The 2002 National Emissions Inventory Shakeout: The First Step in Development of EPA’s 2002 Emissions and Air Quality Modeling Platform
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ABSTRACT

The Environmental Protection Agency (EPA)’s Office of Air Quality Planning and Standards (OAQPS) has performed a “shakeout” of version 1 of the 2002 National Emissions Inventory (NEI) as a first step in using the 2002 NEI for the 2002 Emissions and Air Quality Modeling Platform. The shakeout consisted of two major steps: (1) comparison of the emissions with those used from the latest version of the 2001 platform, and (2) air quality modeling for the purpose of comparing emissions-induced air quality changes from an existing year 2001 platform. The 2001 platform was used for many regulatory analyses, the most recent being the Final PM NAAQS standard. The Sparse Matrix Operator Kernel Emissions (SMOKE) processor was used to process the emissions for subsequent CMAQ 36km air quality modeling. We substituted a particular significant emissions inventory sector with emissions from Version 1 of the 2002 NEI and compared CMAQ results as a first step towards migrating to the 2002 NEI. Meteorology, CMAQ model version, and chemical mechanism were retained from the 2001 platform. The SMOKE input ancillary files were modified primarily to update cross references as was necessary to process emissions from new emissions source category codes. Each 2002 sector was processed separately through SMOKE and CMAQ creating a distinct “shakeout” run that was used to identify the air quality changes resulting strictly from changes in the emissions for a particular sector.

This paper will discuss the methods the OAQPS emissions modeling team used to prepare the 2002 NEI for a 2002 platform, the quality assurance routines used throughout the emissions and air quality modeling process, and the CMAQ results for some inventory sector shakeouts and how those results were used to inform the NEI developers, ultimately leading to a more robust (Version 2) of the 2002 NEI.

INTRODUCTION

Air quality modeling plays a crucial role in the development and evaluation of emissions control programs, policies and rules across EPA offices. The backbone of this modeling is a “modeling platform” which includes the following components: emissions and meteorological
inputs for a base year and the underlying models used to develop these data, air quality model(s), and evaluation data consistent with the base year. The modeling platform may also include emissions and air quality inputs projected from the base year. In this paper we use the term “emissions platform” for the emissions-related aspects of the modeling platform. The introduction of a new base year for a modeling platform can be very resource intensive, as is creating a new emissions inventory. In the same timeframe as the development of the first version of the 2002 NEI, EPA has been working on a 2002-based multi-pollutant modeling platform, where “multi-pollutant” is defined as both criteria air pollutants (CAPs) and hazardous air pollutants (HAPs) including mercury (Hg). The emissions platform component of the 2002 modeling platform includes the following major components:

- a multi-pollutant version of the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system\(^1\) used for converting emissions inventory data to the structure and formats required by air quality models (AQMs);
- the 2002 National Emission Inventory (NEI) for CAPs and HAPs, which has the most integrated CAP and HAP inventories prepared to date;
- ancillary input data for SMOKE that are compatible with the 2002 NEI; and,
- the Emissions Modeling Framework (EMF)\(^2\) for managing data (e.g., editing, documenting, organizing), quality assuring data, and using data in SMOKE.

The first step in the development of this platform, which began in early 2006, was the 2002 National Emissions Inventory Shakeout. This Shakeout uses version 1 of the 2002 NEI (February 2006) and is defined as modeling case 2002aa. There were multiple purposes of the shakeout. One primary purpose that is the focus of this paper was to identify potentially large differences in the AQM predictions of pollutant concentrations between the most recent 2001 modeling platform [for reference, see the PM NAAQS Final RIA\(^3\)] and the 2002 platform that would be caused by large changes in the emissions. We would want to explain any such large emissions platform-related changes and ensure that they were not caused by potential errors in the inventory that were not caught in the QA/QC process in developing the inventory. Likewise, we would also need to inspect the SMOKE ancillary input files as a potential source for changes in air quality between the platforms. SMOKE ancillary input files provide a cross-reference of inventory source classification codes (SCCs), and possibly other inventory variables, such as country-state-county FIPs codes, to various information needed to convert the inventory to AQM-ready emissions. Examples include speciation, spatial and temporal allocation, and projections.

Quite often, potential inventory errors result in large, unexpected changes in air quality model predictions but do not show up as obvious outliers in emissions summaries or even emission density maps such as those discussed in a previous inventory conference\(^4\). Another purpose of the shakeout was to update some of the SMOKE ancillary input data files - the cross reference files that use the source classification codes (SCCs) in the inventory. Any SCCs in the 2002 NEI that are not in the 2001 NEI were added to these files.
METHODOLOGY

The shakeout involved substituting 2002 emissions for 2001 platform emissions inventory sectors, one or two at a time, and running the “mixed” 2002/2001 emissions through both SMOKE and CMAQ\(^5\). In this manner, the only change would be the emissions-related inputs for the one (or two) sectors. All other inputs such as meteorology and the chemical mechanism used in SMOKE were retained from the 2001 modeling platform. By replacing only one or two sectors for each air quality model run, any large differences in predicted pollutant concentrations could be isolated to the particular sector(s) being “shaken out.” As seen in Table 1, examples of inventory sectors are “onroad mobile” and “afdust”. It is worth noting that the composition of each sector changed slightly as we migrated from the 2001 platform to the 2002 platform. For example, the “nonroad” sector in the 2001 platform included “alm” emissions — emissions from aircraft, locomotives, and commercial marine vessels. However, the “alm” emissions are not provided by the same emissions model as the remainder of the National Mobile Inventory Model (NMIM)-based nonroad mobile emissions. We also slightly simplified the 2002 platform by absorbing the “pfdust” sector into the “ptnonipm” sector for 2002 because pfdust emissions were very small. Other differences were separating most non-NEI-based emissions inventories, such as Canada, Mexico, and offshore oil production into their own distinct sectors. The overall goal when redefining the emissions sectors for the 2002 platform was to group inventories based on what data elements are likely to undergo revision at the same time.

Table 1. Emissions inventory sector definitions for the 2001 Platform and 2002 Shakeout**

<table>
<thead>
<tr>
<th>2001 sector(s)</th>
<th>2002 sector(s)</th>
<th>Shakeout Run</th>
<th>SMOKE sector</th>
<th>Description for 2002 sector</th>
</tr>
</thead>
<tbody>
<tr>
<td>oarea</td>
<td>nonpt</td>
<td>nonpt plus ag</td>
<td>Area</td>
<td>NEI non-point inventory, excluding: (1) non-point fires, (2) agricultural ammonia, and (3) fugitive dust</td>
</tr>
<tr>
<td>ag</td>
<td>ag</td>
<td>nonpt plus ag</td>
<td>Area</td>
<td>Agricultural ammonia from the NEI non-point inventory</td>
</tr>
<tr>
<td>ptipm</td>
<td>ptipm</td>
<td>N/A</td>
<td>Point</td>
<td>NEI point source emissions deemed Electrical Generating Units (EGUs) as determined through source matching with Integrated Planning Model (IPM) input data</td>
</tr>
<tr>
<td>ptnonipm</td>
<td>ptnonipm</td>
<td>ptnonipm</td>
<td>Point</td>
<td>Remaining point sources from NEI after removing ptipm</td>
</tr>
<tr>
<td>pfdust</td>
<td>ptnonipm</td>
<td>ptnonipm</td>
<td>Point</td>
<td>For 2001, subset of point PM2.5 emissions related to fugitive dust sources</td>
</tr>
<tr>
<td>onroad</td>
<td>onroad</td>
<td>onroad</td>
<td>Mobile</td>
<td>Onroad mobile emissions</td>
</tr>
<tr>
<td>nonroad</td>
<td>nonroad</td>
<td>nonroad plus alm</td>
<td>Area</td>
<td>Nonroad mobile emissions, not including aircraft, locomotives, and commercial marine (alm)</td>
</tr>
<tr>
<td>nonroad</td>
<td>alm</td>
<td>nonroad plus alm</td>
<td>Area</td>
<td>Aircraft, locomotive and commercial marine</td>
</tr>
<tr>
<td>fire</td>
<td>ptfire</td>
<td>ptfire plus nonptfire</td>
<td>Area (2001), area &amp; point/fire (2002)</td>
<td>Day-specific, point source wildfires and prescribed burning</td>
</tr>
<tr>
<td>fire</td>
<td>nonptfire</td>
<td>ptfire plus nonptfire</td>
<td>Area</td>
<td>Subset of NEI non-point emissions containing open and agricultural burning and prescribed emissions for one state</td>
</tr>
<tr>
<td>afdust</td>
<td>afdust</td>
<td>afdust</td>
<td>Area</td>
<td>Subset of NEI non-point emissions related to fugitive dust sources</td>
</tr>
</tbody>
</table>

** includes only those sectors subject to the 2002 Shakeout (e.g., not listed are emissions from Canada, Mexico, and offshore drilling
Although the 2002 Platform includes both HAPs and CAPs, the 2002 Shakeout was limited only to CAPs. Other than Hg, we had no air quality model results for which to compare the HAPs. We designed the Shakeout to isolate the air quality differences due to emission inputs; therefore the 2002 shakeout runs retained the same meteorological inputs (year 2001 MET), chemical speciation mechanism (CB04), and the same version of SMOKE (V2.1) and CMAQ (V4.5) as the 2001 platform.

Updates to the spatial surrogate files were required because of the additional county in the 2002 NEI which was not in the 2001 platform (Broomfield, Colorado, FIPS = 08014). The updated surrogates were created using the Spatial Surrogate tool with the same underlying data GIS shapefiles. The Spatial Surrogate tool and the 2002 surrogates can be found at: http://www.epa.gov/ttn/chief/emch/spatial/.

The ptipm shakeout was not performed due to time constraints in receiving year 2002-specific continuous emissions monitoring (CEM) data for consistent comparisons to the 2001 platform. We did not present the onroad mobile shakeout results because the 2002 onroad mobile inventory was completely replaced after the onroad shakeout run.

SHAKEOUT SECTOR COMBINATIONS AND RESULTS

The progression of 2002 shakeout runs was essentially determined by the availability of the 2002 inputs and the expected impact of the sector on air quality concentrations. We did not perform a shakeout run for each and every distinct emissions sector. The shakeout runs were limited to those sectors with the largest emissions and therefore the largest impact on air quality concentrations.

The shakeout consisted of two parts: 1) comparing emissions to 2001, and 2) comparing air quality concentrations from the shakeout run to those from the 2001 base. Emissions shakeouts involved preparation of the 2002 emissions for input into SMOKE, and comparing various emissions summaries between 2002 and 2001. Examples of the emissions summaries include state-(SCC)/tier-pollutant summaries across multiple sectors and for the larger-emitting facilities (ptipm and ptnonipm sectors), a comparison of emissions between 2001 and 2002 facilities. The following SCC or tier summaries were developed to compare 2002 vs. 2001 emissions (see Table 1 for a description of these sectors):

- afdust 2002 vs. afdust 2001;
- stationary sources excluding afdust (ptipm, ptnonipm, and oarea/nonpt) 2002 vs. 2001;
- nonroad mobile (including 2002alm), 2002 vs. nonroad 2001;
- onroad mobile July, 2002 vs. onroad mobile July 2001

The summaries were inspected to identify state/SCCs with large differences, between 2001 and 2002, in PM$_{2.5}$, NH$_3$, NO$_X$, SO$_2$, and/or VOC. The state/SCC combinations with large differences were then provided to the emissions inventory developers to investigate the reasons for these differences.
One of the most difficult summaries to analyze because of its size was the state-SCC tier summaries comparing 2001 and 2002 stationary sources. This summary involved combining nearly all stationary source sectors except agriculture, for which we developed a separate summary, and summing emissions by state and by the first two SCC tiers (first 4 SCC digits for “AREA” source categories and the first 3 SCC digits for “POINT” source categories) for PM$_{2.5}$, NH$_3$, NO$_X$, SO$_2$, and VOC. The state-SCC tier summary contained approximately 4,000 records. We used conditional formatting to highlight differences greater than 5,000 tons between the two years for each pollutant and identified potential issues to further pursue. Among the issues that were raised were: much higher fertilizer NH$_3$ emissions for numerous states in 2002 than 2001, catastrophic releases due to severe tire fires that are specific to year-2002 and which we chose to remove from the platform, and, an error in Georgia’s surface coating emissions. The 2002 fertilizer emissions were obtained from the RPO-funded Carnegie Mellon University (CMU) model and were therefore accepted as being an improvement over what had been used for 2001. The catastrophic releases were removed from the 2002 Platform (but not from the NEI) and the error in Georgia’s surface coating emissions was corrected in Version 2 of the NEI. Documentation of the 2002 v1 inventory issues resulting from the shakeout and other reviews is maintained and posted on Chief (http://www.epa.gov/ttn/chief/net/2002inventory.html).

The shakeout of stationary sources also included a comparison of emissions for the top 10 facility in both the ptipm and the ptnonipm sectors. The top 10 facilities (based on the PlantID, or “strStateFacilityIdentifier” in the NEI) for each state in both the 2002 and 2001 Platforms were listed along with their rank (from “1” to “10”). These 2002 facilities did not easily match to the 2001 facilities due to changes in the plant name or PlantID. Nonetheless for a given pollutant, one could use these summaries to spot differences in the magnitudes of top 10 sources from the two inventories.

Table 2 shows an example of how such a summary was able to show a potential issue for NH$_3$ in the 2002 Version 1 inventory. Here we see large differences in the top 10 NH$_3$ sources for 2001 and 2002 in Kansas, where the largest NH$_3$ emitting facility in 2002 is more than 4 times greater than the largest emitting facility in 2001. This comparison revealed a problem with the NH$_3$ emissions from EGUs for some states which was corrected in V2 (and all subsequent versions) of the 2002 NEI.

Other 2002 NEI-related issues were identified as part of the shakeout. For example, we found that there were numerous non-traditional source categories in the 2002 point source NEI that were also covered in other sectors. Traditionally (in the 2001 and previous year inventories) the point source NEI contained 8-digit SCCs, while the non-point and onroad/nonroad mobile inventories contained 10-digit SCCs. However, many states reported sources traditionally seen only the non-point and onroad/nonroad mobile inventories -10-digit SCCs- in the 2002 point source NEI; SMOKE allows for 10-digit SCCs in the point source inventory. These include agriculture (NH$_3$) emissions from animal (farm) waste, aircraft emissions at airports, and onroad and nonroad mobile source emissions at a ski resort (very small emissions). Furthermore, aircraft emissions were also reported as point sources using a point source SCC related to jet engines. It was useful to have as many of these issues as possible identified because, as seen in an example later in the paper, they were sometimes able to explain the emissions shakeout information. Some issues (10 digit SCCs in the point source inventory) did not require inventory
changes; however, some required changes to quality assurance/summary or processing techniques. The results of the air quality modeling shakeouts, discussed in the following sections, will describe some of these changes to how we quality assure the emissions data.

Table 2. 2002 V1 emissions compared to the 2001 Platform – Example of a top 10 summary that helped identify a 2002 V1 inventory issue which has been subsequently fixed.

<table>
<thead>
<tr>
<th>Rank in Inventory</th>
<th>FIPS</th>
<th>Dummy PlantID</th>
<th>State</th>
<th>NH3 tons/yr</th>
<th>Inventory Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>20173</td>
<td>L</td>
<td>Kansas</td>
<td>13</td>
<td>2001</td>
</tr>
<tr>
<td>2</td>
<td>20173</td>
<td>N</td>
<td>Kansas</td>
<td>10</td>
<td>2001</td>
</tr>
<tr>
<td>3</td>
<td>20057</td>
<td>A</td>
<td>Kansas</td>
<td>6</td>
<td>2001</td>
</tr>
<tr>
<td>4</td>
<td>20155</td>
<td>AG</td>
<td>Kansas</td>
<td>6</td>
<td>2001</td>
</tr>
<tr>
<td>5</td>
<td>20149</td>
<td>A</td>
<td>Kansas</td>
<td>3</td>
<td>2001</td>
</tr>
<tr>
<td>6</td>
<td>20107</td>
<td>E</td>
<td>Kansas</td>
<td>2</td>
<td>2001</td>
</tr>
<tr>
<td>7</td>
<td>20055</td>
<td>Z</td>
<td>Kansas</td>
<td>2</td>
<td>2001</td>
</tr>
<tr>
<td>8</td>
<td>20175</td>
<td>A</td>
<td>Kansas</td>
<td>2</td>
<td>2001</td>
</tr>
<tr>
<td>9</td>
<td>20009</td>
<td>B</td>
<td>Kansas</td>
<td>1</td>
<td>2001</td>
</tr>
<tr>
<td>10</td>
<td>20125</td>
<td>B</td>
<td>Kansas</td>
<td>1</td>
<td>2001</td>
</tr>
</tbody>
</table>

AIR QUALITY MODELING SHAKEOUT

Each “Shakeout” subsection that follows describes the separate SMOKE/CMAQ runs that were performed to isolate the impacts on air quality concentrations resulting from the new 2002 emissions. For this shakeout, CMAQ was run using the 36km CONUS domain (identical to the 2001 Platform 36km CONUS domain) for two months: January and July with the exception of the ptfire sector which was run for the entire year. Sectors (Table 1) were combined to save on model runs or due to the particular attributes between the sector definitions. For example the “alm” sector could not be run by itself because it was included in the nonroad sector in the 2001 platform.

Non-point and Ag Shakeout

The first shakeout we processed was the non-point and agriculture (“nonpt” plus “ag”) shakeout. As seen in Table 1, this shakeout involved replacing the 2001 oarea and ag sectors with the 2002 nonpt plus ag sectors. The ag sector consists of NH₃ emissions from fertilizer applications and animal husbandry. The 2001 oarea and 2002 nonpt sectors contain similar
emissions source categories from the NEI non-point inventories; the main difference being that the nonpt sector includes agricultural and managed burning emissions while the oarea sector does not. In order to avoid double counting these emissions, the ag and managed burning emissions were removed from the 2001 platform fires sector before running the air quality model.

The results of the nonpt plus ag shakeout are interesting because the resulting air quality differences were not easily explained by a simple analysis of the annual emissions differences. For example, Figure 1 shows the differences in January nitrate (NO₃) concentrations in the nonpt plus ag shakeout. Significant increases in NO₃ concentrations are seen in eastern Kansas southward through eastern Texas, as well as in northwestern Ohio. Meanwhile, significant decreases in NO₃ concentrations appear in western Kansas, New York, and southern Saskatchewan Canada.

Figure 1. Nonpt Plus Ag Shakeout NO₃ concentration changes: 2002 minus 2001

Analysis of NH₃ emissions shows some of the most significant NH₃ differences in the fertilizer application category: SCC=2801700099. As far as correlation to the January nitrate concentration changes in Figure 1, Figure 2 shows some corresponding significant increases in NH₃ emissions from this category in eastern Texas, and some smaller increases in portions of northwest Ohio.

Figure 2 does not explain the significant decreases in January NO₃ concentrations in New York, western Kansas and southern Saskatchewan. The decrease in NO₃ concentrations in New York was determined to be from an error in stationary residential combustion emissions; this issue was corrected in subsequent 2002 inventories. For Canada however, the Canadian inventories in all 2002 shakeout runs were identical to the 2001 platform; in addition, there was
no significant differences in July NO3 concentrations in Canada. After investigating the SMOKE ancillary file changes used to process 2002 emissions, we discovered that the new monthly temporal profile for fertilizer application used in processing the 2002 emissions resulted in a decrease in the allocation of annual fertilizer emissions in January, compared to 2001. Figure 3 shows that the 2001 platform used a default “flat” monthly temporal allocation profile for fertilizer application, whereas the profile used for 2002 has monthly variations with the lowest fraction of emissions in January. This source category includes some of the highest NH3 emissions in Saskatchewan, and the result of applying the new profile yields about an 85% reduction in NH3 in January for fertilizer application emissions.

Figure 2. Fertilizer Application Emissions (NH3) Changes: 2002 minus 2001
The ptnonipm shakeout helps explain the nitrate differences in the nonpt plus ag shakeout in Kansas and Minnesota.

The nonpt plus ag shakeout also revealed some large increases in PEC (elemental carbon) concentrations in Kansas. These increases resulted from large crop burning emissions (SCC 2801500170) which were part of the data submitted by the RPOs and included in the NEI. We are still investigating the issue of whether this ag burning source should include emissions of both PM2.5 and NH3. For most counties this SCC does not contain both NH3 and PM2.5. These inconsistencies become apparent when investigating the SCC tier emissions for tier 2801 in the nonpt plus ag sector for Kansas and Oklahoma (see Table 3). In the discussion of the ptnonipm shakeout below, we further examine the SCC tier summaries in relation to both the nonpt plus ag and ptnonipm shakeout results.
Figure 4. Nonpt Plus Ag Shakeout EC concentration changes: 2002 minus 2001

Non Pt w/Ag vs 2001ai Jan EC

Table 3. Select SCC Tier Emissions Comparisons for Nonpt Plus Ag and Ptnonipm Shakeout

<table>
<thead>
<tr>
<th>SCC tier</th>
<th>description</th>
<th>sector</th>
<th>state</th>
<th>NH3 2001</th>
<th>NH3 2002</th>
<th>Delta NH3</th>
<th>PM2.5 2001</th>
<th>PM2.5 2002</th>
<th>Delta PM2.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>302</td>
<td>Industrial Processes;Food and Agriculture ptnonipm</td>
<td>Kansas</td>
<td>2</td>
<td>57,611</td>
<td>57,609</td>
<td>454</td>
<td>396</td>
<td>-59</td>
<td></td>
</tr>
<tr>
<td>2801</td>
<td>Miscellaneous Area Sources;Agriculture Production - Crops</td>
<td>ag</td>
<td>Kansas</td>
<td>37,290</td>
<td>63,994</td>
<td>26,704</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2805</td>
<td>Miscellaneous Area Sources;Agriculture Production - Livestock</td>
<td>ag</td>
<td>Kansas</td>
<td>96,168</td>
<td>33,381</td>
<td>-62,787</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>302</td>
<td>Industrial Processes;Food and Agriculture ptnonipm</td>
<td>Minnesota</td>
<td>0</td>
<td>25,934</td>
<td>25,934</td>
<td>858</td>
<td>646</td>
<td>-212</td>
<td></td>
</tr>
<tr>
<td>2805</td>
<td>Miscellaneous Area Sources;Agriculture Production - Livestock</td>
<td>ag</td>
<td>Minnesota</td>
<td>101,460</td>
<td>72,405</td>
<td>-29,055</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2801</td>
<td>Miscellaneous Area Sources;Agriculture Production - Crops</td>
<td>ag</td>
<td>Ohio</td>
<td>7,999</td>
<td>41,316</td>
<td>33,317</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2801</td>
<td>Miscellaneous Area Sources;Agriculture Production - Crops</td>
<td>ag</td>
<td>Texas</td>
<td>60,230</td>
<td>179,640</td>
<td>119,410</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2801</td>
<td>Miscellaneous Area Sources;Agriculture Production - Crops</td>
<td>nonpt</td>
<td>Oklahoma</td>
<td>0</td>
<td>5,124</td>
<td>5,124</td>
<td>2</td>
<td>35,228</td>
<td>35,226</td>
</tr>
</tbody>
</table>
Ptnonipm Shakeout

As shown in Table 1, the ptnonipm sector contains non-EGU (electric generating units) NEI point inventory emissions. One of the more interesting results of the ptnonipm shakeout, presented in Figure 5, was the significant total ammonia (NH₃) increases in Minnesota and western Kansas. Recall from the nonpt plus ag shakeout the large decrease in nitrate emissions in western Kansas (Figure 1). As seen again in Table 3, analysis of emissions changes for the nonpt plus ag and ptnonipm sectors stand out for a couple select source categories in Kansas and Minnesota. Notice the ptnonipm NH₃ increases for SCC Tier 302 in these states. Also notice the ag sector decreases for SCC Tier 2805. In Kansas and Minnesota, these source categories (containing farms) were rolled up as county-level (ag sector) emissions in the 2001 platform, but inventoried as discrete point sources (farms) in the 2002 platform. Therefore, when performing a “shakeout” for the nonpt plus ag sector, these farms were not included in the 2002 shakeout which explains the decrease in nitrate in western Kansas and Minnesota. Likewise, in the ptnonipm shakeout, these farms were in the ptnonipm sector for 2002 and also in the 2001 ag sector which explains the increase in total ammonia for this shakeout in the same two areas. The emissions comparisons in Table 3 also explain some of the increase in nitrate concentrations found in the nonpt plus ag shakeout for Texas, Oklahoma, and Ohio.

Figure 5. Ptnonipm Shakeout NH₃ concentration changes: 2002 minus 2001

Pt Non-IPM vs 2001ai Jan NHₓ

Min= -4.573 at (24,45), Max= 3.661 at (67,52)
Nonroad Shakeout

The nonroad shakeout revealed an error in the allocation of ports in New York and New Jersey as seen in the elemental carbon (EC) concentration estimate differences in Figure 6. This was the result of a misallocation of a port from New York City to Syracuse, NY. This error, which was corrected for the 2001 platform, was remedied in subsequent versions of the 2002 inventory. The differences in EC in Louisiana, as seen in Figure 6, were also the result of a spatial misallocation of emissions. This was corrected in the updated 2002 inventory. In addition, differences in Mecklenburg and Wake counties in North Carolina and Phoenix Arizona are due to differences in PM2.5 emissions from aircraft (commercial for NC and military for Phoenix) -in these areas, aircraft emissions are state-reported for 2002.

Figure 6. Differences in July Nonroad Shakeout EC (elemental carbon) Concentrations

![Image of Figure 6](image)

Ptfire Shakeout

The ptfire shakeout was the most challenging from a quality assurance perspective because the format and content of the data for this sector changed dramatically from the 2001 platform to the 2002 platform. As shown in Table 1, the 2001 platform “fire” sector data is represented as annual county total emissions for the following source categories: wildfires, prescribed burning, open/managed burning, and agricultural burning. In contrast, the 2002 “ptfire” sector contains day-specific, discretely-located wildfire and prescribed burning fire emissions in the SMOKE PTFIRE format. This format contains information such as acres burned, fuel loading, and heat content which are used to compute the vertical distribution of emissions from each fire. Note that the ptfire sector does not include agricultural burning; therefore, for the purpose of the ptfire shakeout, these emissions were retained from the 2001 platform.

As a result of the additional spatial and temporal resolution in the 2002 fire emissions, we expected, and did, find more localized and temporally-refined peaks and minimums in predicted air quality concentrations in the results of the 2002 ptfire shakeout. Figure 7 shows elemental carbon (EC) differences from the ptfire shakeout, presented in a time series of four days –
February 28th through March 3rd. The scale on each of the four days is very large (differences of less than 5 µg/m³ are not shown). A very large “hotspot”, in EC concentrations in 2002 appears suddenly on March 1st (top right panel) in southern Georgia. The large fire(s) on March 1st begin to diminish and disperse by March 2nd (lower left panel). By March 3rd (lower right panel), most EC from the southern Georgia fire(s) has dissipated.

Figure 7. Daily Impacts –Feb 28th through March 3rd- of Differences in Ptfire Shakeout EC (elemental carbon) Concentrations

Analysis of the entire year for the 2002 ptfire shakeout produced several other significant peaks in EC for 2002. However, as expected, most of these were in the West during the summer and were usually much less severe in magnitude, compared to the GA case. We inspected the daily distribution of fires in March 2002 ptfire emissions for Georgia in order to understand the cause of the abrupt temporal changes in predicted concentrations. Figure 8 shows the counts of daily fires for wildfires, prescribed burning, and managed burning. The huge spike in EC emissions appears to be related to the large number of wildfires on March 1st. While the daily distribution of wildfires appeared at least plausible, the daily distribution of the prescribed burning and managed burning emissions solely on March 1st appeared suspicious. Analysis of the other months showed the same temporal behavior in that all prescribed and managed burning emissions were assigned to the first day of the month. Further investigation of these emissions...
revealed that the emissions were not actually assigned to the actual fire—logically, they could not be because they were placed at the same fire (day) for every month. It was discovered that these fires were inventoried at the county level (i.e., as county totals) and assigned as point sources to county centroids. In order to properly process and model the prescribed burning emissions in Georgia, these data were split out of the ptfire sector and placed into a “nonptfire” sector (see Table 1). This same situation was found in several other states.

Another outcome of the ptfire shakeout is the managed burning emissions in the ptfire sector—in the limited number of states where provided—have been aggregated to a SMOKE area format where they are spatially allocated using spatial surrogates and temporally allocated consistent with the 2001 platform. This “smoothes” the managed burning emissions over the month and spatially to the grid cells of activity; however, we believe this is less incorrect than fires aggregated to county centroids during a single (most likely wrong) day (the first day) each month.

**Figure 8.** March Fire Counts in Georgia 2002 Ptfire Inventory

![Figure 8: March Fire Counts in Georgia 2002 Ptfire Inventory](image)

**CONCLUSIONS**

The 2002 shakeout was a successful part of the development of the 2002 Emission Modeling Platform in numerous ways. It helped us to identify inventory errors in the first version of the 2002 NEI, which were remedied in subsequent 2002 NEI versions. By performing the shakeout we became more familiar with certain characteristics of the inventory that relate to the ancillary files prepared for processing and summarizing the emissions data. Both the comparison of platform emissions (emissions shakeout) and concentrations (air quality shakeout) played an important role in this process. The emissions shakeout provided a preview of what we would see in the model results and helped us to better understand the air quality impacts of the new inventory. We also caught some inventory errors as part of the emissions shakeout that were not evident in the modeled concentrations.

The ptnonipm, nonpt plus ag, nonroad mobile, and ptfire 2002 shakeout model runs were useful in identifying emissions inventory errors and characteristics that affect emission processing and data summaries. We also learned that inventory fixes are sometimes forgotten in
new model years. Specifically, the nonpt plus ag shakeout revealed the effects of a newly-added monthly temporal profile to unmodified emissions, and raised the question as to how the EPA accepts and confirms PM and NH₃ emissions factors from state-reported emissions sources. Combined with the results of the ptnonipm shakeout, we discovered that some farms were inventoried more specifically (as point sources) in the 2002 emissions platform than in the 2001 platform (as county-level emissions). The nonroad & alm shakeout revealed how the port location corrections to the 2001 emission platform were not included in the 2002 inventory. The nonpt plus ag shakeout also reaffirmed the potential large effect of replacing of EPA-generated data with state data for a single emissions source category. For several reasons, we expected and found some of our most profound and acute air quality concentration differences from the ptfire shakeout. Through this shakeout, we also indirectly (surreptitiously actually) discovered inventory errors and a SMOKE bug that have also been corrected. As a result of the shakeout we not only have an improved inventory, but we have also gained a greater understanding of the basis and characteristics of the 2002 emissions data.

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KEY WORDS

SMOKE, CMAQ, emissions, 2002 NEI, shakeout