity method, which is a common approach of large systems [50]. Resistance losses between regions are disregarded, but more general formulations could calculate losses as dependent on voltage, power line length, and amount of flow. Unit commitment constraints on generator dispatch (e.g., ramp rates, start-ups, or minimum output levels) are not modeled, consistent with NEMS, but could also be incorporated if desired. The structure of this optimization-based electricity model resembles traditional production cost models, with two important exceptions. One is that our model also includes constraints that require that certain energy outputs of an aggregate model (here, NEMS) be matched (namely, the sum over TDM hourly dispatched generation in time block equals the total generation in that NEMS time block). Second, the TDM optimization model includes more than the usual amount of detail on temporal variations in resource availability and load, and their correlations, because the timing and amount of generation and emissions from thermal generation are closely coupled and influenced by the joint distribution of wind and solar output and loads, and these effects depend strongly on the exact generation mix associated with the energy transition scenario being considered [51], [52].

2.2 Case Study Assumptions

As a case study, we implemented the TDM to downscale NEMS outputs in 2050 in the SRVC region (Figure 2). Results for other years from NEMS could be downscaled similarly using appropriate inputs. Based on a power plant and demand location model derived using the SAG model [49], we downscale energy (MWh) generation projections (by fuel type, technology type, time block, and sub-region) from a scale of nine NEMS time-blocks per year to 8760 hours per year (Section 3.1). Then we convert the hourly generation scenario into chronological emissions profiles which we use to modify the basic emission profiles in SMOKE-CAMQ [18],[54].

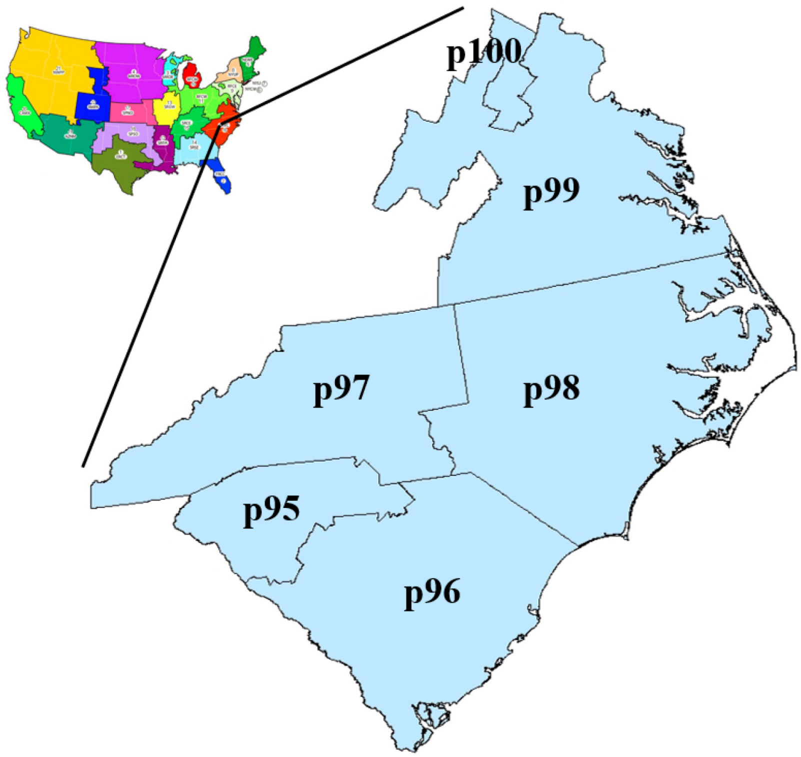


Figure 2. Map of six ReEDS balancing areas (p95-p100) comprising the NEMS SRVC (SERC Reliability Corporation, Virginia and Carolinas) region

The inputs for this downscaling method are of four types: 1) a meteorological scenario of hourly temperatures, cloudiness, and wind speeds (disaggregated to subregion); 2) assumed locations of generation capacity by subregion (from either the SAG method or the more traditional GIP method [49]) with a multi-state region for a future scenario year, 3) energy generation by sub-period (NEMS' nine time-blocks in our case), and 4) local siting or emissions policies that impact dispatch. The outputs are hourly energy and pollutant emissions, in particular: 1) Hourly electricity demand and generation from all generation types (including variable renewables) in each subregion that are consistent with assumed hourly weather, as well as 2) Hourly emissions (especially SO_2, NO_x) by generator type and subregion. After downscaling each subregion's chronological emissions further to individual point sources (e.g., by assuming an allocation in proportion to the capacity of each source present in a point source emissions inventory), those emissions can then be input into an air pollution fate and transport model such as the CMAQ system.

Our application repeats this process for each of four aggregate energy and emission scenarios from NEMS model:

- A base case or reference scenario uses AEO 2017 scenario, without the Obama administration Clean Power Plan [54] (scenario refnocpp),
- Abundant natural gas resources (scenario highNG) [55],
- High electric vehicle penetration (scenario highEV) [56], and
- High building energy efficiency (scenario highEE) [57].

The required additional information on subregional transmission, hourly load profiles, and renewable sources originate from the ReEDS database [58]. This downscaled emission information will be, by definition of the methodology, consistent with NEMS totals by region and by load block (nine demand blocks per year). Finally, we compare the TDM downscaled hourly emissions with the downscaled hourly emissions from SMOKE's output in terms of temporal variation and O_3 formation implications for each of the scenarios (Sections 3.2 - 3.4).

Emissions policies are key assumptions that affect the results of downscaling analyses, and are reflected either in the boundary conditions imposed on the downscaling, or the downscaling process itself. Assumptions about federal or regional policies (such as seasonal NO_x or annual SO_2 caps or the Regional Greenhouse Gas Initiative) constrain solutions of the aggregate energy models that define boundary conditions for downscaling, such as total emissions by jurisdiction or season. Downscaling method then enforces those boundary conditions so that the disaggregated emissions are consistent with the aggregate model solutions and the federal policies they reflect. However, many states impose their own specific emissions policies that should be reflected in downscaling procedures. Examples include state or local CO_2 targets or caps on criterion pollutants within non-attainment areas. In our case study, all emissions are incorporated in the boundary conditions defined by NEMS, but such limits on timing or location of local emissions could readily be included.

In general, there exist important uncertainties that should be recognized when using emission downscaling methods. Some of these are broad federal policy, economic, and technology uncertainties that impact mixes of generation investment and their emissions rates. These are best reflected in sensitivity analyses of the national or regional models whose aggregate results are the boundary conditions that constrain the total investment and energy generation by type within the region being studied. Other uncertainties, such as state or local land use and climate policies that influence the generator siting and operations, should be considered by downscaling under a range of assumptions about those policies to assess if the resulting emissions patterns change in ways that could have significant implications for health or other impacts. For conciseness, this case study does not include such sensitivity analyses.

3 Results

3.1 Hourly Generation Dispatch and Emission Profiles

The scenario-by-scenario NEMS-SAG projected and downscaled generation capacity mixes are shown in Figure S8 in the SI. In this subsection, given the projected 2050 systems, we present TDM downscaled and optimized SRVC power system hourly operation under four scenarios (Figure S9. a-d). The figure reveals that nuclear, coal, natural gas, and solar energy are the primary resources meeting electricity demands in SRVC. In the refnocpp scenario, most of the coal and nuclear power plants operate as baseload generators, while coal was called upon occasionally during peak hours. A significant amount of solar production resulted in gas plants cycling more frequently to meet demand when insufficient solar energy was available. In the highNG case, gas plants dominate power generation instead, accounting for over 50% of total electricity production, leading to changes in coal plant operations which in that case only serve as baseload generators. The operation patterns in the highEE scenario were similar to those in the refnocpp case, but with more fluctuations during peak periods due to EV charging. Coal plant operations also changed in the highEE scenario due to reductions in overall electricity demand. By considering weather-dependent load and renewable variations, the TDM downscaling method can precisely and quantitatively assess how different energy transition scenarios affect emissions timing and amounts by capturing operating interactions of different resources in a quantitative manner.

As shown in Figure 3, temporal variations in thermal plant operation strongly affect power emissions profiles, which are the SO_2 and NO_x hourly emission profiles projection in 2050 in the various scenarios. The emissions are calculated based on the MWh operation of thermal plants multiplied by corresponding emissions factors. The SO_2 profile is driven by the timing of coal combustion, while variations in NO_x result from the operations of both coal and natural gas plants. Emission profiles also exhibit seasonal trends, with higher emissions occurring in summer or winter due to increased cooling and heating demands, respectively. In contrast, emissions in spring or fall tend to be lower. The diurnal pattern shows that there are more fluctuations in NO_x during peak hours compared to SO_2, reflecting the flexible operation of gas plants relative to coal plants and their interactions with solar production.

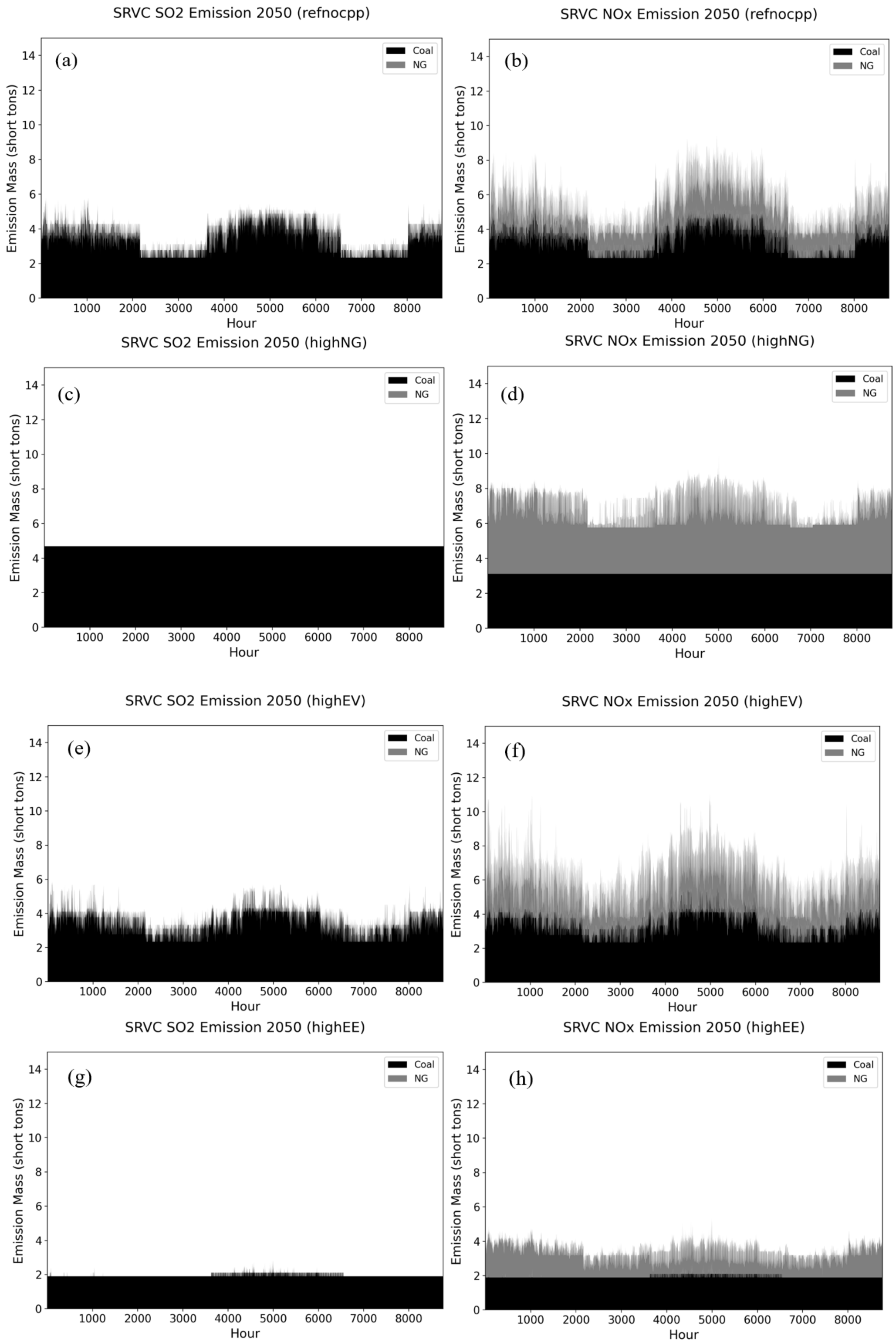


Figure 3. Hourly power emissions in region SRVC under different 2050 scenarios (a. Refnocpp SO_2; b. Refnocpp NO_x; c. HighNG SO_2; d. HighNG NOx; e. HighEV SO_2; f. HighEV NO_x; e. HighEE SO_2; f. HighEE NO_x)

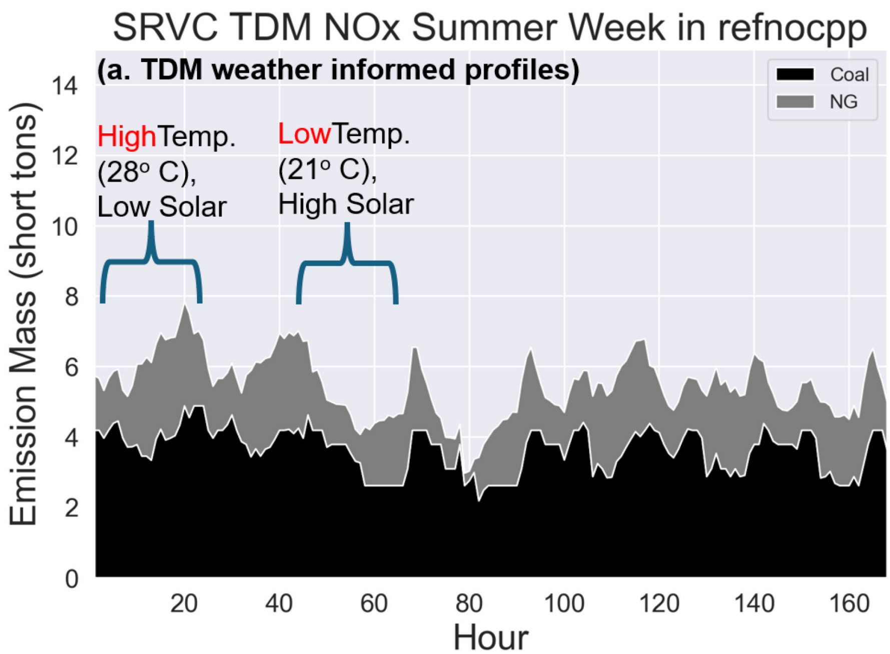
Differences in generation mix and location among scenarios also lead to distinct power system operations and corresponding emission profiles. For instance, in the highNG and highEE scenarios, the emissions of SO_2 from coal facilities remain relatively constant over time due to their baseload mode of operation. This pattern differs from the other scenarios, in which coal generates more power, expanding to include both baseload and cycling roles. Furthermore, the NO_x emission profile in the highEE scenario demonstrates less fluctuation over the seasons compared to the other three scenarios. This is due to the lower demand and lower investment in new power resources in that scenario, especially wind and solar, which reduce the overall variability of net loads faced by fossil units. Thus, the TDM approach effectively captures emission variations arising from different power system configurations and operations across different energy transition scenarios.

As discussed in the next three subsections below, many of the differences in emissions patterns arise from the interactions of weather and particulars of the generation mix, which are captured by the hourly TDM method but not the commonly used SMOKE downscaling method.

3.2 TDM vs SMOKE: Comparison of Emission Profiles

Figure 4 focuses on comparing the diurnal patterns of NO_x emissions profiles obtained using the TDM method and the SMOKE default method. It represents the hourly emissions of one week in the summer season for the 2050 projection. In Figure 4a, we can observe that the NO_x variation patterns are correlated with weather. For example, comparing the first day (high temperature and low solar radiation) with the third day (low temperature and strong solar radiation), we can see a higher demand on the first day and a gradually increased NO_x emission during the afternoon (due to thermal plants gradually ramping up to compensate for decreasing solar power). In contrast, the third day has a lower demand but a duck-curve-like NO_x emissions profile (due to strong solar production replacing thermal plant operation in the afternoon). The TDM simulated profile is the result of system operation informed by impacts of weather on load demand and renewable energy production.

However, the SMOKE profile only relies on historical operation patterns based on generation mixes dominated by thermal power plants, whose day-to-day patterns emission are less affected by weather than renewable-dominated systems that have thermal plants as back-up. As shown in Figure 4b, the corresponding SMOKE NO_x profile has a repeating and simple pattern mimicking the traditional operation of thermal power system, ignoring the impacts of weather on power system operation. The peak emission occurs around noon every day at the same time as peak load demand. However, this is no longer accurate for a power system with a large amount of solar where the timing of peak emission is postponed to later afternoon around 7-8 pm. The timing of power emission is significant because the reaction and transport of air pollutants and formation of secondary air pollutants are highly correlated with when pollutants are emitted into the atmosphere and the local weather conditions. Therefore, the emission profile based on the historical power operations may be inappropriate for a future clean power system with a large amount of variable renewable energy, especially in the context of climate change where the impacts of weather information should be considered for more accurate estimates of power operation and emissions.



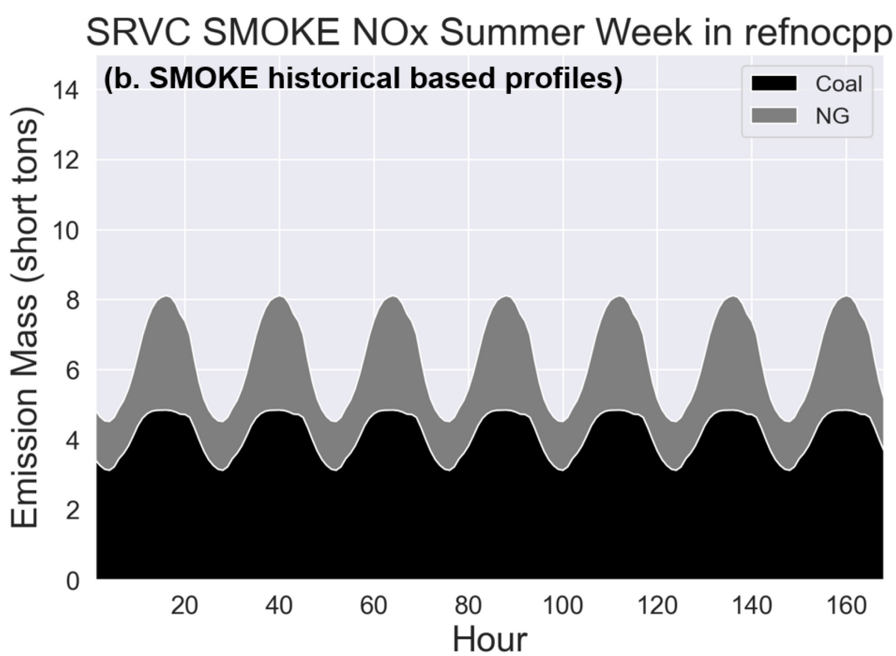


Figure 4. Hourly NO_x emission profiles in summer week in region SRVC in scenario refnocpp (a. TDM downscaling; b. SOMKE default profile)

3.3 TDM vs SMOKE: Weather Indices

To illustrate the influence of weather information on pollutant formation, we develop a simple index of the meteorological potential for tropospheric O_3 formation [59], [60] and analyze its covariation with NO_x emission profiles of TDM and SMOKE at the subregion level in Figure 5. The O_3 formation index is calculated as an equally weighted sum of a 0-1 rescaled wind speed and a 0-1 rescaled solar radiation, where a higher value of the O_3 index for a given hour indicates a greater risk of O_3 formation-favorable weather conditions characterized by low wind speed and high solar radiation. When the peak time of power emission coincides with a high value of the O_3 index, there could be a higher risk of forming secondary O_3 in the atmosphere.

Comparing subregions, we can expect a variety of patterns of local power NO_x emissions and their relationship of local weather conditions because of their different generation mixes. In Figures 5a and 5b, subregions p100 and p95 are unlikely to be exposed to secondary O_3 from the local power system due to low levels of power NO_x emissions. On the other hand, subregions p96 and p98 (Figure 5c and 5e) have a similar generation mix with large amounts of thermal plants and a significant amount of solar energy, which suggests that weather conditions may interact strongly with power resource operation in these areas. From Figures 5c and e, we observe a strong correlation between the resulting SMOKE NO_x emission profile (blue curve) and O_3 index, particularly during peak hours when NO_x emission and O_3 index are both at their maximum. In contrast, the resulting TDM profile (black curve) shows an opposite trend, with lower NO_x emissions when the O_3 index is at its peak, which reflects the impacts of solar penetration on the operation of thermal plants, leading to postponed peak emissions hours. Meanwhile, in p97 (Figure 5d), a similar phenomenon can be observed on some days, except for the first two days of the week, although there is only a relatively small amount of solar power in the local generation mix. This contradiction implies that using the SMOKE profile for a system with high solar penetration could result in overestimating O_3 concentrations in air quality simulations compared to using a profile generated by a TDM method, with the latter providing a more trustworthy estimate of the risk of O_3 penetration due to the changing operation of future power systems. Finally, in p99 (Figure 5f), because the local generation mix is purely dominated by thermal plants with limited renewable penetration, both the SMOKE profile and TDM results can correctly represent emissions patterns in such a case.

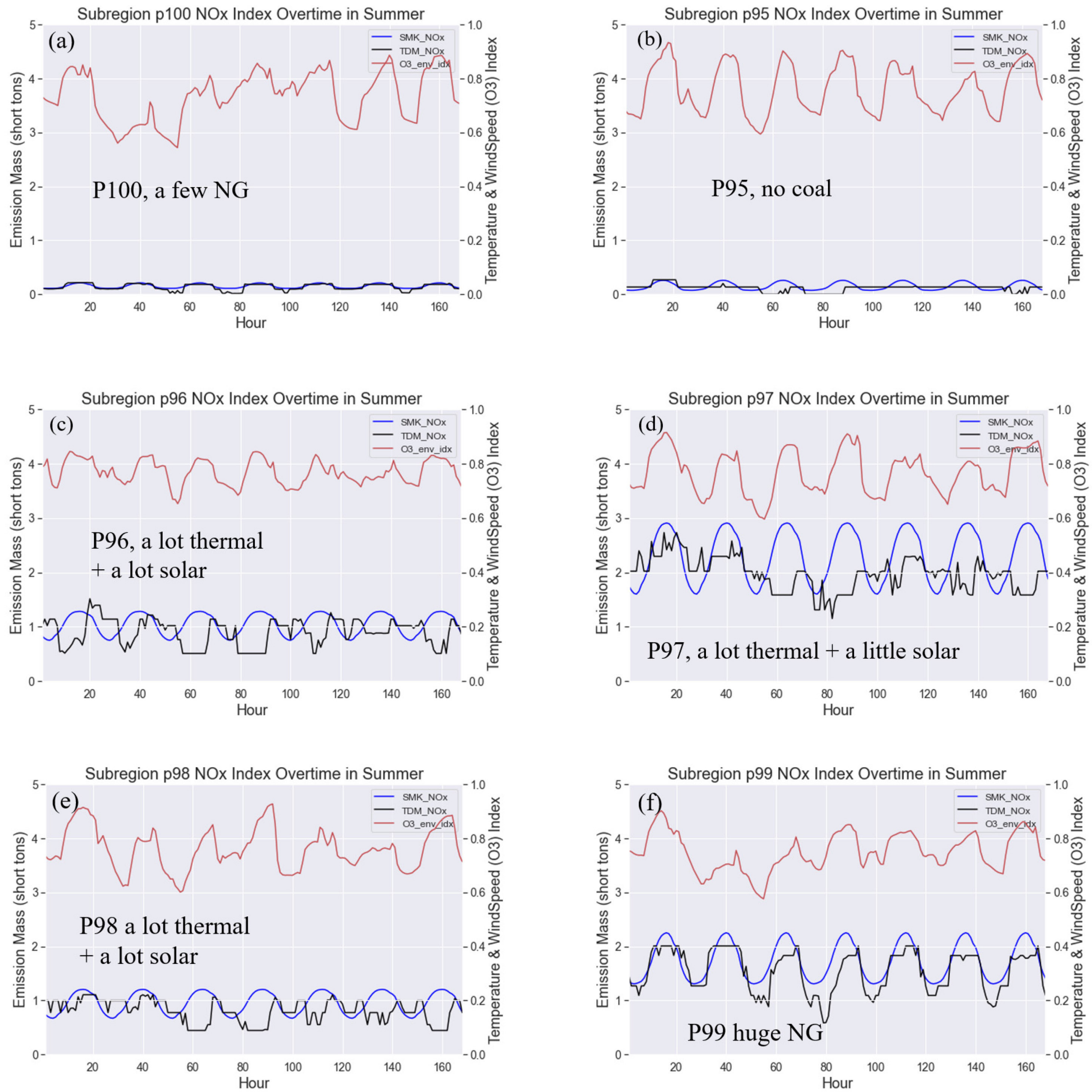


Figure 5. Hourly NO_x emission profiles and O_3 formation index in summer week in subregions of SRVC in refnocpp (a. P100; b. P95; c. P96; d. P97; e. P98; f. P99)

3.4 TDM vs SMOKE: Scenarios

In this section, we compare TDM and SMOKE NO_x emissions in summer (Figure 6) and winter (Figure 7) weeks under different scenarios. The TDM profiles in summer exhibit diverse NO_x emission patterns and levels across the scenarios. The refnocpp case and the highEV case share a similar (and highly variable) TDM NO_x pattern, reflecting the influence of gas and solar operations during the daytime. Their pattern is distinct from the corresponding SMOKE profile whose diurnal pattern is the same every day. In contrast, the highEE and highNG cases include more conventional thermal units, leading to different NO_x emissions compared to refnocpp and highEV cases. The highEE TDM pattern closely resembles the SMOKE pattern, suggesting that the SMOKE profile can sometimes suffice for simulating power emissions if the future system configuration does not shift towards greater reliance on variable renewable energy. In the highNG case, however, the TDM pattern appreciably deviates from the SMOKE pattern despite being dominated by thermal plants. This is due to the presence of a large amount of gas generation, which flattens the peak emissions of coal plants and shifts emissions to non-peak periods, resulting in an overall different emissions pattern compared to the SMOKE profile. Also, the highNG scenario shows approximately 25% fewer daily peak emissions, and 15% higher non-peak emissions compared to SMOKE. By comparing the profiles among different scenarios, we see that the TDM profiles provide plausible estimates of changes in system operation and emission patterns under different scenarios. In contrast, the SMOKE profiles exhibit implausibly similar emission patterns across the scenarios, with differences only in the total emissions levels. SMOKE profiles tend to misrepresent emission profiles, basin them on increasingly irrelevant historical patterns.

Compared to summer patterns, the differences between the TDM and SMOKE profiles in winter are less pronounced (Figure 7). The winter SMOKE profiles exhibit two daily peaks and account for the impacts of solar and load demand changes, which are generally similar to the TDM profile patterns. However, differences still exist in the accuracy of representing peaks and fluctuations across days. For instance, in the refnocpp and highEE scenarios, the extreme peaks observed in the TDM profile on the first day are smoothed out by the SMOKE profiles when averaged over the remaining days. Furthermore, SMOKE profiles may show distinctive daily fluctuation patterns compared to the TDM profile, with SMOKE being more variable than the TDM profile in the highEE or highNG scenarios, while being less so in the refnoccp or highEV scenarios. Therefore, although the winter SMOKE profile is more realistic, it fails to capture the detailed changes in peaks and variations that the TDM profile can capture, which could significantly impact air quality simulations.

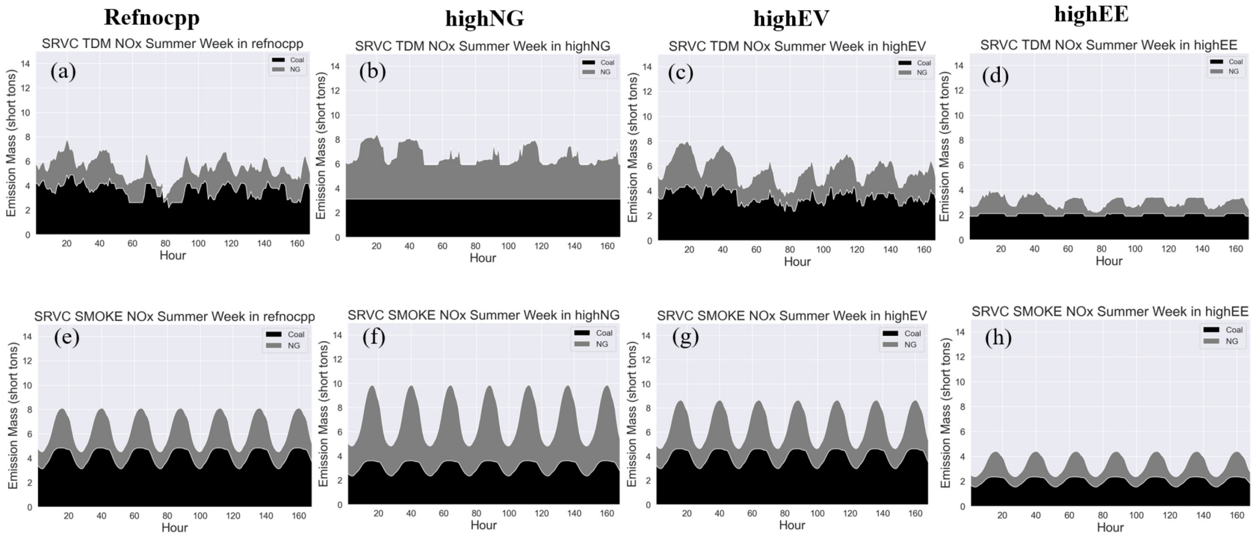


Figure 6. Hourly NO_x emission in summer week of SRVC (a. TDM-refnocpp; b. TDM-highNG; c. TDM-highEV; d. TDM-highEE; e. SMOKE-refnocpp; f. SMOKE-highNG; g. SMOKE-highEV; h. SMOKE-highEE)

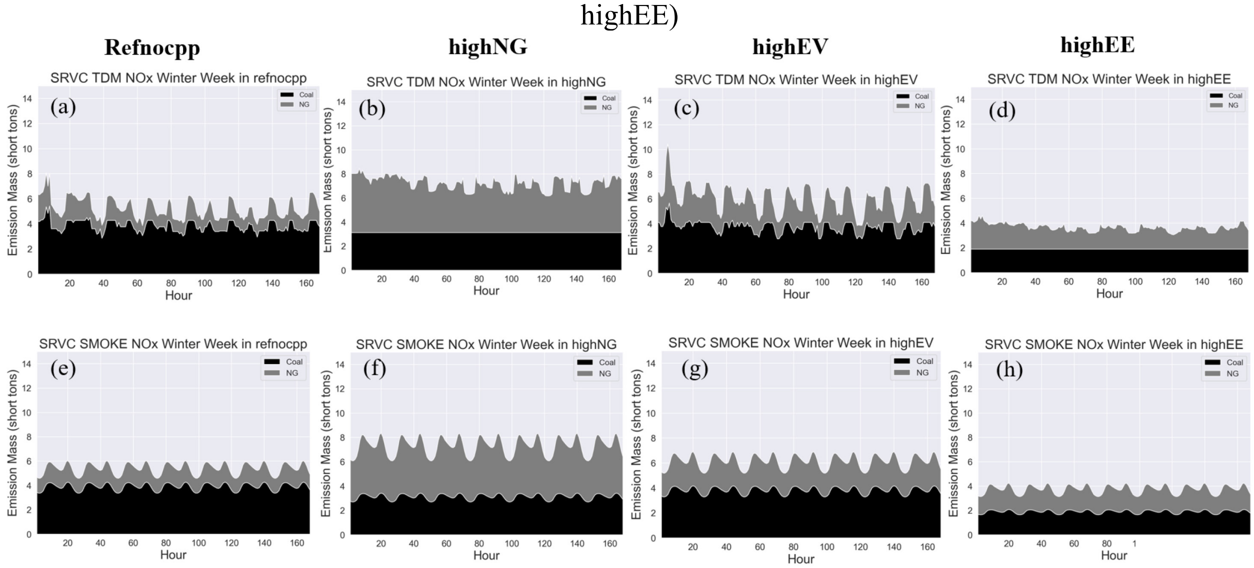


Figure 7. Hourly NOx emission in winter week of SRVC (a. TDM-refnocpp; b. TDM-highNG; c. TDM-highEV; d. TDM-highEE; e. SMOKE-refnocpp; f. SMOKE-highNG; g. SMOKE-highEV; h. SMOKE-highEE)

4. Discussion

In this paper, we have introduced a novel fundamentals-based temporal downscaling method called the Temporal Dispatch Model. TDM is a procedure for translating temporally aggregated emission results from aggregate electric power sector models, such as NEMS, to the detailed plant-level hourly inputs required by air pollutant simulation models, such as the emissions processing model SMOKE. TDM, when paired with the Site-and-Grow (SAG) method in [49], develops spatially and temporally granular emissions projections under a given future technology and policy scenario. Because TDM captures the rich detail of the power networks and generation technology in its dispatch model, the downscaled system's generation mix and operations at the subregional level not only reflect the scenario-specific fundamental structural changes in power systems resulting from a scenario's various technologic, economic, and weather drivers, but also reveals the spatial and temporal heterogeneity in system operations and emissions among those scenarios.

As a numerical case study, we made a comprehensive comparison of the proposed temporal downscaling method TDM with traditional SMOKE profile-based downscaling in the SRVC region power system of the NEMS model. We consider various aspects of the results, including resulting power emission profiles, correlations with weather indices, and consistency with scenario information. The findings reveal that the TDM emissions profiles effectively capture how system operations respond to the impacts of weather on demand and renewable energy production patterns. In contrast, SMOKE profiles, which are based on historical operations, were found to be potentially biased and unresponsive to changes in the pattern of dispatch when representing future power emissions, particularly in the context of climate change and renewables expansion. Furthermore, our analysis of smog season weather indices (representing meteorological conditions such as wind speed and solar radiation that favor O_3 formation) indicates that relying on the SMOKE NO_x emission profile could lead to an overestimation of O_3 concentrations for a system that has relatively higher penetration of solar capacity. This overestimation is attributed to SMOKE's misrepresentation of the timing of peak emissions relative to their occurrence in the presence of solar generation. TDM shifts emissions to the morning and evening peak demand periods due to mid-day solar energy production, which we conjecture would lessen the potential for tropospheric O_3 formation [61]. Finally, our analysis of four policy scenarios demonstrates that the SMOKE profiles exhibited no discernible differences in emission patterns timing across the scenarios, only differences in their integrals (total emission levels). This inflexibility may result in an understatement of the impact of different scenarios on system operations and power emissions, particularly during the summer. In contrast, the TDM profiles result in more credible changes in system operation, variations in emission patterns, and timing of peak emissions that can be causally linked to weather patterns.

In summary, while GIP-SMOKE methods provide relatively quick assessments, they may introduce biases due to oversimplified emission patterns that fail to capture the dynamics of the energy transition, or insufficient consideration of uncertainties and complex interactions. As a result, these methods can anchor on historical emission patterns and average trends. In contrast, SAG-TDM methods are generally more responsive to policy and technology trends and better model system responses to weather. Thus, the SAG-TDM approach provide a more nuanced description of evolving emissions, better reflecting the distinctive characteristics and greater variability of renewable-based systems.

While the SAG-TDM downscaling method offers several advantages over traditional GIP-SMOKE approaches and is better suited for capturing the evolving characteristics of future power systems and emissions, it does come with a tradeoff. The implementation of SAG-TDM introduces an increased computational burden and adds complexity to the modeling framework. Consequently, for future research, we recommend conducting quantitative analyses and comparisons of air quality simulations and their ultimate human health impacts using emission scenarios generated by both the SAG-TDM and GIP- SMOKE methods. In particular, that method introduces additional complexity and requires additional model setup and coding effort. To apply SAG-TDM downscaling, researchers must con-vert the boundary conditions from the chosen aggregate model into the fine-grained in-puts required for the SAG-TDM model while maintaining consistency with assumptions about local power markets and policies. External data may also be needed to capture finer features or dynamics that are not present in the aggregate model. However, although more effort is needed for model and data development, computational speed becomes less of a concern (the difference in computation time between the two methods is typically within an hour in our experience). Altogether, this suggests that GIP-SMOKE may be preferable for policy makers needing quick, high-level insights when policy development timelines are tight. However, once the SAG-TDM model capability is developed, it will offer more detailed insights on locality-specific impacts to inform more extended and detailed policy processes.

Therefore, for future research, we first recommend conducting quantitative analyses and comparisons of air quality simulations and their ultimate human health impacts using emission scenarios generated by both the SAG-TDM and GIP-SMOKE methods. This comparative analysis could focus on evaluating the accuracy of results, computational efficiency, and identifying which methods are suited to various applications. Furthermore, validating downscaled results is essential. Future work could involve comparing historical simulation data with real-world observations (e.g., EPA CEMS data) to ensure accuracy. Lastly, we suggest additional applications, especially studies addressing equity issues in the energy transition process to assess how the benefits of overall emissions decreases are distributed. And for rapidly growing economies where coal generation will likely continue to dominate in coming years, fine-grained downscaling methods can address impacts of policies such as those in China that have emphasized conversion to natural gas in urban areas.

Support Information

Additional literature review on downscaling methods, model, data and processing methods, and additional simulation results and analysis for power system operations.

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