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MOVES-Matrix 3.0 for High-Performance On-Road Energy and Emission Rate Modeling Applications

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# MOVES-Matrix 3.0 for High-Performance On-Road Energy and Emission Rate Modeling Applications

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A White Paper from the National Center for Sustainable Transportation

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# MOVES-Matrix 3.0 for High-Performance On-Road Energy and Emission Rate Modeling Applications

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A National Center for Sustainable Transportation White Paper

February 2023

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## TABLE OF CONTENTS

Executive Summary.....	i
1. Introduction .....	1
2. Methodology.....	3
3. Results and Discussion .....	6
4. Conclusions and Ongoing Work .....	9
References .....	10
Data Summary.....	13

## List of Tables

Table 1. Fuel Formulation Regions for Gwinnett County, GA in MOVES 2014b vs. MOVES3 ..... 8

## List of Figures

Figure 1. MOVES-Matrix Conceptual Flow (Liu et al. 2019a).....	4
Figure 2. MOVES-Matrix Data Processing Overview (Liu et al. 2019a).....	5
Figure 3. Fuel Supply Scenarios in MOVES 2014b (Left) vs. MOVES3 (Right) for Georgia.....	8

# MOVES-Matrix 3.0 for High-Performance On-Road Energy and Emission Rate Modeling Applications

## Executive Summary

This white paper summarizes the development process for MOVES-Matrix 3.0, which will be based on EPA's latest energy use and emission rate model known as MOVES3 (version 3.0.4). The MOVES-Matrix system developed by the Georgia Tech team can be used to conduct on-road energy consumption and emissions modeling more than 200-times faster than using MOVES directly. The concept of using iterative model processing and matrix generation was first applied with the MOBILE model many years ago (Guensler et al. 2004, 2000; Guensler and Leonard II 1995). MOVES-Matrix follows the same iterative approach, where a multidimensional array is generated from MOVES model run outputs. MOVES-Matrix for Atlanta, GA was originally created by running the MOVES 2014 model 146,853 times (across all combinations of input variables). The iterative runs populate matrices that can be queried for energy and emissions analyses using Python scripts and/or other applications (for any set of fleet compositions, model year distributions, environmental conditions, and on-road operating conditions) for each modeling region (which are defined by unique combinations of fuel specification and inspection and maintenance programs). The MOVES-matrix lookup system provides the exact same emission results as using MOVES 2014 directly for each analysis of an individual transportation road link, ensuring the validity of using the matrix outputs in regulatory analysis. The resulting emission rate matrices allow users to connect link-by-link vehicle activity data for large projects with applicable emission rates, and to evaluate changes in emissions for dynamic transportation systems in near-real-time, without having to launch MOVES (because all possible MOVES runs for the modeling region have already been pre-processed).

In developing MOVES-Matrix 3.0, the research team applied the same conceptual design used in MOVES-Matrix 2.0; however, all of the programs employed in generating matrices on the distributed computing servers had to be updated to account for changes in MOVES3 data structures and vehicle source sub-types. The development required significant code modifications to integrate new source type physics parameters (vehicle specific power/scaled-tractive power configurations for various source types by model year), to address changes in input parameters, and to process significantly greater numbers of mandatory iterations within each individual model run. The team currently anticipates a 10% increase in run time per modeling region to generate matrices for MOVES3, given the more complicated source type VSP/STP variables and internal iterations.

MOVES3 also employs more unique combinations of fuel supply regions and inspection and maintenance (I/M) programs than the team faced in developing the original MOVES-Matrix; with 40 fuel scenarios and 87 I/M scenarios in MOVES3 vs. 22 fuel scenarios and 84 I/M scenarios in MOVES 2014b. The increase in fuel scenarios represents changes to fuel formulation regions and one-to-many relationships between counties and fuel formulation

regions by year. MOVES-Matrix is processed for each unique combination of fuel scenario and I/M scenario, which MOVES-matrix defines as a modeling region. The number of MOVES-Matrix modeling regions has increased from 109 regions in MOVES 2014b to 122 regions in MOVES3 (representing a 12% increase in resources required to develop all matrices for the nation). Each iterative process to develop matrices for a modeling region takes about five days to process on the PACE supercomputing resources (Georgia Tech, 2022), given the allocation of nodes currently assigned by PACE (a Georgia Tech supercomputer Co-op) to the modeling team. The research has continued to develop MOVES-Matrix 3.0 and generate matrices for the Atlanta Metro Area and the rest of Georgia as part of an ongoing 2022-2023 research project for NCST.

## 1. Introduction

The MOtor Vehicle Emission Simulator (MOVES) model (U.S. EPA, 2020a) provides significantly improved emission rates compared to the older MOBILE series of models (U.S. EPA, 2016), primarily because MOVES emission rates are more modal in nature, better representing emissions as a function of instantaneous (1Hz) speed and acceleration. Coupling high-resolution on-road vehicle activity data with appropriate MOVES emission rates further advances research efforts designed to assess the environmental impacts of transportation design and operation strategies (U.S. EPA 2022a). Hot spot analysis and near-road dispersion modeling for environmental impact assessment also benefit from using more accurate vehicle activity data in time and space, and the application of high-resolution emission rates to actual on-road driving conditions (Guensler et al. 2021; Liu et al., 2019b). MOVES3 is now the latest official version of MOVES and has been updated and improved from the previous version by: 1) incorporating the latest data on vehicle populations, emission rates, and regional fuels; 2) better accounting for engine starts, truck hoteling, idling; 3) incorporating the forecasted impacts of new truck and passenger vehicle standards (U.S. EPA, 2022b).

Because emissions are a complex function of many locally-dependent variables, and because MOVES integrates a number of aggregation functions for use in emission estimation at state and county levels, the interface is complex and requires numerous user inputs to properly characterize any specific emission scenario. Extensive labor is required to prepare MOVES input files. In addition, running MOVES is time consuming, because emission calculations begin with base emission rates, which are internally adjusted by various correction factors such as temperature, humidity, fuel property, etc. This also makes MOVES difficult to use for large-scale transportation networks that experience dynamic changes in on-road fleet composition and operating conditions that affect corrections factors during the day (CRC, 2017).

The latest Atlanta Regional Commission (ARC) Travel Demand Model network now includes 148,000 roadway segment links (nearly doubling the number of links compared to the 2019 model with 74,500 links). It is nearly impossible to perform emissions modeling for a dynamic network of this size using individual MOVES emission rates for each link when fleet composition and on-road operating conditions change dynamically over the course of a day. On a typical personal computer (PC), depending on the pollutant types to be modeled, MOVES requires around 10-30 seconds to process emissions for one link for a unique fleet and operating condition. To obtain the composite emission rates for 1,000 roadway links in Atlanta, where the fleet composition and operating conditions vary every hour on every road segment, and where temperatures and humidity values vary by hour of day and month, and for the three Atlanta fuels (summer, winter, and transition), would require nearly 32 million individual MOVES runs, which would take ten years to run on a typical PC. This is based on 1,000 road segments, with operations of each hour across 24 hours, in 21 temperature bins scenarios (10-110 °F in 5 °F bins), 21 humidity bins scenarios (0%-100% in 5% bins), and 3 fuels supply scenarios (summer, winter, and transition fuel supply), which yields 31,752,000 individual MOVES runs. Shortcuts can be taken to reduce the number of model runs required (e.g., many runs yield the exact same emission output across a certain temperature/humidity ranges as they are insensitive to

several pollutant types, and there is no need to run the model for low temperatures during summer months). However, modeling across all such operating conditions on a PC is impractical. High-performance modeling approaches are needed to assess large-scale dynamic networks.

Regulations require the latest approved regulatory model (i.e., MOVES3) be used in all transportation and air quality planning and assessment work (U.S. EPA, 2020a). To improve modeling efficiency, but at the same time ensure that regulatory requirements for use of MOVES (2014 at that time) are met, the research team developed MOVES-Matrix (Liu et al. 2019a). For an individual MOVES2014 modeling region, the MOVES model is run more than a hundred thousand times on the PACE supercomputing cluster, which takes three to seven calendar days to complete. Time to completion depends upon how many cores in the supercomputing cluster are assigned to the activity (the cluster is essentially a co-op, and spare cores are automatically assigned by PACE to processes when they are available). The iterative process generates a multidimensional array of energy use and emission rates for all combinations of MOVES input variables for that modeling region (i.e., MOVES runspecs and user csv supplied data, see U.S. EPA 2020e). The array for each region contains around 90 billion cells and is about 2Gb in file size.

Modelers can query MOVES-Matrix emission rates generated through the iterative modeling process, and apply these emission rates in any analytical activity that can be performed with MOVES outputs, without ever having to launch MOVES or transfer MOVES modeling output files into the analyses. The scenario runs demonstrate that MOVES-Matrix can finish the emissions computation tasks more than 200 times faster than using the MOVES batch mode and the results generated are exactly the same (Liu et al. 2019a).

MOVES-Matrix can be used to model the emissions from individual vehicles and eco-driving applications (Xu, et al., 2018; Guensler, et al., 2017), and can be easily coupled with vehicle activity analysis (Li et al. 2017, 2016; Xu et al. 2017; Liu et al. 2019b) by importing second-by-second vehicle operations. The matrix structure also facilitates sensitivity analysis and uncertainty assessment of MOVES algorithms (Lu et al., 2021) and can be integrated with large-scale transit operation data for energy use modeling (Fan et al. 2022). MOVES-Matrix can also be applied to different transportation models, such as travel demand models (Xu, et al. 2018), dispersion models (Kim, 2020; Kim et al., 2020; Liu et al., 2019b, 2017; Lu et al., 2022), and microscopic traffic simulation models (Xu et al. 2016). For example, assessment of the emissions and energy consumptions of the ARC network (149,000 roadway segment links as described above) based on output from activity-based model (ABM) only takes a few hours to run using MOVES-Matrix (Zhao, 2020). In 2017/2018, the team also developed MOVES-Matrix 2.0, which also supported the rapid analysis of engine starts, truck hoteling, evaporative sources, brake/tire wear (Xu et al. 2018).

Georgia Tech continues to collaborate with an expanding set of MOVES-Matrix users. The research team integrated MOVES-Matrix in various EPA meetings and presentations, and provided FHWA with model set and the matrices of Washington D.C. The team provided the

matrices of Texas to researchers at Texas A&M Transportation Institute, and the modeling tool has been integrated into their statewide live online roadway performance assessment tools. Georgia Tech has collaborated with CARTEEH to implement MOVES-Matrix online repository. We are also working with the University of Wyoming (matrices of Wyoming and Utah), Pennsylvania State University (matrices of Pennsylvania), the University of Vermont (matrices of Vermont), Rensselaer Polytechnic Institute (matrices of New York), Beijing Jiaotong University in Beijing (matrices of Atlanta, GA), and Tongji University in Shanghai (matrices of California) by providing the matrices that they need for their research. Consulting firms such as AECOM and Rybinski Engineering (matrices of Delaware) are also using MOVES-Matrix for their projects. The continued advancements in the state-of-art techniques to distribute MOVES in Georgia Tech's high-performance parallel computing system (PACE) system was highlighted in the PACE Newsletter in Spring 2020.

The U.S. Environmental Protection Agency (U.S. EPA) requires that MOVES3 be employed (the grace period of MOVES 2014 ended January 2023). Hence, the research team must ensure that any modeling approach that employs MOVES3 outputs in a lookup matrix process yield exactly the same emission rates as when applying any individual MOVES run output directly to the same transportation operating conditions.

In this project, the team identified all of the major updates within MOVES3 by reviewing the EPA documentation (U.S. EPA, 2020b, 2020c), and assessed changes in the MOVES3 default database (movesdb20220802). The changes in terms of the updated vehicle specific power (VSP)/ scaled tractive power (STP) parameters, I/M programs, fuel supply configurations, and the running environment of MOVES are summarized in this white paper.

## 2. Methodology

MOVES-Matrix is composed of the outputs from a tremendous number of MOVES model runs. The basic process is to run MOVES across all variables that affect output emission rates, where each MOVES run yields pollutant emission rates for all vehicle source types, model years, vehicle fuel types, and on-road operating conditions (by average speed and road type, and across all of the on-road VSP/STP operating mode bins) for all specified combinations of calendar year, temperature, humidity condition, and other applicable regional regulatory parameters (fuel properties, I/M program characteristics). After conducting more than one hundred thousand runs, the resulting MOVES emission rate matrix (MOVES-Matrix) can be queried to obtain the exact same emission rates that would be obtained for any MOVES model run, without ever having to launch MOVES again, or transfer MOVES outputs into the analyses.

Figure 1 provides an overview of MOVES-Matrix application process (Liu et al. 2019). The MOVES-Matrix run module uses user input to identify the regional matrix (defined by fuel properties and I/M programs) and any sub-matrices that will be required for the specific analyses from the large array. Rather than carrying the entire regional 90-billion cell array into analyses, the user-specified calendar year, fuel month, and meteorology data are used to create analytical matrices. The user can then access each cell that contains an emission rate for a specific vehicle class and model year from MOVES-Matrix and weight each emission rate by

on-road activity to reassemble the fleet emission rate. Because the weighting process is exactly the same as used in MOVES to generate a fleet composite emission rate for a link, the MOVES-Matrix process yields the exact same emission rates as a direct MOVES run, but in a fraction of the time. Figure 2 shows the emission rate assembly process for MOVES-Matrix. Because each MOVES run already performed the complex emission rate calculations and adjustments for temperature, humidity, fuel composition, I/M program, etc., and MOVES-Matrix simply contains the resulting emission rates, for the user, applying MOVES-Matrix is significantly faster than running MOVES, and efficient enough to enable large-scale and real-time emission estimation.

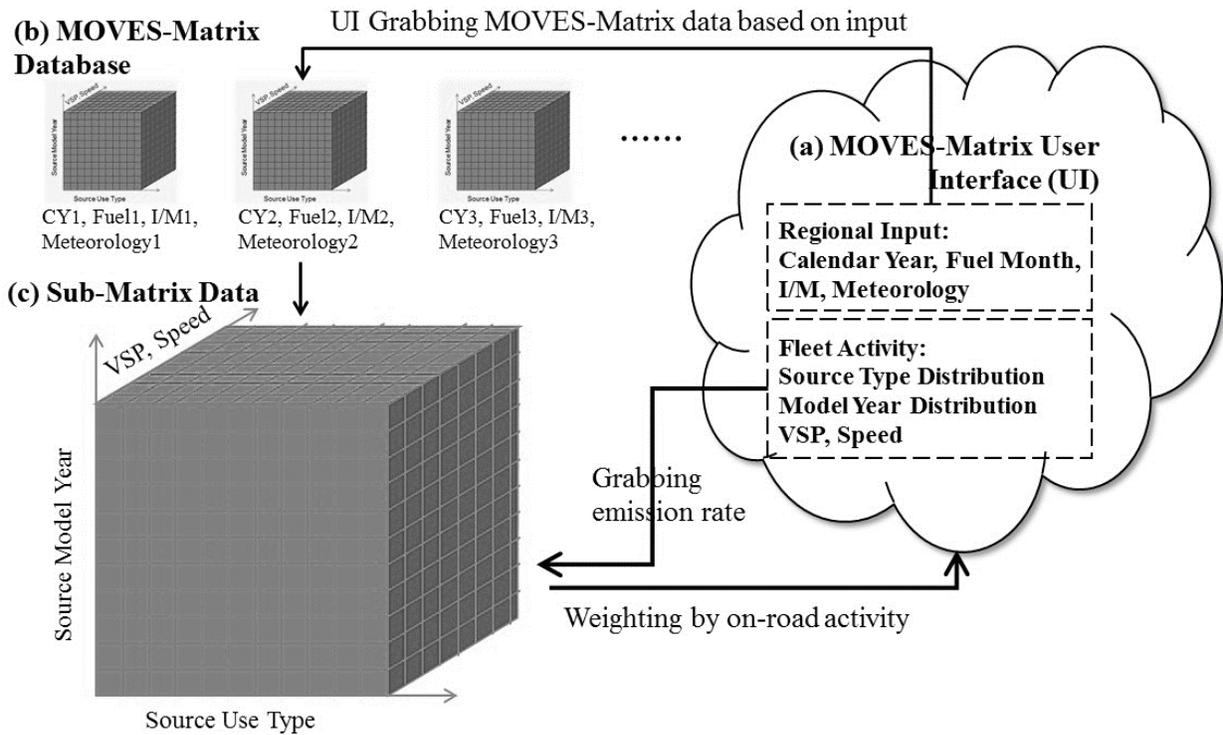
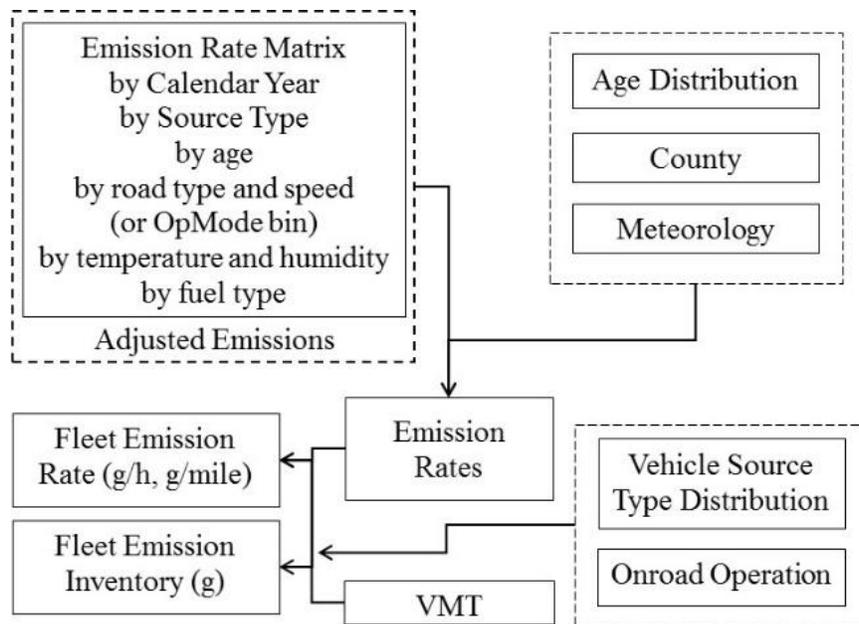


Figure 1. MOVES-Matrix Conceptual Flow (Liu et al. 2019a)



**Figure 2. MOVES-Matrix Data Processing Overview (Liu et al. 2019a)**

The team performed a thorough review of the configurations of fuel and I/M programs in MOVES3 and compare these settings vs. MOVES 2014. The team updated the MOVES-Matrix region directory accordingly (added new regions due to any finer break of fuel and I/M combinations, and removed redundant regions as needed to reduce run time), and developed a comprehensive estimate of run time required to complete the runs for all modeling regions in the nation.

The research team has priority access to the Partnership for an Advanced Computing Environment (PACE) high performance computing (HPC) clusters of Phoenix. PACE is a collaboration between Georgia Tech faculty and the Office of Information Technology, and was established for the primary purpose of providing an environment for distributed high performance computing. The configuration of MOVES3 (version 3.0.4) on PACE requires that internal MOVES model updates accommodated, which includes support of Java 17 and the operating system update to Red Hat Enterprise Linux (RHEL) 7.9 from RHEL 7.6 (a major update in February 2021 that changed the Linux Kernel). The team is again updating previous MOVES3 scripts to account for the PACE cluster changes (especially those due to the Linux Kernel update) in terms of MariaDB, Java, and the compilers of Fortran and Go.

When a MOVES job is launched on a cluster machine, the scripts first install MOVES on the machine by unzipping the MOVES source files on the disk. The script then proceeds to install a thin version of MariaDB server (MySQL for MOVES 2014) by unzipping its files onto the disk, and starts the SQL server on an available port. MOVES command line Java processes are then launched to create input and output database files respectively. The output files are zipped and stored on PACE persistent storage. More details on launching MOVES in PACE can be found in Liu et al. (2016). Given PACE's limits on the number of jobs that can be launched simultaneously (500 jobs according to the PACE policy) and on the number of computational nodes that can be

used at the same time (3,000 nodes per research group), the team will further optimize the scripts to better utilize the computational resources (e.g., by minimizing the nodes needed for each job, while not significantly increase the average run time per job).

For each new region (Matrix not generated based on MOVES 2014), a total of 21 calendar years × 3 fuel months × 23 temperature bins (0-110 degrees with 5-degree interval) × 21 humidity bins (0-100% with 5% interval) = 30,429 runs of MOVES is required. Generating matrices for a region takes approximately 3 to 7 days for MOVES 2014, and currently take around 15 to 20 days for MOVES3 due to the increased number of sub-source types (VSP/STP configurations). A conservative estimate of the run time increase is at least 10%. A more precise assessment will be available once all of the PACE clusters that the team has been using have migrated into the new Slurm supercomputing system and model processing scripts have been updated for the new cluster configuration. Re-generation of a Matrix for a region that has already been processed via MOVES 2014 should take less time once the scripts are modified to exclude unnecessary emission rates (i.e., those that have not changed between MOVES2014 and MOVES3), but the process will still likely take up to three days to complete per modeling region. The research team will prioritize running the regions that are currently using MOVES-Matrix for MOVES 2014, starting with Atlanta, Georgia. All energy use and emission rate data will be uploaded to the DOE OEDI server system for open source access.

In the next stage of NCST research, the research team will bring the MOVES3 matrix results into case studies to ensure that MOVES-Matrix 3.0 generates the exact same results with MOVES3. The speed performance associated with running MOVES-Matrix vs. launching MOVES for individual will also be reassessed to compare with the prior MOVES-Matrix model version. The team will prepare a report that summarizes the work prepared by the team and the four tasks above and provides recommendations for model applications and additional research. Each task deliverable will serve as an Appendix to the full report. The team will place the open source code in the NCST repository.

### **3. Results and Discussion**

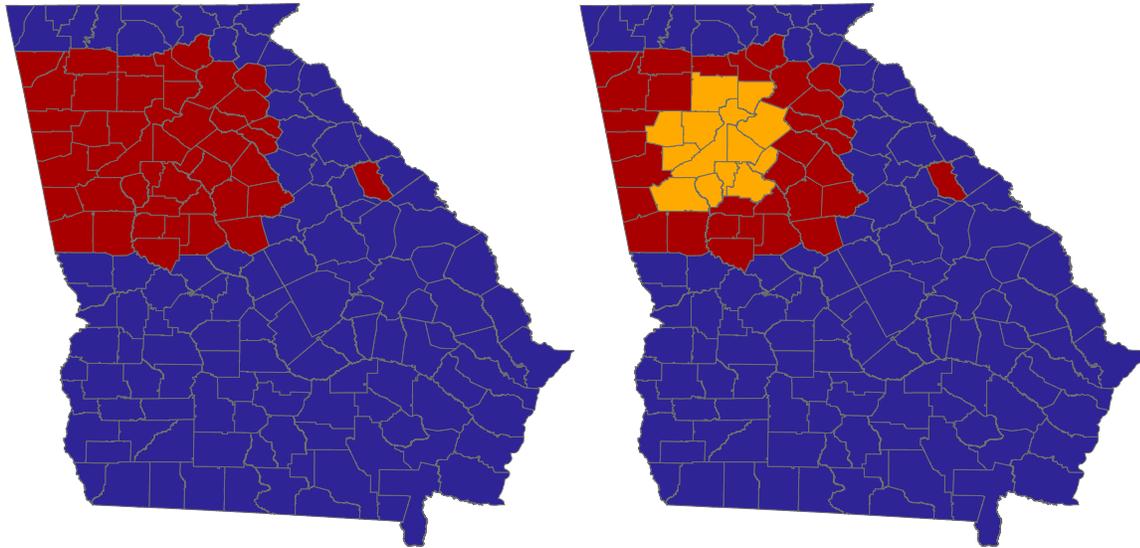
One of the major updates in terms of emissions and energy use modeling is the new source type physics parameters for vehicle-specific-power/scaled-tractive-power configurations (U.S. EPA, 2020d, 2020e) for various source types based on model year (listed in the “sourceusertypephysics” table within the MOVES3 database). The updated MOVES3 database introduced 185 unique combinations of VSP/STP parameters (out of 206 combinations), while MOVES 2014 only employed 22 unique combinations. The team updated the corresponding code for both the generation of the matrices and the MOVES-Matrix running module to address the changes in input parameters. The parameter updates led to a significant run time increase for matrix generation (iterative MOVES3 runs) on the supercomputing cluster, due to the larger number of iterations, and increased time in model applications, due to the assembly of emission rates across a larger number of combinations (and a slightly increased time for input/output).

MOVES 2014b includes 3229 counties. MOVES3 introduced Kusilvak Census Area, Alaska to the county list (but users can still use its former name of Wade Hampton Census Area). Otherwise, the lists of modeled counties are identical for the two versions of MOVES. The Kusilvak Census Area and Wade Hampton Census Areas are marked with different county IDs in MOVES, but their fuel supply and I/M programs are exactly the same in the MOVES3 database (not surprising given they are essentially referring to the same administrative division).

The fuel supply updates in MOVES3 yield 40 fuel supply scenarios, given the increased number of fuel formulation regions and the updated one-to-many county-to-region relationships (there are only 22 fuel supply scenarios in MOVES 2014b). The review of the fuel supply updates (“fuelsupply” table in the default MOVES databases) identified 23 fuel formulation regions in MOVES3 (fuel formulation region #700000000 that covers various Boroughs and Census Areas in Alaska) rather than 22 regions in MOVES 2014b. A major change introduced by MOVES3 is the one-to-many corresponding relationships between counties vs. the fuel formulation regions. In MOVES 2014b, every County corresponds to only one fuel region (across all the years), while in MOVES3, one County can correspond to various fuel regions (one fuel region per year). An example is provided below, where Gwinnett County, GA (County ID #13135) corresponds to three fuel formulation regions (#100000000, #170000000, and #178000000) in MOVES3 while it only corresponds to one (#170000000) in MOVES 2014b. The fuel scenarios for the state of Georgia is shown in Figure 3, where the updated fuel supply settings can be observed for the metro Atlanta area (two scenarios in MOVES 2014b and three in MOVES3).

**Table 1. Fuel Formulation Regions for Gwinnett County, GA in MOVES 2014b vs. MOVES3**

Database	Fuel Formulation Region # (1990 to 2001)	Fuel Formulation Region # (2002 to 2015)	Fuel Formulation Region # (2016 to 2019)	Fuel Formulation Region # (2020 to 2060)
MOVES 2014b	170000000	170000000	170000000	170000000
MOVES3	100000000	170000000	178000000	100000000



**Figure 3. Fuel Supply Scenarios in MOVES 2014b (Left) vs. MOVES3 (Right) for Georgia**

The team updated the examining algorithm to check the unique I/M programs, and found 87 I/M scenarios in MOVES3 (version 3.0.4), whereas MOVES 2014b has 84 scenarios. Major updates on the I/M programs include a finer division of New Jersey, allocating I/M programs to various counties in North Carolina and Louisiana (no default I/M programs in MOVES 2014b for these counties), etc.

The review of the default fuel supply configurations and I/M programs were reviewed by examining the MOVES3 database (the tables of “fuelsupply” and “imcoverage”) vs. MOVES 2014b indicated that MOVES3 introduced finer resolution in terms of defining the regions, and it was found that MOVES 2014b defined a total of 109 regions (unique combinations of fuel vs. IM programs), and that MOVES3 (version 3.0.4) defined 122 regions. An increase of 10.9% more regions are found in MOVES3, which is anticipated to increase the running time to finish the matrices across the nation.

## 4. Conclusions and Ongoing Work

This white paper documents the internal model review of program software updates and default fuel supply configurations and I/M programs in MOVES3 vs. MOVES 2014b. A total of 122 regions are defined in MOVES3 compared with 109 regions in MOVES 2014b, and the team anticipates at least 10% more running time to generate matrices for MOVES3, given the larger number of regions and the more complicated source type VSP/STP variables.

The team has prioritized the runs of Atlanta metro area (Fulton County, Georgia) in the previous efforts, and will conduct matrix runs for additional regions. The team is working with the PACE support team to move forward with running MOVES3 on the supercomputing cluster and to address the challenges in running iterative processes on the cluster given the software updates that have been required.

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## **Data Summary**

### **Products of Research**

No data were collected for the study. All analyses are based upon manual review of the model code and databased employed in the MOVES 2014 and MOVES3 models and model run testing on the PACE supercomputing cluster at Georgia Tech.

### **Data Format and Content**

Not applicable.

### **Data Access and Sharing**

Readers can access the MOVES 2014 and MOVES3 models and modeling support documentation via the EPA modeling website: <https://www.epa.gov/moves>

### **Reuse and Redistribution**

MOVES modeling materials are open source and there are no restrictions on redistribution.