Overview of Progress and Findings from the Cross-EPA Coordination Effort for Understanding and Evaluating NOx Emissions Discrepancies

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Overview of Progress and Findings from the Cross-EPA Coordination Effort for Understanding and Evaluating NOx Emissions Discrepancies

U.S. Environmental Protection Agency
Office of Transportation and Air Quality
Assessment and Standards Division
Ann Arbor, MI

U.S. Environmental Protection Agency
Office of Research and Development
Atmospheric and Environmental Systems Modeling Division
Research Triangle Park, NC

U.S. Environmental Protection Agency
Office of Air Quality Planning and Standards
Air Quality Assessment Division
Research Triangle Park, NC

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1. Executive Summary

During 2013-2017, external groups published analyses suggesting that mobile source nitrogen oxide (NO_x) emission estimates developed by the U.S. Environmental Protection Agency (U.S. EPA) were too high by a factor of up to two. From 2015 to 2020, a cross-EPA workgroup met to coordinate complementary ongoing efforts in the Office of Air Quality Planning and Standards (OAQPS), the Office of Transportation and Air Quality (OTAQ) and the Office of Research and Development (ORD) to evaluate NO_x emissions and modeling. The workgroup's aim was to understand discrepancies between modeled estimates of atmospheric NO_X and total reactive nitrogen (NO_Y) concentrations and ambient measurements and determine whether these discrepancies were driven by mobile source emissions estimates or other model processes. The workgroup identified key parameters and processes impacting NO_x and NO_Y model predictions including: MOtor Vehicle Emission Simulator (MOVES) inputs and results, spatial and temporal allocation of emissions, meteorology, mixing, and dispersion treatment in air quality models, air quality model chemistry, and air quality model treatment of deposition. Smaller teams were formed to investigate key hypotheses addressing each of the parameters listed above. In a related effort, the Technical discussions on Emissions and Atmospheric Modeling (TEAM) team was formed as part of a cross-agency coordination effort between the U.S. EPA, the National Oceanic and Atmospheric Administration (NOAA) and the National Aeronautics and Space Administration (NASA).

Several major findings came out of the analyses undertaken by the workgroup. First, the overestimates were most common in the summer, with distinct morning and evening peaks. EPA's modeling system tended to underestimate NOx in winter. While the analyses did not find a unique explanation for the summer over-prediction of NO_x and NO_Y concentrations, they identified several plausible hypotheses, while ruling out others, for the NO_x positive biases seen at certain times and locations in the modeling. Model over-predictions were likely due to multiple compounding factors that each contributed to a portion of the bias.

Based on our review of the evidence, the most important contributing factor to the summer NOx bias was:

- Planetary boundary layer (PBL) and vertical mixing algorithms in the Community Multiscale Air Quality (CMAQ) model (version 5.0.2 and earlier) led to too little vertical mixing at certain times and in some locations. These algorithms have been improved in CMAQv5.1 and later versions of CMAQ. These changes substantially reduced the NOx bias, as well as the NOx diurnal bias pattern in simulations run with more recent CMAQ versions.

We also demonstrated that there is important uncertainty in the model bias caused by NO_X and NO_Y measurement uncertainty, as well as chemical mechanism used. Caution should be taken in using modeled NO_X bias to constrain NO_X emissions or processes incorporated into air quality modeling.

Through this effort, we identified aspects of the mobile source NO_x emissions that were overestimated in the evaluated air quality platforms. These could lead to important overestimation of NOx emissions, but based on our analysis so far, only had a modest impact on the magnitude and pattern of the bias in modeled NOx concentrations. We have identified and developed improvements to the NO_X mobile source emission inventory to address the summer overestimation of mobile-source NO_X, which include:

- MOVES light-duty NO_X emissions rates.
    - MOVES light-duty gasoline NO_X emissions were reduced in MOVES3 compared to MOVES2014b. The MOVES3 light-duty gasoline NOx rates are generally lower due to updated modeling of high-load operation and updated deterioration trends.
- MOVES inputs in the 2011 National Emissions Inventory (NEI) and EPA platforms
    - MOVES inputs used in the 2011 NEI and EPA modeling platform were not consistent with the ambient datasets to which they were compared when estimating bias. For example, speed and acceleration assumptions were not consistent with vehicle activity at remote sensing locations, long-haul truck hoteling activity was overestimated nationally, and MOVES inputs did not accurately model local variability in age distributions and car/truck splits. These inputs have been improved in MOVES3, the 2016v1 platform (U.S. EPA, 2021a) and the 2017 NEI.
- National nonroad equipment populations.
    - Nonroad equipment populations were overestimated in the 2015 and earlier platforms. These estimates were updated in the 2016 platform using updated nonroad population and activity data incorporated into MOVES2014b. These changes had a noticeable, but relatively small, impact on the NO_X bias.

EPA members of this workgroup have shared results and engaged with the scientific and regulated communities through continued participation in scientific conferences, workshops, journal articles and other outreach opportunities. Members of the workgroup chaired four special sessions focused on this topic at conferences which included 14 EPA presentations and 26 relevant presentations from outside groups (See Table 2). Findings from this work have also been shared in 24 conference presentations at 11 conferences (See Table 3). Analyses from this workgroup have resulted in five journal articles led by EPA authors (Referenced in Section 7.4).

Although the NOx evaluation workgroup is no longer active, work continues among EPA offices and staff to update and improve aspects of the emissions and modeling systems. This document serves to summarize our efforts and understanding of the NOx evaluation effort at the present time.

2. Problem Statement

This document describes the EPA exploration of a reported discrepancy between modeled estimates of nitrogen oxides (NO_X) and reactive nitrogen (NO_Y) concentrations and ambient measurements, particularly summertime overestimates. NOx is defined as NO + NO_2. Reactive nitrogen includes both NOx and oxidation products of NOx such as nitric acid (HNO_3). The mass of reactive nitrogen is more conserved in the atmosphere than NOx or individual reactive nitrogen species (Seinfeld & Pandis, 2006). The criticism and subsequent analysis focused on results from modeling systems using 2011-based inventories and centered on NO_X emissions from onroad mobile sources. Most of this work was done in 2016-2020.

3. Motivation/Background

Mobile source NO_X emissions have received considerable attention from the scientific community over the past 15 years since mobile sources are a major component of the inventory. For instance, mobile sources account for 58% of the NO_X in the U.S. EPA 2014 National Emissions Inventory (NEI) (Toro et al. 2021). In addition, many major point sources are better characterized than mobile sources since large point sources are generally equipped with Continuous Emission Measurement Systems. Therefore, when discrepancies between measured and modeled NO_X are identified, mobile sources have been a major focus.

EPA estimates air pollution emissions from onroad mobile sources (cars, trucks, buses, and motorcycles) using emission models that account for the turnover of the vehicle fleet to vehicles meeting newer emission standards. Over time, these models have been updated to account for changing vehicle and fuel regulations, improvements in vehicle technology, the impact of fuels and ambient parameters, new assessments of real-world vehicle activity patterns, and improved understanding of the various processes that contribute to vehicle emissions. The MOBILE series of models was developed beginning in 1978 and culminated with MOBILE6.2 in 2004. In 2002, EPA began work on the MOtor Vehicle Emission Simulator (MOVES) (https://www.epa.gov/moves), which was first released for official use as MOVES2010. MOVES was first used to calculate mobile source emissions for the NEI in 2008. Recent versions of MOVES also incorporated EPA's NONROAD model that estimates emissions from nonroad mobile sources such as construction and lawn and garden equipment. The data and detail in these models of onroad emission inventories has improved substantially over the last few decades as summarized in Table 1.

Table 6.1: MOVES Version History

Public Releases	Release Date	Key Features
MOBILE1-MOBILE6.2	1978-2004	• Predecessor to MOVES • Estimated g/mi onroad emissions • Increased scope and complexity over time
NONROAD	1998-2010	• Predecessor to MOVES • Estimated emissions for nonroad sources
MOVES2010	2010	• New model for onroad emissions • Incorporated vehicle activity • Designed to model at project, county, and national scales
MOVES2010a	2010	• Modeled 2012+ Light-Duty (LD) Green House Gas (GHG) rule
MOVES2010b	2012	• Performance improvements • Improved vapor venting calculations
MOVES2014	2014	• Modeled Tier 3 and 2017+ LD GHG rules • Updated gasoline fuel effects • Improved evaporative emissions • Improved air toxics • Updated onroad activity, vehicle populations and fuels • Incorporated NONROAD model
MOVES2014a	2015	• Added nonroad VOC and toxics • Updated default nonroad fuels • Added new options for user Vehicle Miles Travelled (VMT) input
MOVES2014b	2018	• Improved emission estimates for nonroad mobile sources • Updated outputs used in air quality modeling
MOVES3[1]	2020	• Updated onroad exhaust emission rates, including Heavy-Duty (HD) GHG Phase 2 and Safer Affordable Fuel Efficiency (SAFE) rules • Updated onroad activity, vehicle populations and fuels • Added gliders and off-network idle • Revised inputs for hotelling and starts
MOVES3.0.1	2021	• Fixed several small issues with processing and aggregation, making it easier to use the model for variety of applications. • Included scripts to assist with checking MOVES3 submissions for the 2020 National Emissions Inventory

[1] MOVES3 and subsequent minor releases and "patches", are documented at https://www.epa.gov/moves/moves3-update-log and https://github.com/USEPA/EPA_MOVES_Model.

Air quality models are often used to predict the fate and transport of atmospheric pollutants such as NO_X. Photochemical air quality models such as the Community Air Quality Model (CMAQ; U.S. EPA 2021b) and the Comprehensive Air quality Model with extensions (CAMx; Ramboll, 2020) simulate the impacts of pollutant emissions, dispersion, chemical reactions, and deposition on air pollution concentrations across a 3-dimensional grid. Air quality model output can be applied to project compliance with National Ambient Air Quality Standards (NAAQS) and to estimate the human health benefits of regulations that reduce air pollution emissions. Emissions are an important input into these models and are often derived from the NEI in the U.S., which is released in full on a triennial basis, although point source emissions are released annually. The NEI includes emissions estimates from a variety of sources including onroad and nonroad mobile sources. Prior to 2008, the NEI onroad emissions were estimated using the MOBILE series of models. MOVES2010b was used for the 2008 NEI and the 2011 NEI, and versions of MOVES2014 were used for the 2014 and 2017 NEI (U.S. EPA, 2013; U.S. EPA, 2015; U.S. EPA, 2018d; U.S. EPA, 2021e; Toro et al., 2021). NEI emissions are generally reported at spatial and temporal resolution that is not sufficiently resolved for photochemical air quality models. In order to address this, NEI emissions are processed through the Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System to create gridded, speciated, hourly emissions for input into a variety of air quality models such as CMAQ and CAMx. SMOKE supports area, biogenic, mobile (both onroad and nonroad), and point source emissions processing for criteria and toxic pollutants. Note that for 2008-and-later NEIs, hourly, gridded onroad emissions are calculated using the SMOKE-MOVES tool and then totaled for the NEI.

Some studies in the literature have used comparisons between model predictions and ambient measured pollutant concentrations to evaluate the accuracy of emissions inventories. Prior to the release of EPA's 2011 NEI, published studies found varying model performance for NO_X. Kota et al. (2014) compared CMAQ modeling of Houston using inventories generated with MOBILE6.2 and MOVES2010, finding that use of MOVES increased the overestimation of NO_X, particularly in areas where mobile sources represent more than 90% of the NO_x. Brioude et al. (2011) performed inverse modeling for NO_Y using flight data from the Texas Air Quality Study in 2006 (TEXAQS II) and found good agreement with NEI 2005 (based on MOBILE6 for onroad emissions) for urban Houston as a whole, but there were large overestimates for the Houston Ship Channel. Marr et al. (2013) found good agreement in Norfolk between measurements and hourly inventory estimates based on EPA's 2008 NEI which used the MOVES model.

EPA's 2011 NEI and the associated 2011 emissions modeling platform were widely applied for scientific and regulatory purposes. Scientific investigations compared emissions based on the 2011 NEI or model outputs from simulations using those emissions to measurements made in various field campaigns in the summers of 2011 and 2013 as well as other available ambient measurement and satellite data. Several external groups produced analyses suggesting that EPA's 2011 NEI estimates of NO_X emissions were too high. Anderson et al. (2014) compared NEI estimates of emitted carbon monoxide (CO) to NO_Y ratios to measurements made on aircraft flights of the Baltimore/Washington D.C. metro area in July 2011 and concluded that 2011 EPA mobile source NO_x emissions were overestimated by 51%-70%. They specifically recommended scaling EPA mobile emissions by a factor of 0.5 to improve model performance. Canty et al. (2015) expanded on the

work from Anderson et al. (2014) and reported that cutting mobile NO_X emissions in half improved modeled predictions of NO_X concentrations across the eastern U.S. Souri et al. (2016) applied satellite NO_2 estimates in an inverse modeling analysis over southeast Texas for the summer of 2013 to constrain NO_X emissions from different source types. Their model results point to overestimates of NO_X emissions from area, point and mobile sources in urban areas and underestimates of soil and area source NO_X emissions in rural areas. Souri et al. found that reducing mobile source emissions by 30% improved agreement between modeled and measured ground-level NO_2 from the 2013 DISCOVER-AQ Texas Campaign. Travis et al. (2017), also investigated summer 2013 NO_X emissions estimates (scaled from 2011 emissions) in the Southeastern U.S. Travis et al. used a variety of data sources including satellite NO_2, aircraft NO_X measurements from the SEAC4RS field campaign, and routine NADP nitrogen deposition measurements to conclude the 2011 NO_X emissions were too large. They found that reducing NO_x by 63% from all sources other than power plants led to improved model performance. One caution about using satellite NO_2 data to constrain emissions came from Kemball-Cook et al. (2015) who found large differences between two Ozone Monitoring Instrument (OMI) NO_2 retrievals. When applying these two different satellite retrievals to an inverse modeling problem, one suggested that NO_X emissions inventories in Texas were too high while the other suggested that NO_X emissions inventories in Texas were too low.

Separately, McDonald et al (2018) developed mobile source emissions rates per mass of fuel burned derived from near-road remote sensing data. These emissions rates were multiplied by state-level fuel sales to estimate total NO_X emissions. When McDonald et al. (2018) compared their inventory to the 2011 NEI-based emissions, they found that the fuel-based inventory had 50% lower NO_X emissions for onroad gasoline vehicles but 10% higher NO_X emissions for onroad diesel sources than the 2011 inventory. Overall, these results led to 10% lower total NO_X emission (from all sources) in rural areas and 20% lower total NO_X emissions in urban areas than the 2011 NEI.

While individual studies have uncertainties and limitations, together they suggested that ambient NO_X and NO_Y estimates produced by various modeling systems using 2011-based inventories were high and that additional investigations by EPA were warranted.

4. Cross-EPA Coordination Effort for Understanding and Evaluating NO_x Emissions Discrepancies: Structure and EPA Participants

In 2015, various U.S. EPA offices were involved in independent complementary efforts to understand and characterize mobile source emissions. OTAQ simultaneously conducted MOVES development, quality assurance, and validation activities. Within OAQPS, there were projects evaluating CMAQ and CAMx NO_X predictions using the 2011v2 emissions. Staff in EPA's former National Exposure Research Laboratory had projects underway to evaluate CMAQv5.1 for 2011, as well as projects analyzing satellite data and field measurements to understand NO_x sources. Finally, staff in EPA's former National Risk Management Research Laboratory (NRMRL)and OAQPS examined the NO_X measurement data from near-road field campaigns in Detroit and Las Vegas.

A cross-EPA coordination group was initiated to 1) increase communication and coordination between the groups that were already working on various aspects of evaluating EPA NO_X emissions and model estimates and 2) allow for cross-office prioritization of analyses and research questions that would advance our understanding of NO_X emissions, atmospheric transformation and fate.

The coordination group held conference calls 5-10 times per year. In addition, six smaller subsets of the coordination group formed teams that focused on specific topics. Those teams evolved, and new efforts and collaborations are continuing.

The foci of the initial six working teams were:

1. Use Detroit and Las Vegas near-road measurements to evaluate MOVES emissions factors
2. Use traffic counts from Detroit, Las Vegas, and other sources to develop/evaluate temporal patterns to inform temporal allocation of mobile source emissions
3. Conduct in-depth and targeted photochemical model (CMAQ and CAMx) evaluation of NO_Y species to diagnose important model processes contributing to bias in predictions of these chemical constituents
4. Evaluate MOVES against roadside, tunnel, and on-road measurements from the literature
5. Conduct targeted MOVES sensitivity simulations to understand the range of MOVES results that could be obtained different input assumptions such as vehicle speed and acceleration and fleet age and composition.
6. Further evaluate $CO:NO_Y$ to determine the usefulness of this metric for understanding NO_X emissions errors.

Cross-EPA coordination team members[2] included:

- Office of Air and Radiation
    - Office of Air Quality Policy & Standards
        - Pat Dolwick
        - Alison Eyth
        - Barron Henderson
        - Shannon Koplitz
        - Chris Owen
        - Sharon Phillips
        - Norm Possiel
        - Venkatesh Rao
        - Heather Simon – Coordination Team Lead
        - Brian Timin
        - Jeff Vukovich
    - Office of Transportation and Air Quality
        - Chad Bailey
        - Sudheer Ballare[3]
        - Megan Beardsley
        - David Choi
        - Jaehoon Han
        - Harvey Michaels
        - Sarah Roberts
        - Darrell Sonntag

[2] Some people have retired or moved on to other roles since the start of the project

[3] Former ORISE participant hosted by EPA, supported by an interagency agreement between EPA and DOE

        - Claudia Toro[3]
        - James Warila
        - Margaret Zawacki
- Office of Research and Development, Center for Environmental Measurement & Modeling
        - Wyat Appel
        - Jesse Bash
        - Kristen Foley
        - Deborah Luecken
        - George Pouliot
        - Havala Pye
        - Luke Valin
        - Sue Kimbrough

5. EPA Assessment as of 2016

An initial evaluation of NO, NO_2, and NO_Y was conducted for EPA's 2011 emissions modeling platform (including mobile emissions from MOVES2014b), and air quality modeling using CMAQ. Figure 1 shows modeled NO_X bias for summer months at all Air Quality System (AQS) monitors across the U.S. for three consecutive public releases of CMAQ, shown by hour of day. The evaluation found that NO_x and NO_Y (not shown) were overpredicted at night and during morning and evening rush-hour but were unbiased or even underpredicted at mid-day, forming a "bridge pattern." NO_X biases progressively decreased as CMAQ matured. CMAQv5.0.2 was the model that was employed by Anderson et al. (2014). The largest improvement occurred from CMAQv5.0.2 to CMAQv5.1 because substantive updates were made to the model's treatment of vertical mixing in the boundary layer. The increased vertical mixing in the CMAQv5.1 version contributed to decreasing the ground level NO_X and NO_Y concentrations at night and during morning and evening transitions, which reduced model overpredictions. Other updates in model processes and inputs also had moderate impacts on predicted NO_X concentrations.

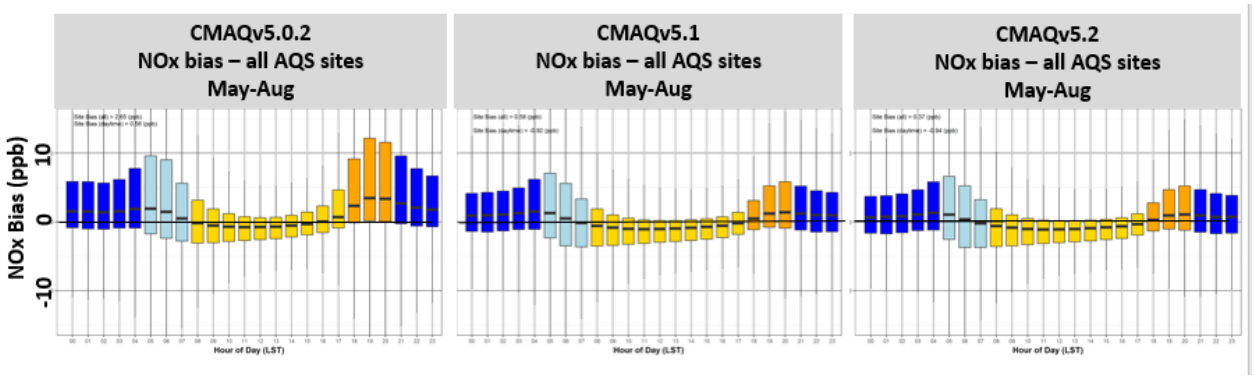

Figure 1: CMAQ 2011 summertime NO_x bias shown by hour of day. Boxes show the interquartile range of bias for each hour of day.

A comprehensive model evaluation was conducted for the CMAQv5.1 modeling system using a series of 2011 simulations (Appel et al. 2017). While NO_X evaluation was not the primary focus of this paper,

diurnal profiles of NO_X performance were included for each season across all AQS NO_x monitors (Figure 2). This figure shows a similar summertime pattern of NO_X bias as Figure 1, with overpredictions overnight, peaking during morning and evening rush-hours, but minimally biased or underpredicted NO_X values at mid-day. Appel et al (2017) provided additional insight into the seasonal nature of this bias by showing that while the evening rush-hour overprediction was a common feature in all seasons, the model tended to underestimate NO_X overnight and during morning rush hour and during daytime hours for fall, winter, and spring seasons.

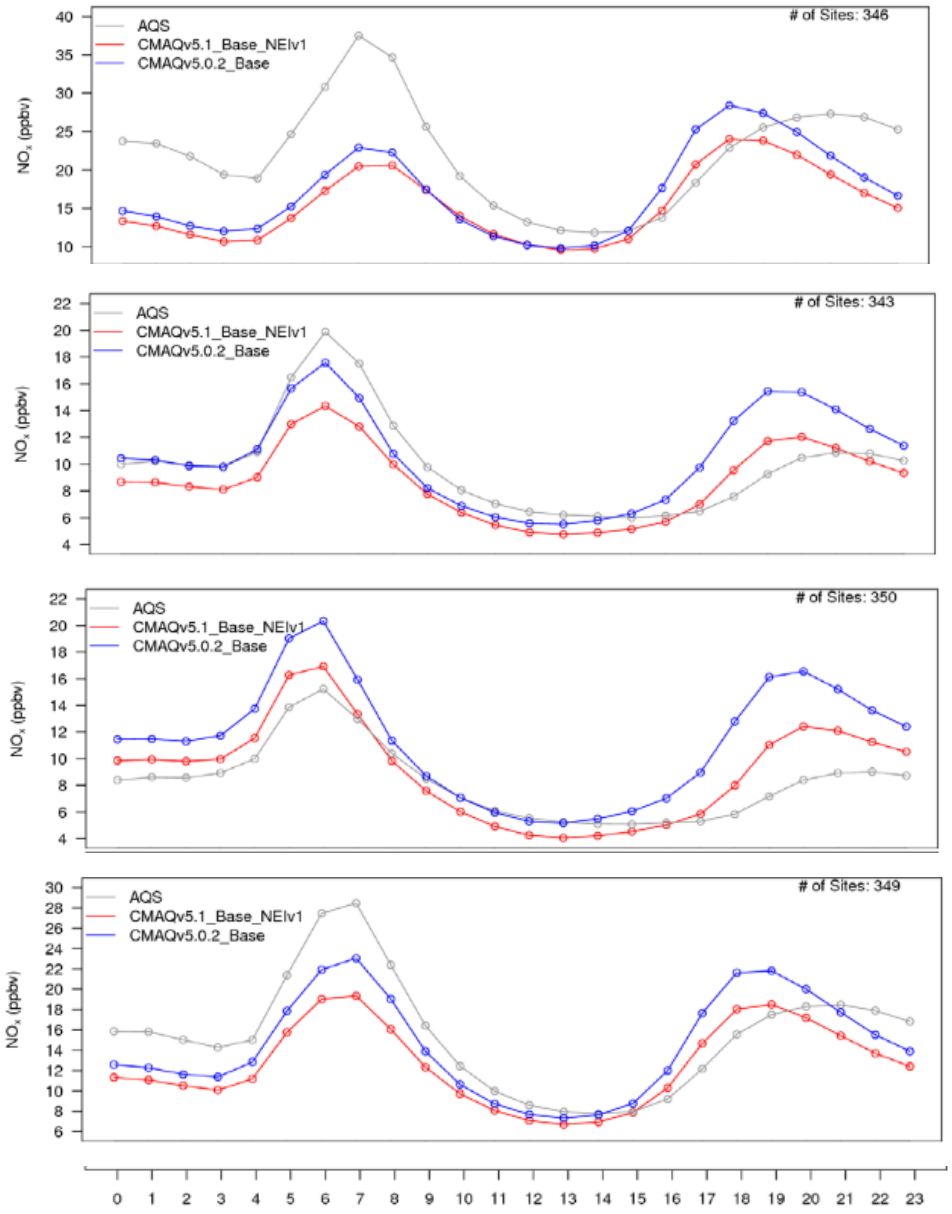

Figure 2 (adapted from Appel et al., 2017): Diurnal time series of NO_x (ppb) from AQS observations (gray), CMAQv5.0.2 (blue) and CMAQv5.1 (red) for winter (top), spring (top middle), summer (bottom middle) and fall (bottom).

Several EPA evaluations of the 2011 modeling system suggested the need to conduct additional bottom-up comparisons, and targeted model evaluations of specific aspects of MOVES, SMOKE, CMAQ, and CAMx. EPA staff recognized the complex and multifaceted nature of the modeling system, which includes emissions from many different sources with varying spatial and temporal patterns and model treatment of chemical and physical atmospheric processes that impact NO_Y composition, transport, and lifetime. In addition, comparisons between models and measurements are not always straightforward. Measurement artifacts and uncertainties must be considered as well as differing spatial and temporal resolution of the models and the measurements as described below. Figure 3 shows a schematic of the modeling systems and shows how different parties are responsible for different portions of the system underscoring the need for a collaborative process to evaluate NO_X emissions inventories and model predictions.

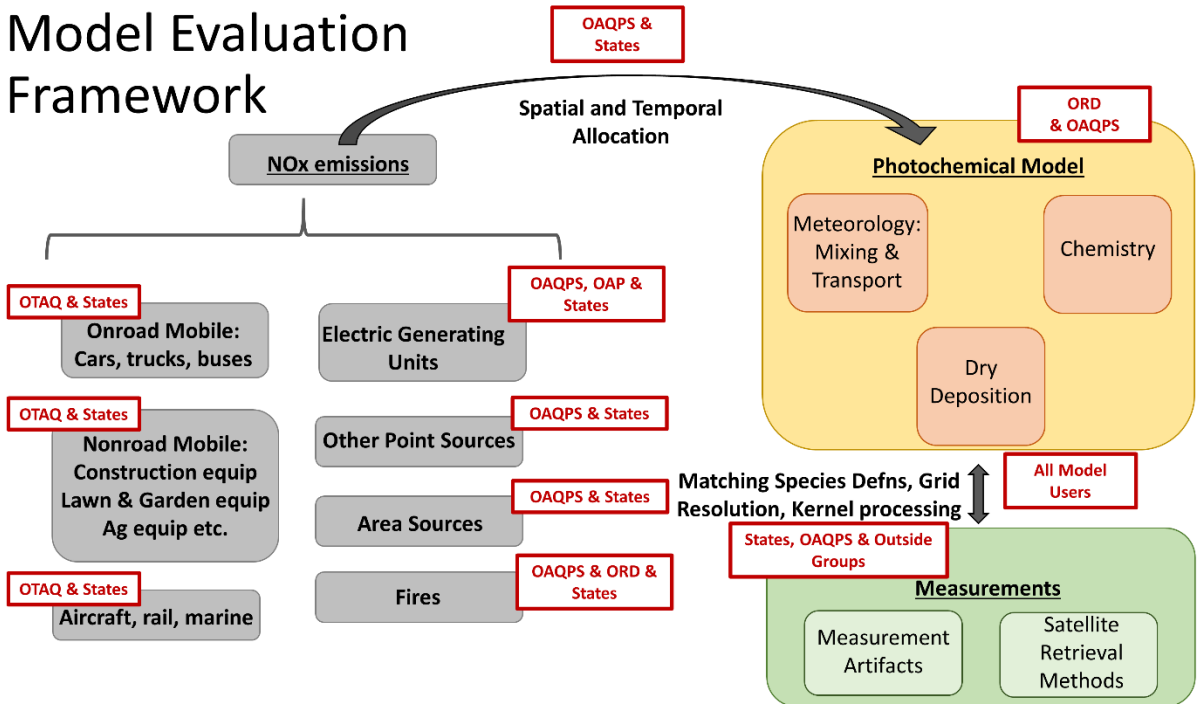

Figure 3: Schematic of NO_X model evaluation framework and parties responsible for different aspects of the system.

6. Key Hypotheses and Progress

The NO_X evaluation coordination group identified a list of potential hypotheses to explain discrepancies between modeled and observed NO_X concentrations. These hypotheses included errors or uncertainties in the air quality models (i.e., treatment of meteorology, chemistry, dry deposition and grid-resolution), issues with the measurement data (i.e., uncertainties in satellite retrieval algorithms, spatial representativeness of measurements, and NO_Z (i.e. NO_Y-NO_X) measurement artifacts for AQS NO_X monitors) and assumptions built into the emissions inventories (i.e., mobile source emissions rates and vehicle fleet/activity assumptions, as well as emissions estimates from other sources of NO_X).

The details of U.S. EPA investigation of these and other hypotheses is provided below.

6.1 Model biases related to uncertainties in specifying photochemical processes in the air quality model or model evaluation methods

Hypothesis 1.1: Model bias is caused by NO_X and NO_Y measurement uncertainty

Status *with regard to aircraft measurements taken from the DISCOVER-AQ Baltimore field campaign: This hypothesis has been investigated and found to have an important impact on air quality model NO_X bias.*

Comparison of model output to NO_Y measurements made from aircraft during the DISCOVER-AQ Baltimore field campaign using different types of instruments results in very different model biases (Figure 4). NO_Y component species were measured both using the chemiluminescence and the thermal-dissociation laser-induced fluorescence (TD-LIF) instruments. The chemiluminescence instrument measured total NO_Y and provided the data used in Anderson et al. (2014). Summing the NO_Y component species ($\sum NO_{Y,i}$) measured by both the chemiluminescence and TD LIF instruments provides an independent estimate of measured NO_Y. CMAQ model simulations using the CB05 chemical mechanism had normalized mean NO_Y biases of 76% and 49% when comparing to the chemiluminescence NO_Y and $\sum NO_{Y,i}$ measured values, respectively. CMAQ model simulations using the CB6 chemical mechanism had normalized mean NO_Y biases of 51% and 28% when comparing to the chemiluminescence NO_Y and $\sum NO_{Y,i}$ measured values, respectively. These results were presented in Simon et al (2018a,b) and Toro et al (2021).

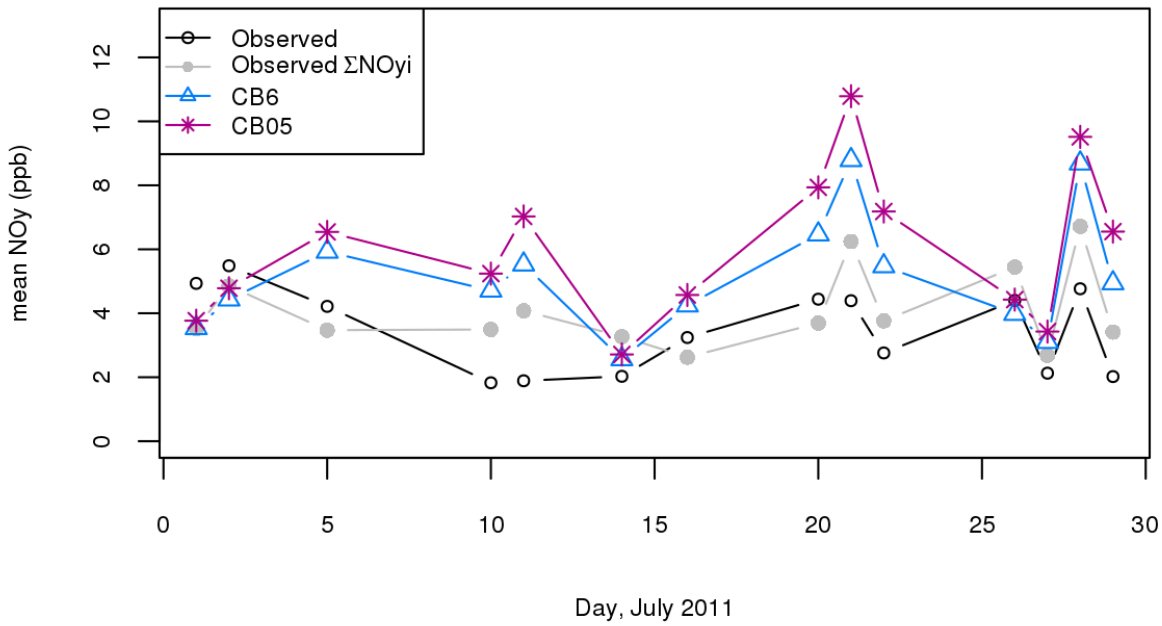

Figure 4: Daily average NO_y values of all DISCOVER-AQ Baltimore aircraft measurements taken within the planetary boundary layer. Black and gray lines represent measurements made using chemiluminescence and TD-LIF instruments, respectively. Blue and purple lines represent daily average of all modeled NO_y values that were matched in space and time to the DISCOVER-AQ Baltimore aircraft measurements.

***Status** with regard to ground-based monitors: This hypothesis has been explored and suggests likely NO_X bias may be underestimated by comparisons against ground-based monitors.*

Ground-based NO_X monitors commonly used in state and local monitoring networks reported in the AQS have known measurement artifacts. Monitors using EPA's Federal Reference Method (FRM) are known as chemiluminescence instruments. Within the instrument, NO is oxidized into excited NO_2 which fluoresces at specific wavelengths. The FRM monitors alternately sample ambient air to measure NO concentrations and air that has been routed over a catalyst to reduce ambient NO_2 to NO before directing the sampled air to the chemiluminescence instrument. In this way, the instrument is intended to measure both NO and NO_2 concentrations. The catalyst, however, is non-specific and will reduce other NO_Z compounds to NO. In monitors intended to measure NO_X as opposed to NO_Y, the catalyst is often located at the end of a sampling line such that a portion of reactive NO_Z compounds will adsorb to the line and not reach the sensor. Despite some adsorption to the sample line, these monitors often report NO_Y species as part of NO_x measurements (Dunlea et al., 2007; Dickerson et al., 2019). As a result, measurements are artificially inflated, suggesting that model overpredictions from comparisons against ground-based monitors might be amplified, if this impact were not considered.

Hypothesis 1.2: Model bias is caused by comparing modeled grid-cell average concentrations to measurements made at a finer spatial resolution.

Status *<u>with regard to aircraft measurements:</u> This hypothesis has been explored and is not likely a driving cause of air quality model NO_X bias*

During DISCOVER-AQ (Baltimore/Washington, Houston, and Denver/Front Range) P-3 spirals were approximately 4 km in diameter which is a finer resolution than model grid-cells for simulations conducted at 12km resolution. Analysis of different ways to match modeled grid concentrations to DISCOVER-AQ aircraft measurements showed that model bias is sensitive to sampling error, but all tested sampling schemes generally still result in an NO_Y overprediction (Figure 5). These results were presented by Simon et al. (2018b).

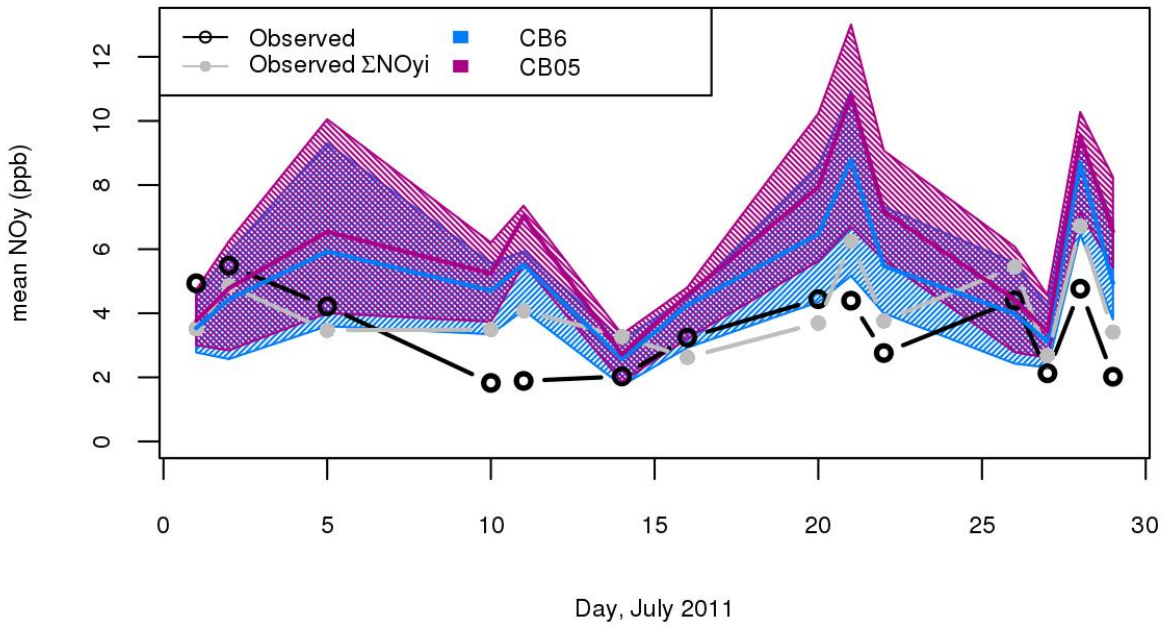

Figure 5: Daily average NO_y values of all DISCOVER-AQ Baltimore aircraft measurements taken within the planetary boundary layer. Black and gray solid lines represent measurements made using chemiluminescence and TD-LIF instruments, respectively. Blue and purple solid lines represent daily average of all modeled NO_y values that were matched in space and time to the DISCOVER-AQ Baltimore aircraft measurements. For solid lines, model values represent matching a measurement location to a grid cell (horizontal and vertical) and measurement time to the closest hour. Shading represents the range of model values from sampling +/- 1 grid cell in each direction and +/- 1 hour.

Status *<u>with regard to ground-based monitors</u>: Hypothesis has not yet been actively explored*

This hypothesis has not yet been explored in-depth for ground-based monitors. A potential follow-up would include analyzing modeled vs. measured concentrations from 2017 and 2018 field campaigns using forthcoming 4km resolution modeling simulations. Some insight may be gained by comparing performance of multiple model simulations conducted using different grid resolutions and examining within-cell variability in measured data by identifying locations with multiple monitors within a single modeled grid cell.

Hypothesis 1.3: The planetary boundary layer (PBL) and vertical mixing algorithms in photochemical models lead to too little vertical mixing at certain times and in some locations.

Status: *This hypothesis has been explored and found to have an important impact on air quality model NO_X bias. Updates to vertical mixing in the CMAQ model substantially reduced the NO_X overprediction, but did not completely resolve the discrepancy.*

Evidence suggests that the PBL and vertical mixing algorithms in CMAQ versions 5.0.2 and earlier led to too little vertical mixing at certain times and locations, especially at night and during morning and evening transition periods when the PBL rises quickly (morning) and collapses quickly (evening).

Extensive work has occurred to update vertical mixing schemes in CMAQ (starting with CMAQv5.1). Specifically, updates were made both to the Pleim-Xiu land-surface model within CMAQ and the asymmetric convective mixing version 2 PBL scheme within both the Weather Research Forecasting (WRF) and CMAQ models. In addition, errors in the CMAQ calculation of the Monin–Obukhov length (MOL) calculation were corrected (Appel et al., 2017). The impacts of improved representation of vertical mixing were shown in Henderson et al. (2017a; 2017b) and in Toro et al (2021). Figure 6 (right) (reproduced from Toro et al., 2021) shows the dramatic improvement in 2011 NO_X bias between model simulations conducted using CMAQv5.0.2 and CMAQv5.1 at monitors in four urban areas. Additional testing showed that most of the NO_X changes between the simulations at these monitors were attributable to the vertical mixing updates included in CMAQv5.1. The changes to the modeled PBL had the largest impact on the air quality model NO_X bias of all the hypotheses evaluated.

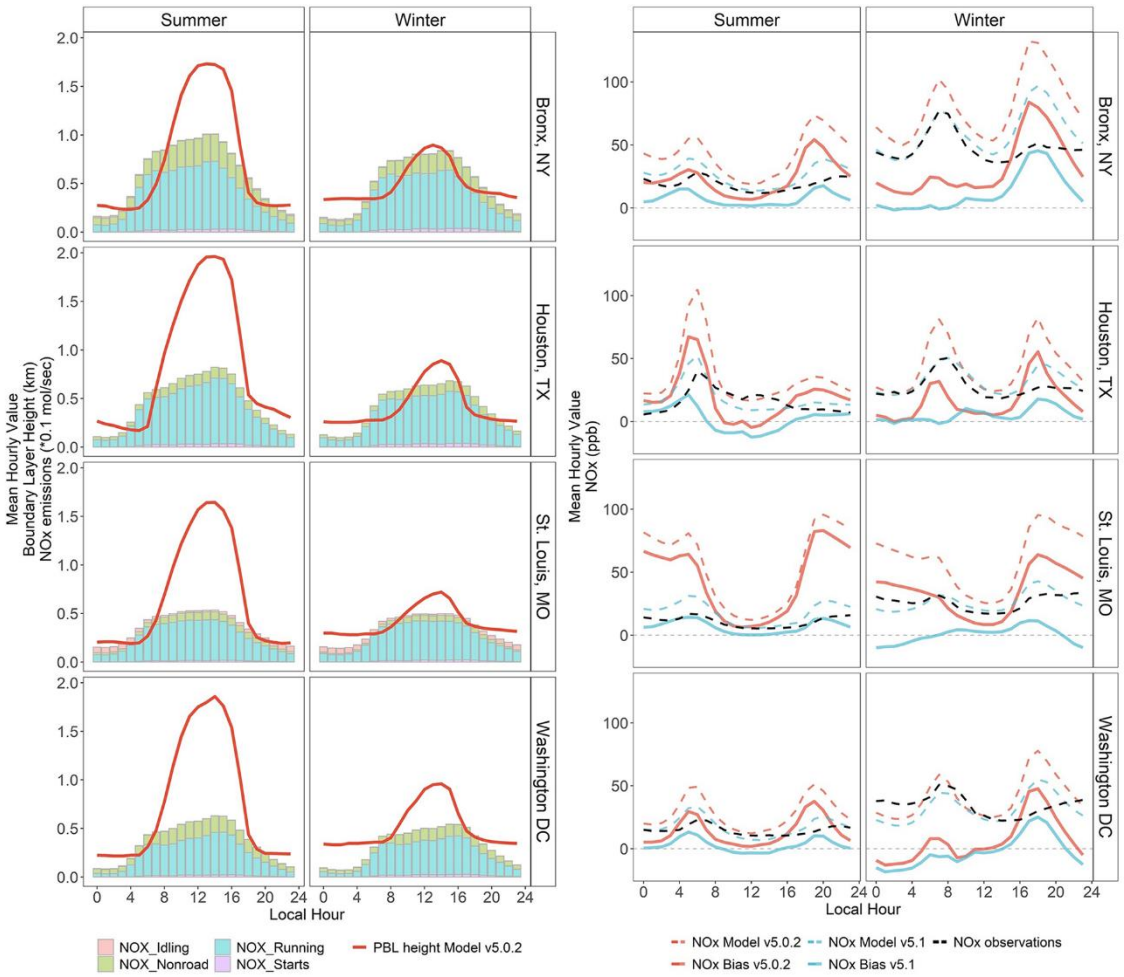

Figure 6 (from Toro et al., 2021) Seasonal differences in diurnal profiles of NO_X bias, mobile NO_X emissions, and modeled boundary layer. Summer and winter diurnal profiles for modeled average boundary layer height, NO_X onroad + nonroad emissions (left panel), NO_X observations, NO_X modeled mixing ratios, and calculated bias (right panel). NO_X bias and mixing ratios are shown for two Community Multiscale Air Quality (CMAQ) versions (v5.02 and v5.1) for multiple urban areas in 2011. Emissions are scaled by 0.1 for all sites. The boundary layer height values for CMAQv5.0.2 come from WRFv3.4.

While the PBL updates substantially reduced NO_X overprediction, the discrepancy between measured and modeled concentrations was not completely resolved. Other groups (e.g., modelers at the state of New York) have continued to explore the impact of different meteorological parameterization of mixing on modeled NO_x concentrations. In addition, new ceilometer measurements that are becoming available as part of the PAMS network and the unified ceilometer network (UCN, https://alg.umbc.edu/ucn/) provide hourly PBL height information that can be used to evaluate modeled PBL schemes. The techniques for interpreting ceilometer measurements are still under development. However, this new dataset will provide a more direct way to evaluate current model PBL estimates, especially during morning and evening hours. EPA staff plan to work with these new measurements and apply them to more fully understand model PBL performance.

Hypothesis 1.4: Dry deposition velocities for NO_Y species are too low in CMAQ

***Status**: This issue has been investigated and is not likely a driving cause of air quality model NO_X bias*

In CMAQ v5.3, the parameterization of NOx and PAN deposition from Pleim and Ran (2011) and alkyl and peroxy nitrates from Nguyen et al. (2015) is used for the stomatal/mesophyll resistance. Laboratory studies showed that approximately 80% vegetative sink of PAN is via stomatal uptake (Sun et al., 2016) while micrometeorological field experiments typically estimate a smaller stomatal sink (25-50%: Wolfe et al., 2009; Turnipseed et al., 2006). However, an equal amount of the measured flux may be explained by thermal decomposition resulting in similar (approximately 20%) non-stomatal fluxes as reported in laboratory experiments (Wolfe et al., 2009). CMAQ v5.3 has a parameterization of PAN deposition (Pleim and Ran, 2011) to non-stomatal surfaces consistent with Turnipseed et al. (2006) and higher than many other contemporary models (Wu et al., 2012). In a sensitivity study, the mesophyll resistance reactivity factor was decreased by an order of magnitude from the initial values of Pleim and Ran, 2011 to match that of O_3, near the values reported by Wolfe et al. (2009), and similar changes were made to the mesophyll reactivity factor for alkyl and peroxy nitrates to bound the impact that this parameter has on the overall modeled **NO_Y** budget. This was a bounding experiment as PAN is the only organic nitrate documented to react with the enzyme nitrate reductase in the mesophyll (Sparks, 2009). The non-stomatal CMAQ deposition velocity was not changed as it is already at the high end of the observed values (Wu et al., 2012). The results of model sensitivity simulations show little impact, less than 1% difference in the modeled ambient concentration, of updates to surface resistance for alkyl nitrates and peroxy nitrates. This is likely due to the high solubility of these species and the limiting resistance is the stomatal resistance. These simulations and previous studies revealed that the dry deposition velocity of NO_z species is already at the high end of the observations (Wu et al., 2012) and further increases would lead to unrealistic deposition rates and is unlikely to be a driver of NO_Y overpredictions. Additional work to update land use (i.e., more accurately specifying land vs. water cells) had both decreased and increased NOy concentrations near coastal areas due to the parameterization of mixing and differences in surface areas between vegetated land and water surfaces. There is ongoing work to investigate updates to VOC deposition, which appears to have some impact on alkyl nitrate and peroxy nitrate concentrations but does not appear to affect other NO_Y species.

Hypothesis 1.5: Model chemical mechanisms may not properly characterize individual organic nitrogen species, particularly their solubility, formation, reaction rates and products, so it is possible that more deposition and decay is occurring than predicted

***Status:** This issue has been explored and results indicated that including additional alkyl nitrate species in the model substantially lowered NO_Y concentrations but had little impact on NO_x concentrations. Understanding the NO_x lifecycle continues to be an active area of mechanism development.*

Evaluation of NO_Y species with different chemical mechanisms shows that the choice of chemical mechanism impacts NO_Y model performance, with the newer CB6 mechanism outperforming the older CB05 mechanism (Figure 4). However, further modifications to the

chemistry cannot reduce total NO_Y without adding to the overpredictions of HNO_3, as shown in Figure 7 reproduced from Toro et al. (2021). The results were first presented at the Atmospheric Chemical Mechanisms Conference (Simon et al., 2018b) and are described in more detail in Toro et al (2021).

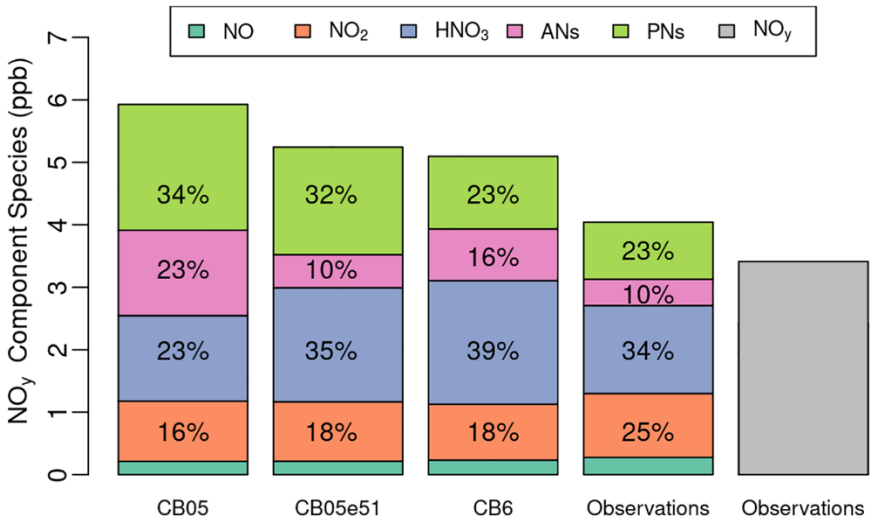

Figure 7 (reproduced from Toro et al., 2021) Aggregated model predictions and measurements of NO_Y species. All measurements considered are within the boundary layer over all flight days part of the July DISCOVER-AQ 2011 field study near Baltimore, MD. Bars representing observations are derived from both LIF (NO_2, HNO_3, alkyl nitrates, peroxy nitrates) and chemiluminescence (NO and NO_Y) instruments. NO_Y is shown as a gray bar. DISCOVER-AQ = Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality.

Separately, EPA researchers led an effort to create a detailed chemical treatment of organic nitrate species. Specifically, Zare et al. (2019) characterized their solubility, formation, reaction rates, and products using an update to the RACM2 chemical mechanism. When modeling a summer 2013 episode, Zare et al. (2019) showed that the updated chemical treatment reduced the model prediction of alkyl nitrate species from a factor of 2 overestimate to a 32% underestimate at a rural measurement site in Alabama. Understanding and representing the sinks of NO_X in atmospheric models continues to be an area of active research (e.g., Vasquez et al. 2020).

Hypothesis 1.6: Model bias is due to some unique feature of the 2011 modeling platform

Status *<u>for summertime:</u> This hypothesis has been explored and is not likely a driving cause of air quality model NO_X bias.*

NO_X bias is not unique to 2011 and is seen throughout 2002-2012 model simulations using CMAQv5.0.2. Model bias decreased over this time period as observed NO_X decreased. The NO_X bias has decreased further in modeling of 2013-2017 that used more recent model versions (e.g., CMAQv5.1, v5.2, and v5.3). The model overprediction in the most recent CMAQ v5.3 simulations using 2016 emissions shows substantially lower bias than was seen in simulations of 2011. These results are shown in Figure 8 and were presented at the 2019 CMAS and AGU conferences (Foley et al., 2019; Simon et al., 2019) and in Toro et al. (2021).

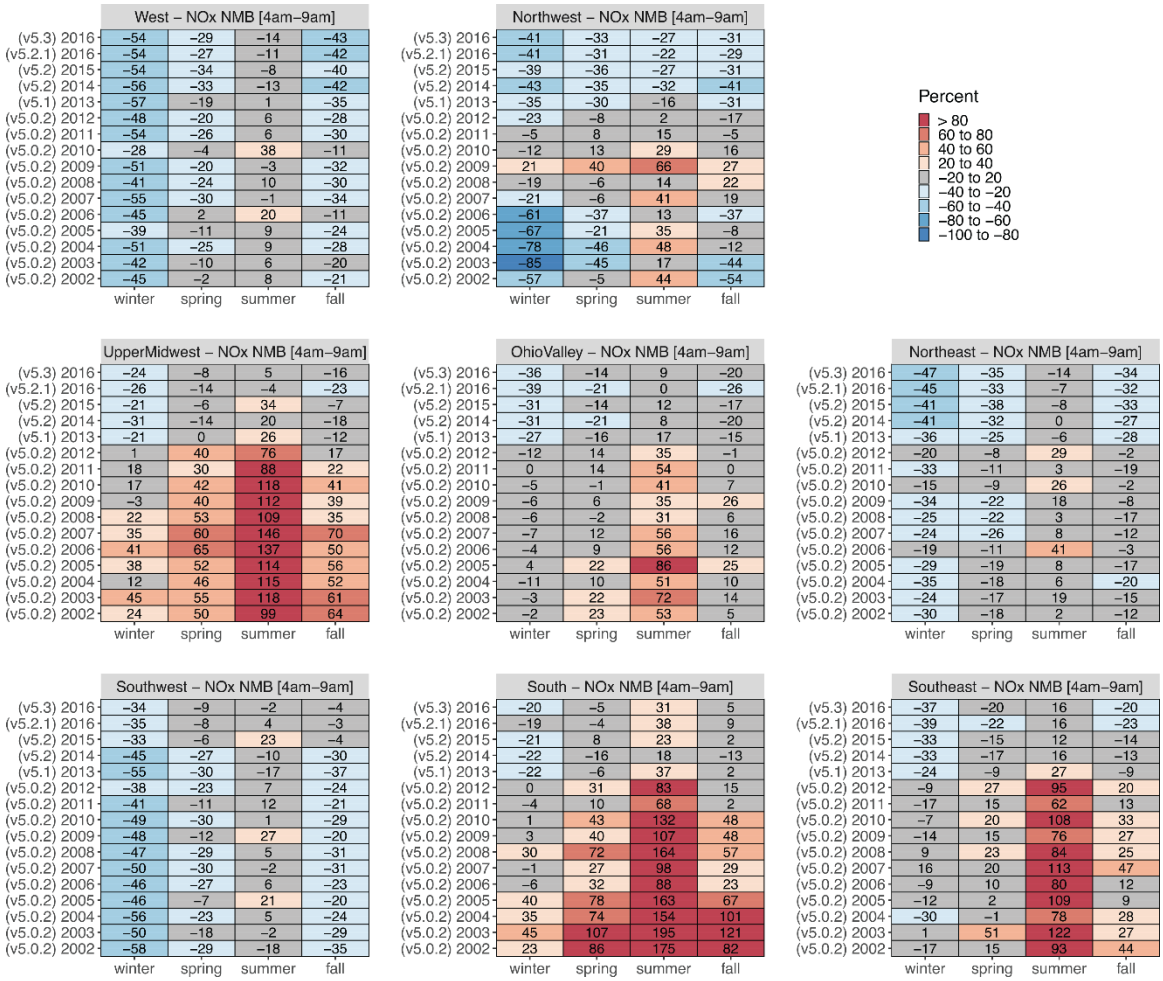

Figure 8 (from Toro et al., 2021) Normalized mean bias of morning modeled NO_X minus observed NO_X. Morning hours are 4–9 AM LST. Morning bias is aggregated by season for each annual simulation across monitors in multiple regions. Community Multiscale Air Quality model version used for each simulated year is shown in parentheses. Reds indicate model overprediction, and blues show model underprediction. West = CA and NV; Northwest (combined with the Northern Rockies and Plains) = OR, WA, ID, MT, NE, ND, SD, and WY; Upper Midwest = IA, MI, MN, and WI; Ohio Valley = IL, IN, KY, MO, OH, TN, and WV; Northeast = CT, DE, ME, MD, MA, NH, MJ, NY, PA, RI, and VT; Southwest = AZ, CO, NM, and UT; South = AR, KS, LA, MS, OK, and TX; and Southeast = AL, FL, GA, NC, SC, and VA.

Status *<u>for seasons other than summer:</u> This hypothesis has been explored and is not likely a driving cause of air quality model NO_X bias.*

In winter months, NO_X is underpredicted during most hours of the day except during evening rush-hour (Figure 9). Similar to findings for summer for simulations from 2002-2016, modeled winter NO_X concentrations have decreased more than observed winter NO_X concentrations. Consequently, at times and locations with NO_X underpredictions, these underpredictions have worsened. Conversely, the evening hour NO_X overpredictions have decreased over this time period. These results were presented at the 2019 CMAS and AGU conferences (Foley et al., 2019; Simon et al., 2019) and in Toro et al. (2021).

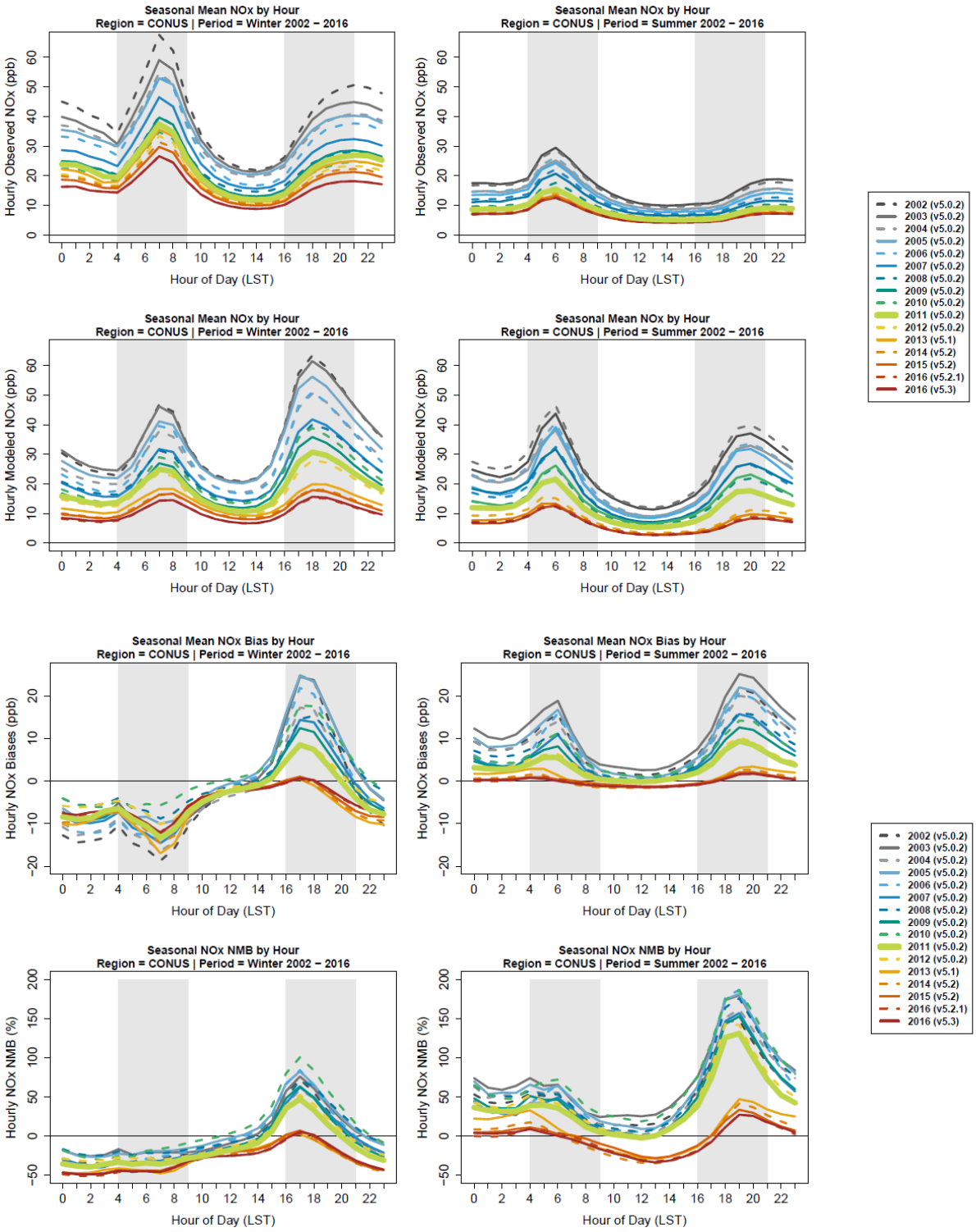

Figure 9 (reproduced from Toro et al (2021)) Diurnal mean NO_X observations (top) and bias (bottom). Profiles for winter (left) and summer (right) are shown by year. Modeled years include 2002–2016.

Hypothesis 1.7: Air quality model bias is unique to summer in the Eastern U.S.

Status: *This hypothesis has been explored and confirmed to be an important characteristic of the air quality model NO_X bias. The model NO_X overpredictions appear to be most prevalent in the Upper Midwest, Ohio Valley, South, and Southeast regions during summer months. The model often underpredicts NO_X concentrations at other times of year and locations.*

NO_X bias appears to be a feature unique to summer in the model, with morning overprediction eliminated in winter. These results are shown in Figure 8 and have been presented in Henderson et al (2017a; 2017b) and documented in Toro et al. (2021). These findings are also consistent with results presented in Appel et al. (2017). In addition, a recent 2015 wintertime field campaign in New England was conducted by external researchers. Two studies from that campaign (Salmon et al., 2018; Jaeglé et al., 2018) both concluded that measurements were in agreement with EPA emissions inventories and resulting model estimates for that time period. The cause of the seasonally changing NO_X bias has not yet been identified and is a topic that needs further research.

6.2 Model biases as related to methods used to process emissions for input to the photochemical model.

Hypothesis 2.1: Spatial allocation (county to grid cell) is incorrect for onroad emissions

Status: This hypothesis has been investigated and is not likely a driving cause of air quality model NO_X bias

Improvements have been made to spatial allocation for onroad emissions in the 2014 and 2016 model simulations. Improvements included more fully resolved data for the road network through the use of Annual Average Daily Traffic (AADT) data by road link in the development of spatial surrogates, although allocation of off-network emissions such as starts and idling may still need improvement. Air quality model-ready emissions were developed based on the AADT, but an air quality model run was not performed because the emissions changes were small and localized. Updates to the surrogates have been documented in the emissions modeling technical support documents for the 2014v7.1 and 2016v7.2 platforms (U.S. EPA, 2018c; U.S. EPA, 2019).

Hypothesis 2.2: Heavy-Duty (HD) onroad vehicle running emissions are at the wrong time of day

Status: *This hypothesis has been investigated and is not likely a driving cause of air quality model NO_X bias*

Sensitivity model simulations in which HD diurnal profiles were altered to allocate more emissions during daytime hours and fewer emissions during nighttime hours had little impact on modeled NOx concentrations. Results from CAMx model simulations were presented at the 2017 CMAS conference (Timin et al., 2017). In addition, CMAQ model sensitivity simulations were included in the Toro et al. (2021) journal article.

Hypothesis 2.3: Emissions from Electrical Generating Units (EGU) without Continuous Emission Monitors (CEMS) may be inappropriately allocated from annual to hourly emissions

Status: *This hypothesis has been investigated and is not likely a driving cause of air quality model NO_X bias nationwide although it may have large impacts on modeled NO_X bias over limited spatial and temporal scales*

An error was found in how temporal profiles were assigned to EGUs without CEMS. This error led to some facilities such as municipal waste incinerators having temporal allocations that resembled profiles that are applied to peaking units. While the municipal waste incinerators and other non-CEMS EGUs did not account for a large fraction of the inventory, this error resulted in annual emissions being predominantly allocated to only a few days in the 2011 modeling at some units. Model simulations were conducted to evaluate the impact of updating the temporal profile to more realistically show these units emitting NO_X throughout the entire year. Fixing daily allocation for non-CEMs EGUs had a large impact for a few locations on a few days. These days and locations happened to coincide with the DISCOVER-AQ Baltimore field study which was used in the Anderson et al (2013) study, so it may have impacted their conclusion that EPA NO_X emissions were too high. This information was described in Simon et al (2018a). The impact of updating this emissions temporalization was evaluated using CAMx sensitivity simulations. The updated temporalization did not have a substantial national impact on NO_X concentrations or model performance, although impacts were important on several days directly downwind for the EGU facilities. Results from CAMx model simulations were presented at the 2017 CMAS conference (Timin et al., 2017). In addition, CMAQ model sensitivity simulation results were included in Toro et al (2021).

Hypothesis 2.4: Monthly, day-of-week, and/or diurnal temporal profiles for nonroad equipment activity are incorrect

Status: *This hypothesis has been investigated and is not likely a driving cause of air quality model NO_X bias*

Model sensitivities in which diurnal profiles for nonroad equipment activity were altered had little impact on modeled NO_X concentrations. Results from CAMx model simulations were presented at the 2017 CMAS conference (Timin et al., 2017). In addition, updated CMAQ model sensitivity simulation results were included Toro et al (2021).

Hypothesis 2.5: Spatial allocation (county to grid cell) of nonroad equipment is incorrect

Status: *Hypothesis has not been actively investigated*

This has not yet been evaluated but is likely less important than national to county equipment allocation (see below).

Hypothesis 2.6: Spatial allocation of nonroad emissions (national to county) is not representative of actual emissions

Status: *This issue needs more analysis*

The surrogate data used to allocate national populations of agricultural and construction equipment to the county level was updated in the 2016v1 emissions modeling platform. These improvements in the spatial distribution of construction and agricultural nonroad emissions have been implemented in the Inventory Collaborative's 2016v1 emissions modeling platform

(U.S. EPA, 2021a). The construction and agricultural equipment spatial allocation update conserved the model's national base equipment population but re-allocated the population such that some states saw an increase in population (and therefore activity and emissions), while others saw a decrease. EPA staff have not conducted a sensitivity analyses of the platform to investigate the individual impact of the updated spatial surrogates for agricultural and construction equipment on the bias. Nationally, emissions didn't change significantly, and the emissions and air quality impacts are anticipated to be localized. Further work is needed to understand the impact of these spatial surrogates and estimated NO_X emissions on local areas.

6.3 Model biases related to overestimates of mobile source emissions from MOVES

Hypothesis 3.1: Onroad light-duty (LD) gasoline vehicle emissions rates are too high.

Status: *We invested significant effort to evaluate and update LD gasoline onroad vehicle emission rates in MOVES. Our early work suggested significant reductions in NO_X LD emission rates in MOVES. In a sensitivity evaluation, these preliminary reductions had a noticeable, but modest effect on the NOx bias evaluated in the 2016 air quality modeling platform. Additional work showed that a smaller change in NOx rates was warranted (U.S. EPA, 2020b), so the final MOVES3 light-duty emission rates are higher than the emission rates evaluated in the sensitivity case. Thus, the sensitivity case serves as an upper bound to the changes in NO_X ambient concentrations in 2016. Despite the modest effect on the NOx bias, we are continuing to compile data to improve LD base emission rates, adjustment factors and activity inputs for future versions of MOVES.*

There are many factors that impact LD emission rates estimated by MOVES—the NO_X base emission rates in the model vary with emission process, operating mode, and age. Emission rates are then weighted together based on estimates of activity and are adjusted to account for fuel effects, Inspection & Maintenance programs, ambient conditions, and air conditioning. Exploring the hypothesis that the emission rates are too high requires analyzing these factors individually. A description of the factors explored to date are listed below:

- Emission rates under high-power driving conditions

  Comparison of trends for NO_X, HC, and CO emissions in relation to vehicle-specific power for Tier 2 vehicles (model year 2004 – 2013) between MOVES2014 and real-world data suggests that MOVES2014 emission rates for operating modes representing high speed and acceleration are likely too high (Sonntag et al. 2018). Revised assumptions for high-power emissions for vehicles in model year 2004 and later result in better agreement with real-world measurements acquired using Portable Emissions Measurement Systems (PEMS). Sensitivity analyses indicate that updating these assumptions has a minor impact (<5% reduction) for pre-2016 calendar year NO_X emissions from light-duty vehicles, but these revisions become important for future years (>20% reduction in calendar year 2028) (Toro et al. 2019a). These emission rates were updated in MOVES3 (U.S. EPA, 2020b). We are continuing to gather and analyze data on emissions under high-power driving conditions and expect to further refine these rates as data become available.

- Deterioration of start emissions

  For emissions immediately following engine starts, comparisons to the In-Use Verification Program (IUVP) suggest that for Tier 2 vehicles, NO_x emissions from starts rise more slowly with vehicle age (in proportional terms) than emissions during hot-running operation. This result differs from the assumptions included in MOVES2014, where both emission processes were assumed to deteriorate at the same proportional rate. Sensitivity analyses using IUVP-based deterioration show a moderate (7-10%) decrease in NO_x emissions for light-duty vehicles for all calendar years evaluated (Toro et al. 2019a). Starts trends with age were updated in MOVES3 (U.S. EPA, 2020b).

- Deterioration of running emissions

  Comparison of MOVES2014 Tier 2 vehicle running emission trends with vehicle age and data from the Denver Inspection & Maintenance (I/M) program suggest that the NO_X deterioration trend included in the MOVES2014 is more aggressive than that seen in the Denver I/M data. Emissions impact sensitivity tests indicate that updates to the deterioration trend result in moderate NO_X emissions reductions for the LD sector, in the range of 5-15% depending on the calendar year (Toro et al. 2019a). Updated deterioration trends and baseline emission rates were estimated for light-duty NO_x vehicles using the Denver I/M data in MOVES3 (U.S. EPA, 2020b).

- Preliminary sensitivity results

Preliminary sensitivity results from the three adjustments to base emission rates described above indicated a cumulative reduction of LD NO_X emissions on the order of 20% for calendar year 2011 and 30% in 2016. An overview of the data and sensitivity analysis was presented at the IEIC 2019 conference (Toro et al., 2019a). The sensitivity of these changes to modeled ambient NO_X concentrations was evaluated using the 2016 beta collaborative platform, with mobile-source emissions estimated using MOVES2014b, and presented at the 2019 AGU Fall Meeting (Toro et al. 2019b). The median NO_X bias for the conterminous U.S. (CONUS) are shown by season and hour in Figure 10. With the sensitivity case, the median modeled NO_X concentrations had a noticeable decrease. The NO_X bias slightly improved for the winter evening hours, and the summer morning, evening, and night-time hours. However, the morning winter bias worsened with the change. While showing noticeable changes to the NO_X concentrations and bias, the overall NO_X bias pattern is relatively unchanged. As discussed in Toro et al. 2019b, results varied regionally. The Southeast showed the most model improvement in the summer morning with the sensitivity change. However, all CONUS regions showed a worse model performance in the winter morning periods.

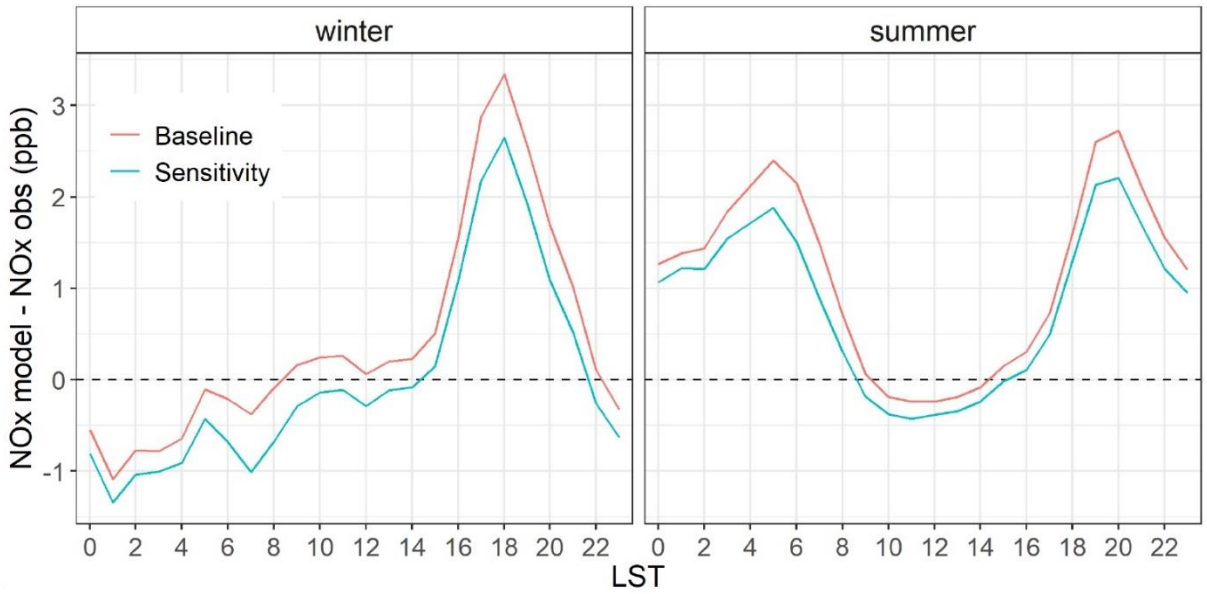

Figure 10 (reproduced from Toro et al. 2019b) Hourly median NOx bias for the Conterminous U.S. (CONUS) by season and hour (local standard time - LST), using a baseline case in 2016 and a sensitivity case with reductions to the light-duty NOx emission rates due to revised high-power rates and deterioration trends.

- Final MOVES3 light-duty emission rates

Since conducting the emissions and air quality model sensitivity analyses discussed above, we developed updated light-duty vehicle emission rates for MOVES3 (US EPA, 2020b). Compared to the sensitivity case discussed above, the new rates account for updated deterioration trend and zero-mile rates estimated using data from the Denver I/M program. The MOVES3 start emission rates also include revisions to the relationship between starts and soak time (time parked before starting), which increases NO_X start emissions during starts at intermediate soak times. The combined updates to the MOVES3 light-duty emission rates still generally decrease the MOVES light-duty emission rates compared to MOVES2014b by individual vehicle regulatory class, operating mode, age, and model year, but to a smaller degree than evaluated in the preliminary sensitivity case discussed above; in some cases the light-duty emission rates actually increase as presented in the MOVES3 light-duty emission rate technical report (US EPA, 2020b).

The impacts of the final MOVES3 light-duty NO_X emission rates on estimated NO_X emissions and NO_X bias have not been evaluated separately. The updates to light-duty NO_X emission rate were made to MOVES3 in conjunction with other changes, including updates to light-duty population and activity that also impact NO_X emissions. Thus, the percent changes in the estimated NO_X light-duty *emissions* at national scale are different than the changes in the light-duty emission *rates*. In fact, despite MOVES3 having generally lower LD NO_X emission *rates* (e.g. gram/mile or gram/start by vehicle regulatory class) than MOVES2014b, MOVES3 estimates higher LD NO_X *total emissions* (kilograms or tons) than MOVES2014b in some calendar years. For example, calendar year 2023 shown in Figure 11 shows higher gasoline NO_X in 2023 due to MOVES3 estimating a higher fraction of light-duty truck populations and activity compared to MOVES2014b (Han, J. 2021). However, future gasoline MOVES3 light-duty NO_X emissions are significantly lower, which is consistent with the updates made to future model year light-duty

emission rates based on our evaluation. A further discussion of uncertainty of population and activity MOVES inputs on the NO_X bias is discussed in Hypothesis 3.3.

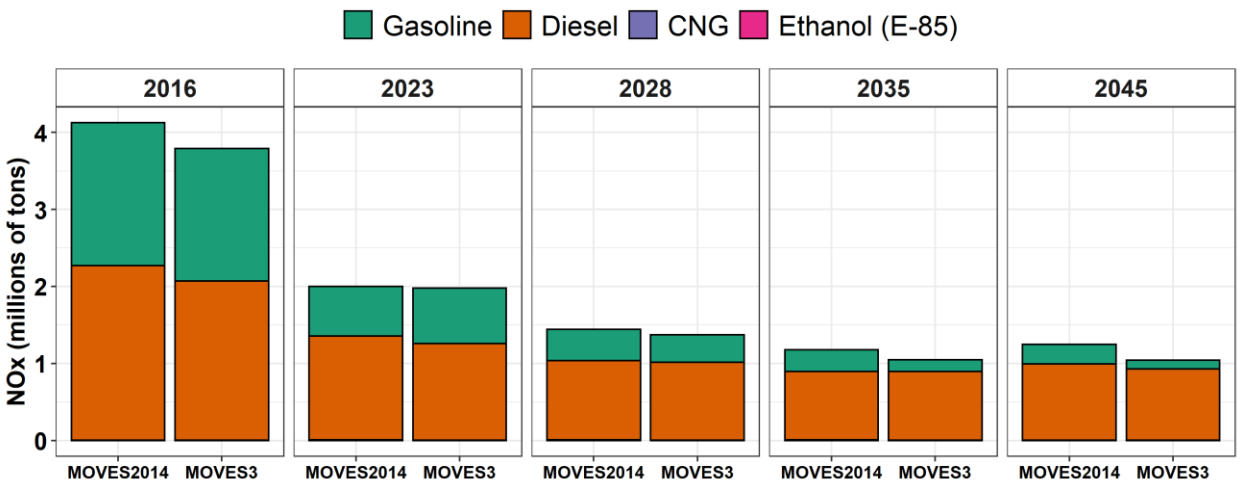

Figure 11 (reproduced from US EPA, 2021c) National onroad NO_X in MOVES3 as compared to MOVES2014b

Evaluation of the air quality model NO_X concentration bias using an emissions platform that incorporates MOVES3 emission rates have not yet been completed. As discussed in the Ongoing Work Section (Section 9), future emissions and air quality modeling platforms will use MOVES3, however the isolated impact of the updated MOVES3 light-duty NO_X emission rates will not be readily apparent given the many other changes to the platform. Because the light-duty NO_X emission rates reductions in the sensitivity case were larger than the reductions to the light-duty NO_X emission rates finalized in MOVES3, the sensitivity case discussed above can serve as an upper bound on the anticipated effect of the final MOVES light-duty NO_X emission rates on NO_X ambient concentrations in calendar year 2016. Additional work would be needed to evaluate the isolated impact of the light-duty NO_X emission rates on the NO_X bias using the updated emissions and air quality modeling platform.

Hypothesis 3.2: Onroad heavy-duty (HD) NO_X emission rates are too high

Status: *This hypothesis has been investigated and is not likely a driving cause of air quality model NO_X bias*

MOVES2014 HD diesel emission rates compare well with road-side measurements (McDonald et al. 2018, Sonntag et al. 2017). More recent analyses suggest that MOVES2014b HD emission rates for model year 2010 and later vehicles are too low for running exhaust, and too high for extended idle emissions. These rates were updated in MOVES3 (U.S. EPA, 2020b). The HD diesel emission rates updates have minimal impact on calendar years evaluated in the NO_X evaluation (2016 and earlier) (Han et al. 2019).

Hypothesis 3.3: MOVES inputs used in the 2011 NEI and EPA platform were not consistent with the ambient datasets to which they were compared. For example, speed and acceleration assumptions were not consistent with vehicle activity at remote sensing locations, long-haul truck hoteling activity was overestimated nationally, and MOVES inputs did not accurately model local variability in age distributions and car/truck splits.

Status: *This hypothesis has been investigated and found to have an important impact on MOVES NO_X emissions. The isolated impact on NO_X bias has not been evaluated.*

- Speed and acceleration assumptions, age distributions, and car/truck splits were identified as influential MOVES inputs on NOx emissions (Choi et al. 2017).
- Average speed distributions were updated for the 2017 NEI and MOVES3 based on telematics data. However, the new distributions show more driving at higher speeds, which can increase emissions. (U.S. EPA 2021b). When compared to four US road-side remote sensing locations, MOVES default speed and acceleration assumptions for the representative county were significantly more aggressive than was measured at the three of the four sites (Choi et al. 2017), likely due to bias in site selection.
- Age distributions were updated for the 2017 NEI and MOVES3. In general, the age distributions show an older vehicle fleet, which can increase emissions. (U.S. EPA 2021c). When compared to four US road-side remote sensing locations, MOVES default age distributions were significantly older than the age distributions at three of the sites. Using the MOVES default age distributions to model these locations led to a significant overestimation in NO_X emissions (Choi et al. 2017).
- The MOVES vehicle classifications do not map perfectly to vehicle activity and registration data. Uncertainties in this classification can impact resulting emissions since, for example, MOVES emission factors for passenger cars are lower than those for passenger trucks and light commercial trucks. For the 2016v1 platform, to ensure consistency in "passenger car," "passenger truck," and "light commercial truck" splits across the country, all state-submitted VMT for these vehicle types was summed and then re-allocated using the splits obtained from county-level registration data from a single data provider (U.S. EPA, 2019). EPA staff have not assessed the impact of this change on NO_X concentrations on the 2016v1 compared to previous platforms, and this approach was not incorporated into the 2016 NEI alpha and 2016 NEI beta platforms evaluated by Toro et al. (2021). This approach is incorporated into the 2016v1, 2017 NEI, and EQUATES emissions and air quality modeling platforms.
- EPA staff identified and implemented improvements to make use of gridded hourly humidity data instead of monthly average humidity and to use speed distributions instead of individual speeds in the NEI and platform (Baek and Eyth, 2019). These updates resulted in temporal and spatial differences in NO_X emissions.
- Based on the latest telematics data, EPA reduced the default hoteling hours for long-haul combination trucks by over a factor of 3 in the 2016v1 platform, compared to the 2014 NEI. (U.S. EPA (2019). This change had a significant reduction in total heavy-duty NO_X emissions. The updated hoteling activity decreased the total national heavy-duty NO_X emissions by 10% to 21% between 2010 and 2020 (Han et al. 2019). County-scale reductions varied, with higher reductions seen in rural counties. Note that these hoteling activity reductions were not included in the 2016 platform evaluated by Toro et al. (2021), but are included in the 2016v1, 2017 NEI, EQUATES emissions and air quality modeling platforms.

Hypothesis 3.4: Nonroad emission rates are too high

Status: *This hypothesis has been investigated and is not likely a driving cause of air quality model NO_X bias. Revisions made to Tier 4 nonroad engine emissions in MOVES2014b likely had a small impact on the NOx bias in the 2016-and-later emissions and air quality modeling platforms. A more comprehensive evaluation of nonroad NO_X emissions has been postponed since there will be future efforts to update nonroad equipment emissions rates.*

In 2018, EPA released MOVES2014b, which incorporated updated NO_x emission rates for Tier 4 (first introduced with model year 2008) nonroad engines based on updated certification data. In addition, compliance provisions available to manufacturers were accounted for (U.S. EPA, 2018a). Based on MOVES national inventory tests, this change had very small impact in calendar year 2011 but resulted in a 3% increase in nonroad NO_X emissions in 2016, and a 1% decrease in nonroad NO_x emissions in 2025. These updates were incorporated in the 2016 platform evaluated by Toro et al. (2021) which estimated mobile emissions using MOVES2014b. However, changes in the NO_X bias in the 2016 platform are not likely driven by this change due to the small change in overall NO_X emissions. We are continuing to evaluate nonroad equipment emission rates as more data become available.

Hypothesis 3.5: National nonroad equipment population and activity are overestimated

Status: *The uncertainty in nonroad population has been investigated and had modest impact on air quality model NO_X bias. An evaluation of nonroad activity is ongoing.*

Updates to the growth of nonroad equipment populations were implemented in MOVES2014b (U.S. EPA, 2018b). Nonroad equipment in MOVES includes off-highway mobile engines from twelve broad economic sectors (including construction, agricultural, and lawn & garden) but excludes locomotives, airplanes and commercial marine vessels which are handled by separate emission models (U.S. EPA 2021c). Adjusting nonroad equipment populations has a moderate impact on national NOx emissions, decreasing national nonroad NOx emissions by 7% in 2011. EPA conducted a sensitivity test using the 2011 platform by adjusting the nonroad emissions to reflect this change and it resulted in decreased NO_X concentrations in the range of 0.5 ppb across large urban areas in the northeast US for July 2011.

Nonroad NO_X emissions from this update had a larger impact for more recent and future years. Based on MOVES national runs, national nonroad NOx emissions decreased by about 13% in 2016 due to this update. The updated nonroad equipment population growth rates were included in MOVES2014b and the 2016 emissions and air quality modeling platform evaluated by Toro et al. (2021). The change in the mean NO_X bias due to all changes in the 2015 and 2016 platforms varied across regions and seasons, increasing as much as 15 ppb in the summer in the South and decreasing as much as 28 ppb in the summer in the Upper Midwest. Thus, while the nonroad equipment population growth has been shown to have an important impact on NO_X concentrations (in the range of 0.5 ppb), it is only a minor contributing factor to the larger changes observed in the 2016 platform NO_X concentrations.

Representative and comprehensive nonroad equipment activity data are sparse and often non-existent for certain sectors and types of equipment. EPA has initiated work to develop updated

estimates of nonroad activity based on equipment activity loggers, auction house records, and other data sources. It is anticipated that activity estimates likely have a similar impact on nonroad emissions as nonroad equipment population and we are looking for data sources to improve and evaluate nonroad activity.

7. Internal and external outreach activities

7.1 Cross-EPA coordination meetings

From 2015-2019, there were regularly scheduled NO_X coordination calls which occurred 5-10 times per year. On these calls, updates were provided on progress for specific projects and analyses. In addition, calls included discussion of outstanding questions and uncertainties and prioritization of new analyses.

7.2 Technical discussions on Emissions and Atmospheric Modeling (TEAM)

The Technical discussions on Emissions and Atmospheric Modeling (TEAM) team was formed as part of a cross-agency coordination effort between national environmental agencies. The group was led by representatives from EPA, NOAA and NASA and focused on communications between federal agency staff on specific topics. The first topic area chosen for TEAM was the use of ambient measurements and satellite to constrain NO_x emissions. During this topic, there were four webinars and three conference sessions. Members of the EPA NO_X coordination group were substantial participants in each webinar and conference session. The webinars included presentations by EPA staff describing emission development techniques, NOAA staff describing fuel-based mobile NOx inventories, NASA discussing satellite assets, and top-down constraint methodologies and results. All three agencies presented results comparing their methodologies to field campaign data. The conference sessions were held at the 2017 International Emissions Inventory Conference (IEIC), the 2017 Community Modeling and Analysis System (CMAS), and the 2017 American Geophysical Union (AGU) Fall Meeting. These conference sessions included presentations from TEAM and EPA NOx coordination group members, as well as contributions from others.

7.3 Seminars, scientific conference presentations and special sessions

EPA has shared results and engaged with the scientific and regulated communities through continued participation in scientific conferences, workshops, and other outreach opportunities. Members of the NO_X evaluation group have organized and chaired four special sessions focused on this topic at conferences which included 14 EPA presentations and 26 relevant presentations from outside groups (Table 2). In addition, findings from this work have been presented in 24 presentations at 11 conferences (Tables 2 and 3). EPA staff have actively engaged in ongoing discussions with researchers from varied institutions and with disparate points of view.

Table 2: List of relevant conference presentations (talks and posters) from special sessions convened or co-convened by members of the cross-EPA NO_x evaluation group at four international scientific conferences. Presentations given by EPA staff are shown in **bold**.

Conference Session	Title	Presenter	Presenter Affiliation
22nd International Emissions Inventory Conference, Baltimore, MD, August 2017 Special Session: Reconciling NO_X Emissions with Ambient Observations (Darrell Sonntag, U.S. EPA & Greg Frost NOAA)	Diurnal, Weekday and Long-term Patterns in NO_X Emissions Based on Decade-long Time Series of Hourly AQS Data and Comparison with Traffic Count Data	B. De Foy	St. Louis University
	Satellite NO_2 for the Evaluation of U.S. NO_X Emissions	M. Harkey	UW Madison
	Evaluation of NO_x Emissions and Modeling	**B. Henderson**	**U.S. EPA – OAQPS**
	MOVES-Based NO_X Analyses for Urban Case Studies in Texas	S. Bai	Sonoma Technology
	United States Light and Heavy-Duty Fuel Specific On-Road NO and NO_X Emission Factor Trends and Their Importance in Inventory Calculations	G. Bishop	University of Denver
	Modeling Ozone in the Eastern U.S. using a Fuel-Based Mobile Source Emissions Inventory	B. McDonald	NOAA
	Comparison of Light-duty NO_X Emission Rates Estimated from MOVES with Real-world Measurements	**D. Sonntag**	**U.S. EPA – OTAQ**
	Technical discussions on Emissions and Atmospheric Modeling (TEAM)	**B. Henderson**	**U.S. EPA – OAQPS**
16th Annual Community Modeling and Analysis System Conference, Chapel Hill, NC Oct 2017 Special Session: Improving the Characterization of the Ambient NO_Y Budget (Heather Simon, U.S. EPA & Darrell Sonntag U.S. EPA)	**Technical discussions on Emissions and Atmospheric Modeling (TEAM)**	**B. Henderson**	**U.S. EPA – OAQPS**
	Evaluation of NO_X Emissions and Modeling	**B. Henderson**	**U.S. EPA – OAQPS**
	Reconciling modeled and observed upper tropospheric NO_2 for the interpretation of satellite measurements	R. Silvern	Harvard University
	Evaluation of Emissions of Nitrogen Oxides in Houston, Texas Using Three-Dimensional Aircraft Observations during the DISCOVER-AQ 2013 Mission	J. Smith	Texas Commission on Environmental Quality
	Real world emissions of NO_X and other pollutants in the Ft. McHenry tunnel	A. Khlystov	Desert Research Institute
	MOVES-Based NO_X Analyses for Urban Case Studies in Texas	K. Craig	Sonoma Technology

Conference Session	Title	Presenter	Presenter Affiliation
	Modeling Ozone in the Eastern U.S. using a Fuel-Based Mobile Source Emissions Inventory	B. McDonald	NOAA
	Comparison of light-duty gasoline NO_X emission rates estimated from MOVES with real-world measurements	**D. Sonntag**	**U.S. EPA – OTAQ**
	Updates on Production of NO_X by Lightning	K. Pickering	University of Maryland
	Influence of different canopy reduction functions on biogenic NO emission patterns in northern Europe	J.A. Arndt	Helmholtz-Zentrum Geeshthacht
	Sensitivity of MOVES emissions specifications on modeled air quality using traffic data and near-road ambient measurements from the Las Vegas and Detroit field studies	**C. Owen**	**U.S. EPA – OAQPS**
	Unconventional Constraints on Nitrogen Chemistry using DC3 Observations and Trajectory-based Chemical Modeling	Q. Shu	University of Florida
	Evaluating CO:NO_X in a near-road environment using ambient data from Las Vegas	**H. Simon**	**U.S. EPA – OAQPS**
	Sensitivity of MOVES-estimated vehicle emissions to inputs when comparing to real-world measurements	**D. Sonntag**	**U.S. EPA – OTAQ**
	CAMx Model Sensitivity Analysis of Emissions Temporal Profiles; Impacts on 2011 Modeled NO_X/NO_Y Concentrations	**B. Timin**	**U.S. EPA – OAQPS**
	Exploring differences in nitrogen oxides overestimation at the seasonal and day-of-week levels to understand potential relationships with mobile source emission inventories.	**C. Toro**	**U.S. EPA – OTAQ**
	Investigating modeling platform emissions for grid cells associated with a near-road study site during a field campaign in Las Vegas	**C. Toro**	**U.S. EPA – OTAQ**
American Geophysical Union Fall Meeting, New Orleans LA, Dec 2017 Session: Leveraging Inventories, Observations, and Models to Improve	Impacts of Aging Emission Control Systems on In-Use Heavy-Duty Diesel Truck Emission Rates	C. Preble	University of California – Berkeley
	Multi-Year On-Road Emission Factor Trends of Two Heavy-Duty California Fleets	M. Haugen	University of Denver
	Comparisons of MOVES Light-duty Gasoline NO_X Emission Rates with Real-world Measurements	**D. Choi**	**U.S. EPA – OTAQ**

Conference Session	Title	Presenter	Presenter Affiliation
the Scientific Basis of Emissions (Greg Frost, NOAA; Barron Henderson, U.S. EPA; Barry Lefer, NASA)	**Evaluation of NO_X Emissions and Modeling**	**B. Henderson**	**U.S. EPA – OAQPS**
	Eddy Covariance Measurements Assessing NO_X Emission in London, UK	W. S. Drysdale	University of York
	Evaluation of a Fuel-Based Oil and Gas Inventory of Nitrogen Oxides with Top-Down Emissions	B. McDonald	NOAA
	Update of NO_X emission temporal profiles using CMAQ-HDDM	C. Bae	Ajou University
	Technical discussions on Emissions and Atmospheric Modeling (TEAM)	G. Frost	NOAA
American Geophysical Union Fall Meeting, Washington DC, Dec 2018 Session: Improving the Science of Emissions Through Inventories, Observations, and Models (Greg Frost, NOAA; Barron Henderson, U.S. EPA; Barry Lefer, NASA)	Satellite and Surface Observations Confirm Steady Decline in US NO_X Emissions over the 2004-2017 Period	R. Silvern	Harvard University
	Unexpected slowdown of US pollutant emission reduction in the past decade	H.M. Worden	NCAR
	A large decline of tropospheric NO_2 in China since 2013 observed from space by SNPP OMPS	Y. Wang	University of Houston
	Recent Advances in Deriving NO_X Emission Estimates from Satellite Data	D. Goldberg	Argonne National Laboratory
	Truck Exhaust Plume Capture and Quantification of Nitrogen-Species Emission Rates: Impact of Diesel Particle Filters and Selective Catalytic Reduction Systems	T. Kirchstetter	Lawrence Berkeley National Laboratory
	Estimates of global biogenic soil HONO emissions using a process-oriented model	H. Su	Max Planck Institute for Chemistry
	Quantification of Global Reactive Nitrogen Emissions from Biomass Burning using Satellite Observations	C. Bray	North Carolina State University

Table 3: List of conference presentations or seminars presented by members of the cross-EPA NO_x evaluation on this topic (excluding presentations already listed in Table 2)

Conference	Title	Presenter
15th Annual Community Modeling and Analysis System Conference, Chapel Hill, NC, Oct 2016	An analysis of sensitivity of MOVES emissions estimates to traffic data and comparison to grid-cell estimates and near-road measurements from the Las Vegas field study	C. Owen
	Modeled Source Contributions to CO and NO_Y Concentrations during the DISCOVER-AQ Baltimore Field Campaign	H. Simon
	In-depth examination of emissions inventories to support EPA evaluation of modeled ambient nitrogen oxides (NO_X and NO_Y)	C. Toro
CRC Real World Emissions Workshop, Long Beach, CA, March 2017	Evaluation of NO_X Emissions Projected by MOVES2014 Using Dynamometer, Remote-Sensing and Tunnel Data	J. Warila
MOVES Review Workgroup meeting, Ann Arbor, MI, September 2017	Update on MOVES model evaluation: NO_X	D. Sonntag
EPA/ORD NERL Computational Exposure Division seminar series, Sep 2017	Ongoing EPA efforts to evaluate modeled NO_Y budgets	H. Simon
EPA Environmental Modeling Community of Practice webinar	Ongoing EPA efforts to evaluate modeled NO_Y budgets	H. Simon
MD and Northeast states Weekly Photochemical Modeling Coordination Call, November 2017	Ongoing EPA efforts to evaluate modeled NO_Y budgets	H. Simon
	Comparing light-duty gasoline NO_X emission rates estimated with MOVES to real-world measurements	D. Sonntag
CRC Real World Emissions Workshop, Garden Grove, CA, March 2018	Updated Evaluation of MOVES Light-duty Gasoline NO_X Emission Rates with Real World Measurements	D. Sonntag
Atmospheric Chemical Mechanisms Conference, Davis, CA, December 2018	Ongoing EPA efforts to evaluate modeled NO_Y budgets	H. Simon
CRC Real-World Emissions Workshop, Long Beach, CA, March 10-13, 2019	Updates to EPA's Motor Vehicle Emission Simulator (MOVES)	M. Beardsley
MOVES Review Work Group, Ann Arbor, MI, April 2019	Updates to "high-power" emission rates and start deterioration for light-duty vehicles	C. Toro

2019 International Emissions Inventory Conference – Collaborative Partnerships to Advance Science and Policy, Dallas, TX, July 2019	MOVES Light-Duty Emission Rate Evaluation in the Context of Reconciling Modeled and Ambient NO_X	C. Toro
	Planned Updates to EPA's MOVES Emission Model for Heavy-Duty Onroad Vehicles	J. Han
	SMOKE version 4.7 Recent Enhancements	B. H. Baek/A. Eyth
18th Annual community Modeling and Analysis System Conference, Chapel Hill, NC, Oct 2019	Evaluation of CMAQ Estimated NO_X from 2002 to 2016	K. Foley
American Geophysical Union Fall Meeting, San Francisco, CA, Dec 2019	Evaluation of CMAQ Estimated NO_x from 2002 to 2016	H. Simon/K. Baker
	Comprehensive bottom up analysis of the onroad mobile emission sector: from NO_X emission rates to air quality impacts	C. Toro

7.4 Journal publications

Several externally peer-reviewed journal publications resulted from this coordination effort.

Simon et al. (2018a) re-examined the methods used by Anderson et al. applying new modeling to understand source contributions of CO and NOy during the DISOCVER-AQ Baltimore field campaign and showed that those results were impacted by the choice of metrics used. This analysis using the 2011 emissions modeling platform showed reasonably good agreement between modeled and measured concentrations of NO_2 aloft in the boundary layer (NMB = 8%) but model over-predictions of aged nitrogen species (NMB = 69%, 118% and 18% for alkyl nitrates, peroxy nitrates and nitric acid respectively). These findings suggest that chemistry plays a key role in how well model predictions of total NO_Y compare against measurements. This analysis also shows that two different measurement methods used in that field campaign (1) total NO_Y measured by chemiluminescence instrument and 2) sum of NO_Y component species measured by chemiluminescence and TD-LIF instruments) produced widely diverging NO_Y values and that model NO_X performance could vary substantially depending on which measurement was used (NMB for NO_Y = 69% when compared against chemiluminescence measurements versus 50% when compared against the sum of measured NO_Y component species). When normalized to CO, the modeled NO_Y was not statistically different from the measured normalized ratio indicating transport and dispersion processes may play an important role in NO_Y model performance issues.

Day et al. (2019) reviewed progress on emissions inventories that has occurred since a 2005 NARSTO report which included recommended areas for improvement. While this article did not focus specifically on NO_X emissions it included several relevant sections, including a detailed description of updates to mobile source emissions modeling that have occurred through incorporation of new vehicle testing data into the MOVES model.

Zare et al. (2019) improved the characterization of organic nitrogen species in the CMAQ model, particularly solubility, formation, reaction rates and products. At a rural Alabama monitoring site these updates reduced the model prediction of alkyl nitrate species from a factor of 2 overestimate to a 32% underestimate and brought the model into better agreement with measurements.

Simon et al. (2020) evaluated various methods for calculating CO:NO_X ratios from measurements taken in near-road environments. For this purpose, Simon et al. leverage an extensive near-road dataset collected next to an interstate in Las Vegas, NV between December 2008 and February 2010. When measured ratios are compared to those derived from MOVES using traffic data from the field location, MOVES values are generally unbiased but the full variability seen in observations was not captured by the model.

Toro et al. (2021) examined model NO_X performance against AQS monitors for 15 years of modeled data. The CMAQ model simulations for more recent years in the 15-year timeseries apply updated emissions inventory methods and model versions which incorporate more recent science and more detailed data. The paper has several key findings. First, it demonstrates the seasonal dependence of the modeled NO_X performance with over-predictions mainly focused on summer months and under-predictions in the winter months. The analysis also highlighted the spatial nature of NO_X model bias with most of the over-predictions occuring in the Upper Midwest, Ohio Valley, South, and Southeast regions of the U.S. Comparisons of the model to measurements made in other regions of the U.S. tended to show model underpredictions of NO_X. In addition, the analysis shows that NO_x over-predictions have decreased substantially or been eliminated in some locations in recent years. Updates to chemical and physical processes in CMAQv5.1 were identified as a major driver in reducing NO_X over-predictions in summer and increased the NO_X underpredictions in winter. In addition, the decrease in over-prediction may also be due in part to decreasing measured ambient NO_X concentrations accompanied by large decreases in modeled NO_X emissions concentrations in the emissions and air quality modeling platforms with more recent calendar years. The paper then looks further into the 2011 calendar year with additional 2011 CMAQ simulations meant to examine sensitivity to model chemistry and emissions assumptions. These sensitivities show several things. First, while timing of NO_X emissions from various source categories can be important to model NO_X predictions at specific times and locations, adjusting temporal assumptions had little overall impact on model NO_X performance. Updates to projected nonroad equipment population did reduce predicted NO_X emissions and improved model performance. In addition, the model performance was sensitive to the chemical mechanism applied with newer chemistry resulting in substantially lower total NO_Y concentrations. Finally, the paper compared model predictions to aircraft measurements from the DISCOVER-AQ Baltimore field campaign that have been the focus of several previous studies that evaluated EPA NO_X emissions estimates. Consistent with the findings in Simon et al. (2018a), this comparison showed that the magnitude of model bias for aloft NO_Y within the boundary layer was sensitive to both the ambient measurements that were used and the model chemical mechanism (model NMB could range from 27% to 77%, depending on these factors). The findings that measurement uncertainty and model chemical and physical processes play key roles in model performance suggest that caution should be taken in using modeled NO_X bias to constrain NO_x emissions.

8. Conclusions

The evaluation of NO_X model bias is complex and multi-faceted. The NO_X bias varies significantly geographically and temporally, including across hourly, seasonal, and yearly timescales. In addition, updated emissions and air quality modeling platforms include an ensemble of changes, making it difficult to attribute changes in the NO_X bias to individual updates. As such, it was useful to coordinate efforts across EPA offices to build upon expertise in emissions modeling, air quality modeling, and ambient measurements. The coordinated effort to evaluate the NO_X bias led to improved methods to evaluate model bias, updated model inputs, as well as an increased understanding of the impacts of model inputs and changes on NO_X concentrations. Overestimation of ambient concentrations of NO_X has been substantially reduced or eliminated with the most recent calendar year emissions and CMAQ air quality modeling platforms. One reason is that the more recent modeling platforms correctly modeled a decrease in NO_X emissions and ambient concentrations which corresponded with real-world NO_X concentration reductions. In addition, EPA staff identified several key changes in the emissions and air quality modeling platform that reduced the NO_X model bias.

At this time, EPA staff have not found a unique solution for the overprediction of NO_X concentrations, but have identified several plausible hypotheses, while ruling out others, for the NO_X positive biases seen at certain times/locations in the modeling. Model overpredictions were likely due to multiple compounding factors that each contribute to a portion of the bias. Based on our review of the evidence, the most important was:

- Planetary boundary layer (PBL) and vertical mixing algorithms in CMAQ led to too little vertical mixing at certain times and in some locations. These algorithms have been improved in CMAQv5.1 and later versions of CMAQ. These changes substantially reduced the NOx bias, as well as the NOx diurnal bias pattern in simulations run with more recent CMAQ versions.

We also demonstrated that there is important uncertainty in the model bias caused by NO_X and **NO_Y** measurement uncertainty, as well as the chemical mechanism used. Caution should be taken in using modeled NO_X bias to constrain NO_X emissions or processes incorporated into air quality modeling.

Through this effort, we identified aspects of the mobile source NOx emissions that were overestimated in the evaluated air quality platforms. These could lead to important overestimation of NOx emissions, but based on our analysis so far, only had a modest impact on the magnitude and pattern of the bias in modeled NOx concentrations. We have identified and developed improvements to the NO_X mobile source emission inventory to address the summer overestimation of mobile-source NO_X, which include:

- MOVES light-duty NO_X emissions rates.
    - MOVES light-duty gasoline NO_X emissions were reduced in MOVES3 compared to MOVES2014b. The MOVES3 light-duty gasoline NOx rates are generally lower due to updated modeling of high-load operation and updated deterioration trends.
- MOVES inputs in the 2011 National Emissions Inventory (NEI) and EPA platforms

    - MOVES inputs used in the 2011 NEI and EPA platform were not consistent with the ambient datasets to which they were being compared. For example, speed and acceleration assumptions were not consistent with vehicle activity at remote sensing locations, long-haul truck hoteling activity was overestimated nationally, and MOVES inputs did not accurately model local variability in age distributions and car/truck splits. These inputs have been improved in MOVES3, the 2016v1 platform (U.S. EPA, 2021a) and the 2017 NEI.
- National nonroad equipment populations were overestimated.
    - Nonroad equipment populations were overestimated in the 2015 and earlier platforms. These estimates were updated in the 2016 platform using updated nonroad population and activity data incorporated into MOVES2014b. These changes had a noticeable, but relatively small, impact on the NO_X bias.

We believe continued collaboration, evaluation, and communication of the model bias within and outside the EPA will lead to increased fidelity of future emissions and air quality modeling platforms.

9. Ongoing Work/Next Steps

EPA is continuing to update NO_X emissions methods and input data and CMAQ model treatment of physical and chemical processes. In addition, EPA is in the process of conducting an updated multi-year modeling evaluation.

- MOVES updates:
    - The EPA is continuing to evaluate and develop future MOVES versions using the latest science and data. In November 2020, the EPA's Office of Transportation and Air Quality released MOVES3 (U.S. EPA OTAQ, 2021c). MOVES3 contains significant updates that impact NO_X emissions, including:
        - Updated light-duty emissions rates based on new inspection and maintenance (I/M) program data, remote sensing, and portable emission measurement system data.
        - Updated start emissions as a function of parked time for light-duty and heavy-duty vehicles
        - Updated heavy-duty emission rates for model year 2010 and later vehicles based on manufacturer in-use testing data
        - Updated heavy duty emission rates for extended idling and auxiliary power units
        - Updated onroad activity, including idling activity, and vehicle populations
        - Accounted for glider vehicles (new heavy-duty vehicles with old engines)
        - Updated and increased resolution in heavy-duty vehicle masses using weigh-in-motion and other datasets
        - Updated fuel properties based on latest fuel compliance data
    - Using MOVES3 code and national default inputs, national onroad vehicle NO_X emissions decreased by 8% in 2016 compared to MOVES2014b. Results will differ for different calendar years, local areas, and for comparisons such at the NEI that use custom inputs to represent local vehicle population and activity. EPA is evaluating the impact of using

MOVES3 on developing national emission inventories and air quality as part of the EQUATES project discussed below.

- CMAQ chemistry updates (CRACMM): The chemical mechanism of an atmospheric chemical transport model like the Community Multiscale Air Quality (CMAQ) system contains the condensed set of reactions that describe the interactions between emitted hydrocarbons and nitrogen oxides as well their reaction products. The mechanism affects the representation of NOy including how it is partitioned among species and the gas and particle phase. Traditionally, mechanisms in regional models were designed for the prediction of ozone under alkane-rich urban atmospheres of the 1990s and are connected to independently developed modules and metadata to compute fine particles and deposition among other endpoints. The Community Regional Atmospheric Chemistry Multiphase Mechanism (CRACMM) is under development in ORD and aims to couple gas- and particle-phase chemistry by treating the entire pool of atmospheric reactive organic carbon (ROC) relevant to present-day emissions.

- EQUATES: **E**PA's Air **QUA**lity **T**im**E S**eries Project (EQUATES) is a cross-agency collaboration between ORD, OAR/OAQPS, and OAR/OTAQ to develop modeled meteorology, emissions, air quality and pollutant deposition for 2002 through 2017. Modeled datasets cover the Conterminous U.S. (CONUS) at a 12km horizontal grid spacing using WRFv4.1.1 for meteorology and CMAQv5.3.2 for air quality modeling. New CONUS emissions inventories were developed using (to the extent possible) consistent input data and methods across all years, including MOVES3 modeling for onroad emissions. Evaluation of model estimated trends will be used to inform model development and build confidence in the use of the modeling system to quantify the impact of meteorological and emissions changes on air quality.

Disclaimer: The views expressed in this report are those of the authors and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency.

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11. Appendix A: Acronyms

CMAQ – Community Multiscale Air Quality Model

CAMx – Comprehensive Air Quality Model with extensions

EQUATES – EPA's Air Quality Time Serie Project

MAR – Mileage accumulation rate

MOVES – Motor Vehicle Emission Simulator

NO_X – nitrogen oxides: NO + NO_2

NO_Y - Reactive nitrogen compounds including: NO, NO_2, HNO_3, NO_3, HONO, N_2O_5, $ClNO_2$, PAN, other organic nitrates, particulate nitrate

NO_Z – NO_Y-NO_X

OAQPS – U.S. EPA Office of Air Quality Standards and Planning

OTAQ – U.S. EPA Office of Transportation and Air Quality

PBL – Planetary Boundary Layer

SMOKE – Sparse Matrix Operator Kernel Emissions modeling system

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