Task 4: Final Report: Peer Review of

Fuel Effects, Toxics Emissions, Total Organic Gases (TOG) and Particulate Matter (PM) Speciation Analysis Report

in Support of MOVES2013

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Contents

Tables

1. Introduction

The MOtor Vehicle Emission Simulator (MOVES) was developed as part of OTAQ's comprehensive approach to address the impacts of light- and heavy-duty vehicles on air quality and public health. MOVES is OTAQ's current emission modeling system, capable of estimating emissions for a broad range of pollutants from on-road cars, trucks & motorcycles at multiple analysis scales, including the impact on air quality of light duty vehicle (LDV) fleet evaporative emissions. Future versions of MOVES will add various enhancements to this model, including the ability to simulate emissions from non-highway mobile sources.

As part of the development of the next release version, MOVES2013, EPA is preparing five reports/analyses documenting the results of various inquiries into the nature of fuels, vehicle exhaust and evaporative emissions on air quality. These reports detail how EPA intends to update MOVES' ability to model policy outcomes from proposed changes in the understanding of the US vehicle fleet and to help mitigate any adverse air quality impacts associated with future motor vehicle fuels.

This document reports the findings of an external peer review of all or part of five reports:

- Modelling Effects of Fuel Properties in the Motor Vehicle Emissions Simulator (MOVES2014)
- TOG and PM Speciation in MOVES for Air-Quality Modeling
- PM Speciation Appendix
- Development of Emission Rates for Light-duty Vehicles in the Motor Vehicle Emissions Simulator (MOVES2014)
- Estimation of Air-Toxic Emissions from Highway Vehicles in the Motor Vehicle Emissions Simulator (MOVES 2014)

These are referred to here collectively as the MOVES2013 Fuel Effects, Toxics Emissions, Total Organic Gases (TOG) and Particulate Matter (PM) Speciation Analysis Reports.

This peer review was conducted from July 2013 to September 2013 according to *EPA's Peer Review Handbook, Third Edition*. These guidelines specify that all highly significant scientific and technical work products shall undergo independent peer review per specific agency protocols to assure the use of the highest quality science in its predictive assessments and assure stakeholders that each analysis/study has been conducted in a rigorous, appropriate, and defensible way.

This document contains the conclusions of each peer reviewer on each document included in the review, by charge question. Supporting documentation collected from the reviewers, including their curriculum vitae (CV) and conflict of interest (COI) statements, is also provided in Appendix A and Appendix B. The Task 3: Peer Review Process Report describes the process to select reviewers and administer the peer review. At the conclusion of the review, ICF collected all peer review comments and cover letters in order to provide them to EPA, unedited. The following materials are included in this report.

1. Reviewer Responses to Charge Questions (Section 4)
2. Reviewer Supporting Documentation (Appendix A and Appendix B):
    a. Reviewer Delivery Email (i.e., Cover Letter)
    b. Reviewer CV
    c. Reviewer COI Statement

2. Peer Review Process

Full documentation of the process to select reviewers and administer the peer review is included in the Task 3: Peer Review Process Report. This section summarizes the process that resulted in the selection of Dr. Tom Durbin and Dr. Allen Robinson to review the Fuel Effects, Toxics Emissions, Total Organic Gases (TOG) and Particulate Matter (PM) Speciation Analysis Reports.

2.1. Reviewer Selection

ICF identified a pool of independent subject matter experts to conduct this review. Initial contact to each reviewer confirmed the potential reviewer's expertise in the field, their ability to perform the work during the period of performance, any association with whom they have worked that might preclude them from being an independent and objective reviewer, their hourly billing rate, and to confirm their contact information. A curriculum vitae or resume for each peer review candidate that expressed interest and availability was also collected. This list was submitted to EPA for approval and revisions, as necessary. Multiple iterations were made to the list of selected reviewers before a set of available, conflict free reviewers for the Evaporative Report were agreed upon. The final pool of potential candidates was contacted via e-mail and phone. Additionally, a final peer review selection memo was delivered to EPA.

2.2. Administration and Completion of the Peer Reviews

Following acceptance of reviewers by EPA and by reviewers to participate, the review was administered according to the below process:

- A charge for each report was drafted with instructions to provide clear and detailed comments that distinguish between recommendations for improvements and, if appropriate, what conclusions could be drawn from the report and/or subsequent model predictions
- Electronic distribution of the review material, including the report charges,
- For each report, a teleconference was arranged between the selected peer reviewers, the EPA WAM, EPA-identified relevant project-related staff, and ICF staff. The purpose of these calls was to clarify any questions the reviewers had regarding the review material. EPA's purpose on the call was to provide technical and/or background support on the particular report or analysis under review, as needed,
- Any technical reviewer questions were facilitated through ICF to EPA, and
- A deadline for submission of materials.

Dr. Durbin met the submission deadline and his review was submitted to EPA on the 9/30/13 contract end date. Dr. Robinson delayed his submission by several months. This report was eventually collected (during the period of performance of WA2-14) and provided to EPA upon receipt of his review and reauthorization for ICF to proceed with work under this contract. Their full set of review comments,

along with their cover letters, CVs, and Conflict of Interest statements, were gathered and provided to EPA unedited.

Additionally, a technical report documenting the peer review process for each report was assembled to conclude each review. Finally, all contracting and payment issues with each reviewer were managed by ICF to ensure prompt payment of each reviewer for their services.

2.3. Difficulties Encountered

No notable difficulties were encountered in review of the Fuel Effects Report, other than Dr. Robinson's delay in submitting his material.

2.4. Supporting Documentation

Supporting documentation collected from the reviewers and outreach material to Dr. Durbin and Dr. Robinson is captured in Appendices A and B. This includes the reviewers' cover letters, conflict of interest statements, and CVs.

3. Charge Questions and Scope of the Peer Review

The peer reviewers were asked to review the MOVES 2013 Fuel Effects, Toxics Emissions, Total Organic Gases (TOG) and Particulate Matter (PM) Speciation Analysis Reports. These reports consisted of several documents, summarized below in Table 1.

Table 1. Documents Reviewed for the Peer Review of the Fuel Effects, Toxics Emissions, Total Organic Gases (TOG) and Particulate Matter (PM) Speciation Analysis Reports

Type	Title
Chapter	Gasoline Fuel Effects for Vehicles Certified to Tier-2 Standards, IN: *Modelling Effects of Fuel Properties in the Motor Vehicle Emissions Simulator (MOVES2014)*
Chapter	MOVES2014 Sulfate and Sulfur Dioxide Emissions Calculator, IN: *Modelling Effects of Fuel Properties in the Motor Vehicle Emissions Simulator (MOVES2014)*
Chapter	Calculating the Effects of Gasoline Sulfur on Exhaust Emissions, IN: *Modelling Effects of Fuel Properties in the Motor Vehicle Emissions Simulator (MOVES2014)*
Report	*TOG and PM Speciation in MOVES for Air-Quality Modeling*
Appendix	PM2.5 Speciation in MOVES
Section	2.3 Estimating Elemental Carbon Fractions, IN: *Development of Emission Rates for Light-duty Vehicles in the Motor Vehicle Emissions Simulator (MOVES2014)*
Section	2.5 Updates to PM2.5 Emission Rates in MOVES2014, IN: *Development of Emission Rates for Light-duty Vehicles in the Motor Vehicle Emissions Simulator (MOVES2014)*
Sub-section	2.1.3.5 Computation of Elemental Carbon and Non-Elemental Carbon Emission Factors, IN: *Development of Emission Rates for Heavy-Duty Vehicles in the Motor Vehicle Emissions Simulator (MOVES2014)*
Report	*Estimation of Air-Toxic Emissions from Highway Vehicles in the Motor Vehicle Emissions Simulator (MOVES 2014)*

Responses were requested to five general questions and one catch-all question. These are repeated below.

3.1. General Charge Questions

The general charge questions were as follows:

1. Does the presentation give a description of selected data sources sufficient to allow the reader to form a general view of the quantity, quality and representativeness of data used in the development of emission rates? Are you able to recommend alternate data sources might better allow the model to estimate national or regional default values?
2. Is the description of analytic methods and procedures clear and detailed enough to allow the reader to develop an adequate understanding of the steps taken and assumptions made by EPA to develop

the model inputs? Are examples selected for tables and figures well chosen and designed to assist the reader in understanding approaches and methods?

3. Are the methods and procedures employed technically appropriate and reasonable, with respect to the relevant disciplines, including physics, chemistry, engineering, mathematics and statistics? Are you able to suggest or recommend alternate approaches that might better achieve the goal of developing accurate and representative model inputs? In making recommendations please distinguish between cases involving reasonable disagreement in adoption of methods as opposed to cases where you conclude that current methods involve specific technical errors.
4. In areas where EPA has concluded that applicable data is meager or unavailable, and consequently has made assumptions to frame approaches and arrive at solutions, do you agree that the assumptions made are appropriate and reasonable? If not, and you are so able, please suggest alternative sets of assumptions that might lead to more reasonable or accurate model inputs while allowing a reasonable margin of environmental protection.
5. Are the resulting model inputs appropriate, and to the best of your knowledge and experience, reasonably consistent with physical and chemical processes involved in exhaust emissions formation and control? Are the resulting model inputs empirically consistent with the body of data and literature that has come to your attention?

The catch-all charge question was as follows:

1. Please provide any additional thoughts or review of the material you feel important to note that is not captured by the preceding questions.

3.2. Conclusion of the Peer Review

The compiled set of unedited reviewer comments for each charge question are provided in Section 4. Each reviewer's delivery emails (i.e., cover letters), CVs, and COI statements were also gathered and are provided in Appendix A and Appendix B for each reviewer in PDF format or in the referenced attachments. This Task 4 Technical Report concludes the review.

4. Reviewers' Responses to Charge Questions

4.1. All Documents Reviewed

This section provides a verbatim list of peer reviewer comments submitted in response to the general/catch-all review charge question for all documents reviewed as a part of the Fuel Effects, Toxics Emissions, Total Organic Gases (TOG) and Particulate Matter (PM) Speciation Analysis.

4.1.1. Adequacy of Selected Data Sources

Does the presentation give a description of selected data sources sufficient to allow the reader to form a general view of the quantity, quality and representativeness of data used in the development of emission rates? Are you able to recommend alternate data sources might better allow the model to estimate national or regional default values?

4.1.1.1. Dr. Tom Durbin

This particular question I will address globally for all of the reports, as many of the datasets being recommended apply to more than one report. This is also the area of my significant criticisms. The data sets selected for the MOVES2014 development are large, relatively comprehensive, representative, and generally well conducted, and as such represent a good basis in the model development for MOVES2014. These data sets focus predominantly on the EPA Kansas City study, the E-55/59 study, the ACES Phase 1 study, and the EPAct study for fuel effects.

On the other hand, EPA coverage of data is relatively narrow in terms of the larger body of literature, and in particular doesn't consider the relatively significant work being carried out in California. As the MOVES model continues to develop into future years, it is suggested that EPA broadens its coverage of data being collected around the country. Many of the California datasets are just being completed and should be available in time for the next MOVES update.

The issue with the silicone in the Kansas City study for the hot running is another point of consideration. While some corrections can be applied to species profiles that may be reasonable, it also reinforces the idea that a broader range of data sources should be considered.

Some of the areas where additional data could be particularly useful is for vehicle categories for which data is still relatively limited. In particular, gasoline direct injection engines (GDI) are rapidly expanding into the in-use fleet, have considerably different characteristics compared to more traditional gasoline vehicles, and are not included in the data sets currently being used for MOVES2014. Data for heavy-duty vehicles/engines with newer 2007+ and 2010+ are also still relatively limited. Finally, data on natural gas vehicles/engines are relatively limited.

Its difficult to determine how recent the Predictive/Complex model are. In one of the document that discusses fuel effects for sulfur its seems to rely heavily on studies conducted in the early 1990s by CRC

and EPA and then goes to the EPAct Study with almost no consideration of anything done in between. CARB, on the other hand, considered a number of additional and robust dataset in its 2007 update of its predictive model.

Another important consideration is that the heavy-duty pre-2007 data does not seem to include any data from retrofit DPFs, which tend to be more passive in nature and can vary from the OEM DPFs for 2007+ engines.

For the "Gasoline Fuel Effects for Vehicles Certified to Tier-2 Standards" report, there are several other data sets should be considered for inclusion in the fuel effects part of the model as the model continues to be developed. These include the CRC-83 project, which utilizes the same vehicle fleet as the main EPAct study, but evaluated fuel olefin levels. UC Riverside is also conducted an extensive study of ethanol/butanol blends that is nearing completion. In particular, this study includes GDI vehicles that are not covered in EPAct study. This study has some emphasis on California fuels, but should also have more general applicability for evaluated fuels at a national level.

For the "MOVES2014 Sulfate and Sulfur Dioxide Emissions Calculator" report, there are several other data sets should be considered for inclusion in the model as the model continues to be developed. There are several other datasets that are coming out that would be worth EPA considering or at least evaluating with respect to the model, especially on the diesel vehicle side. The California Air Resources Board has been looking at the toxicity of advanced technology vehicles, and some of this data has sulfate emissions that could be of relevance here. The South Coast Air Quality Management District has also conducted a study to evaluate the in-use emission rates of 2007+ technology, heavy-duty diesel and natural gas vehicles. These data will probably not be available until the first part of next year, but they could be considered for future application to the model. Phase 2 of the ACES program is another data set that could be of value for future model revisions.

For the "Calculating the Effects of Gasoline Sulfur on Exhaust Emissions" report, there are several other data sets should be considered for inclusion in the model as the model continues to be developed. Even though M6Sulf is supposed to model Tier 1, LEV, and ULEV vehicles, the majority of the datasets listed are from studies conducted in the early 1990s. Given that early 1990s technologies are not very representative of Tier 1, LEV, and ULEV vehicles, consideration should be given to incorporating more data here. Example data sets include the the CRC E-60 program.

For the "TOG and PM Speciation in MOVES for Air Quality Modeling" and the "Appendix: PM2.5 Speciation in MOVES" reports, there are several other data sets should be considered for inclusion in the model as the model continues to be developed. The California Air Resources Board has been looking at the toxicity of advanced technology diesel vehicles, and some of this data has sulfate emissions that could be of relevance here. The South Coast Air Quality Management District has also conducted a study to evaluate the in-use emission rates of 2007+ technology, heavy-duty diesel and natural gas vehicles. These data will probably not be available until the first part of next year, but they could be considered for future application to the model. Phase 2 of the ACES program is another data set that could be of value for future model revisions.

For CARB studies, see http://www.arb.ca.gov/research/veh-emissions/veh-emissions.htm noting that there have been some publications more recent that those listed on the website.

UC Riverside program with the South Coast Air Quality Management District (SCAQMD), "Determining the Physical & Chemical Composition & Associated Health Effects of Tailpipe PM Emissions"

UC Riverside program with the Coordinating Research Council (CRC), "Biodiesel and Renewable Diesel Characterization & Testing in Modern LD Diesel Passenger Cars & Trucks"

UC Riverside program with the South Coast Air Quality Management District (SCAQMD), "Determining the Physical & Chemical Composition & Associated Health Effects of Tailpipe PM Emissions"

UC Riverside and West Virginia University program with the SCAQMD, "In-Use Emissions Testing and Demonstration of Retrofit Technology for Control of On-Road Heavy-Duty Engines"

Durbin, T.D., Karavalakis, G., Johnson, K.C., Miller, J.W., and Hajbabaei, M. (2013) Evaluation of the Performance and Air Pollutant Emissions of Vehicles Operating on Various Natural Gas Blends – Heavy-Duty Vehicle Testing – Regulated Emissions and PM, Final Report for the California Energy Commission by the University of California at Riverside, June.

Durbin, T.D., Karavalakis, G., Miller, J.W., Hajbabaei, M., Bumiller, K., Villela, M., and Xu, K.H., 2012. Effects of Olefins Content on Exhaust Emissions: CRC Project E-83, Final report for the Coordinating Research Council by the University of California at Riverside, June.

Durbin, T.D., Miller, J.W., Johnson, K.C., Hajbabaei, M., Kado N.Y., Kobayashi, R., Liu, X., Vogel, C.F.A., Matsumura, F., Wong, P.S., and Cahill, T. (2011) Assessment of the Emissions from the Use of Biodiesel as a Motor Vehicle Fuel in California - Biodiesel Characterization and NOx Mitigation Study, Final report for the California Air Resources Board by the University of California at Riverside, the University of California at Riverside, and Arizona State University, October.

Durbin,T.D., J.W. Miller, T. Younglove, T. Huai, and K. Cocker. 2006. Effects of Ethanol and Volatility Parameters on Exhaust Emissions: CRC Project No. E-67. Final report for Coordinating Research Council, CRC Project No. E-67, January.

Durbin, T. D., J. W. Miller, J. T. Pisano, C. Sauer, T. Younglove, S. H. Rhee, T. Huai, and G.I. MacKay. 2003. The Effect of Fuel Sulfur on NH3 and Other Emissions from 2000-2001 Model Year Vehicles. Final report for Coordinating Research Council, CRC Project No. E-60, CE-CERT Technical Report No. 02-VE-59971-E60-04, May.

4.1.1.2. Dr. Allen Robinson

No response directed at all reports.

4.1.2. Clarity of Analytical Methods and Procedures

Is the description of analytic methods and procedures clear and detailed enough to allow the reader to develop an adequate understanding of the steps taken and assumptions made by EPA to develop the model inputs? Are examples selected for tables and figures well chosen and designed to assist the reader in understanding approaches and methods?

4.1.2.1. Dr. Tom Durbin

No response directed at all reports.

4.1.2.2. Dr. Allen Robinson

No response directed at all reports.

4.1.3. Appropriateness of Technical Approach

Are the methods and procedures employed technically appropriate and reasonable, with respect to the relevant disciplines, including physics, chemistry, engineering, mathematics and statistics? Are you able to suggest or recommend alternate approaches that might better achieve the goal of developing accurate and representative model inputs? In making recommendations please distinguish between cases involving reasonable disagreement in adoption of methods as opposed to cases where you conclude that current methods involve specific technical errors.

4.1.3.1. Dr. Tom Durbin

No response directed at all reports.

4.1.3.2. Dr. Allen Robinson

No response directed at all reports.

4.1.4. Appropriateness of Assumptions

In areas where EPA has concluded that applicable data is meager or unavailable, and consequently has made assumptions to frame approaches and arrive at solutions, do you agree that the assumptions made are appropriate and reasonable? If not, and you are so able, please suggest alternative sets of assumptions that might lead to more reasonable or accurate model inputs while allowing a reasonable margin of environmental protection.

4.1.4.1. Dr. Tom Durbin

No response directed at all reports.

4.1.4.2. Dr. Allen Robinson

No response directed at all reports.

4.1.5. Consistency with Existing Body of Data and Literature

Are the resulting model inputs appropriate, and to the best of your knowledge and experience, reasonably consistent with physical and chemical processes involved in exhaust emissions formation and control? Are the resulting model inputs empirically consistent with the body of data and literature that has come to your attention?

4.1.5.1. Dr. Tom Durbin

No response directed at all reports.

4.1.5.2. Dr. Allen Robinson

No response directed at all reports.

4.1.6. General/Catch-All Reviewer Comments

Please provide any additional thoughts or review of the material you feel important to note that is not captured by the preceding questions.

4.1.6.1. Dr. Tom Durbin

No response directed at all reports.

4.1.6.2. Dr. Allen Robinson

Overall I think that EPA has done a good job of developing MOVES2014 and that these chapters provide the reader/user a reasonable description of the model. The models are statistical fits of data; that is probably the best approach given the limitations in our quantitative understanding in the underlying physical and chemical processes that control the emissions. For the most part the models seem to be based on the best available datasets, but there are inevitably gaps. In certain instance there appear to be important data that are not incorporated into the analysis. I have provided many comments on individual chapters. The majority of the comments are focused on improving the usability of the materials. However, there are some important scientific shortcomings (treatment of uncertainty, semivolatile PM, and SOA precursors).

Here are the major comments that apply across most if not all of the sections that I read:

<u>Presentation related:</u>

1. Data sources – the various chapters and report often provide references to the underlying data. However, these references often point to large reports (e.g. the EPAct data analysis), which means that the reader may not be able to figure out what specific data were used. I would encourage EPA

to be as specific as possible about what data are used. I have often been frustrated trying to figure out the exact data underlying models like MOVES and MOBILE.

2. Examples – I think quantitative examples really help the reader understand the model. These exist in a few chapters but not in most. I would encourage EPA to include more examples which will help the reader understand what MOVES is doing. Pointing the reader to online tools, such as the fuel effects spreadsheet are also useful.
3. Tables defining all variables – in some chapter many variables are not defined making it difficult for the reader to understand the model. These tables should also indicate which variables are user inputs and which are derived from existing data. For the user inputs, default values should be clearly defined.
4. Example results – For the reader it would be useful to provide some sample output from the model to understand the effects. Ideally this would be graphical presentation.

Content related:

5. Goodness of fit – Given that the models are statistical fits of data, some description is needed in each chapter on how well the model(s) fit the underlying data is important. These could be some sort of statistical measure and/or scatter plots of model predictions versus underlying data.
6. Uncertainty – There is no discussion of uncertainty of the model predictions. This is my largest substantive concern with the reports. One measure of the uncertainty is the quality of the statistical fit. A better measure is how well the model performs against data that were not used to derive the fitting parameters. I strongly encourage EPA to quantify the uncertainty in the MOVES2014 predictions. Every prediction should be accompanied by a quantitative uncertainty estimate.
7. Data limitations – EPA has done a good job utilizing existing data. However, there are inevitably gaps. Obvious gaps are GDI, higher mileage vehicles, high emitters, etc. The reader should be made aware of these limitations and guidance should be given about how to address.

4.2. Gasoline Fuel Effects for Vehicles Certified to Tier-2 Standards

This section provides a verbatim list of peer reviewer comments submitted in response to the charge questions for the chapter Gasoline Fuel Effects for Vehicles Certified to Tier-2 Standards, IN: *Modelling Effects of Fuel Properties in the Motor Vehicle Emissions Simulator (MOVES2014)*.

4.2.1. Adequacy of Selected Data Sources

Does the presentation give a description of selected data sources sufficient to allow the reader to form a general view of the quantity, quality and representativeness of data used in the development of emission rates? Are you able to recommend alternate data sources might better allow the model to estimate national or regional default values?

4.2.1.1. Dr. Tom Durbin

Refer to response to All Documents Reviewed in Section 4.1.1.1.

4.2.1.2. Dr. Allen Robinson

I think that the presentation of the data sources (specifically test fleet, and fuel composition) could be improved. There is a lot of detailed information in the main EPAct report, which I download and skimmed parts of, but it would helpful for the reader if a bit more information (a few more paragraphs) was provided in the intro about this test program. Here are some examples of the sort of information that would be useful to provide the reader: Were these all relatively new, low-mileage vehicles? What was the variety of emission control technologies? Were the vehicles all port fuel injected? Were all the vehicles 2008 MY? How were the vehicles procured? Recruited from the in-use fleet – if so where? What was the range of each property of the fuels tested in EPAct? What are typical values for each of these properties in actual in-use fuels (summer and winter)?

If all the vehicles were port fuel injected then what is the guidance for gasoline direct injection vehicles which are becoming more prevalent? That seems like the most significant gap in the information.

All of the EPAct vehicles were low mileage, what are the recommendations for higher mileage tier 2 vehicles?

These things seem like important data limitations. Although these issues probably cannot be addressed (these types of vehicles were not in the EPAct test fleet), the document should clearly describe potential limitations of the model so that the reader is aware of them.

4.2.2. Clarity of Analytical Methods and Procedures

Is the description of analytic methods and procedures clear and detailed enough to allow the reader to develop an adequate understanding of the steps taken and assumptions made by EPA to develop the model inputs? Are examples selected for tables and figures well chosen and designed to assist the reader in understanding approaches and methods?

4.2.2.1. Dr. Tom Durbin

The description of the methods and procedures is reasonable. The following are some suggestions in this area.

Section 2.1 should have a reference to a more basic description of the "Z factor" and other elements of the discussion for those looking for a more fundamental discussion of the method.

The first example on page 6 is for aromatics, and then the examples switch to ethanol.

Tables 2 and 3 provide a good description of the different coefficients. It is worth noting that because Table 3 is in log scale it, it is not necessarily straightforward to determine the magnitude of the effects that might be seen for different in arithmetic space. It would be interesting to see what the coefficients would be when they are transformed to arithmetic space, although this is not how they are used in the model. Also, the blanks in table 3 are not explained. Tables 5 and 6 are good, especially Table 6 that goes into detail on each of the terms.

For the means in Table 2, are these based on just a mean for the fuels in the test matrix, or are they weighted based on the number of tests run on each fuel for the dataset being used.

The first example on page 6 is for aromatics, and then the example switches to the quadratic term for ethanol.

How are start and running emissions calculated? Based on bag 1 for start and bag 2 for running?

4.2.2.2. Dr. Allen Robinson

The core statistical model/parameterizations appears to have been derived by the EPAct project and appears to be described in the final report for that project (Assessing the Effect of Five Gasoline Properties on Exhaust Emissions from Light-Duty Vehicles Certified to Tier 2 Standards: Analysis of Data from EPAct Phase 3 (EPAct/V2/E-89) Final Report (EPA-420-R-13-002)). In that (EPAct) report they describe multiple models, but the set of parameters that will be used in MOVES2014 appear to be the same as what is listed in Table ES-1 and ES-2 of the EPAct report (the only exception appears to be the value of the variance listed in Table 3 – why are those different?). This was not clear from reading the fuel effects document. If that is the case (the models were taken directly from the EPAct report), then this document needs to have a short declarative sentencing stating so. "The models used here were derived and described in the EPAct final report (ref)." Right now the introduction only provides a very qualitative discussion of the EPAct process, but does not explicitly say that the analysis was used here. If the model is different than one of the models derived in the EPAct report then this report needs a lot more discussion of the derivation of the model.

Without reading the EPAct report the reader has essentially no "understanding of the steps taken and assumptions made by EPA to develop the model inputs." The EPAct report is very long and detailed. In addition, they fit multiple models to the data. This chapter would benefit if it provided some more discussion of the EPAct modeling process and why this particular model was chosen (as opposed to one of the other models fit by the EPAct team). This would be a page or so of text. This would give every

reader a basic understanding of the model; interested readers could then be referred to the EPAct report for more details. I thought that the air toxics report did a much better job of describing the underlying model(s) than this chapter.

Another shortcoming of this document is that it does not provide some description of the goodness of fit of the model to the original data (part of this should be providing some physical description of what the variance values in Table 3). I skimmed through multiple sections of the EPAct report and could not find that succinctly summarized. A few paragraph (up to a page or two) description of the goodness of fit of the model to EPAct data should be provided as the ability of MOVES2014 to predict fuel effects ultimately depends on the model and how well it describes the data.

Were any exercises performed to test the model with independent data (data not used to fit the model)? Standard techniques such as "leave-one-out" can be used. Alternatively one could use speciated data from other test campaigns to test the model? For example, ARB has extensive data from their surveillance program. This sort of independent evaluation of the model with real world data seems extremely important. This analysis should be performed and described in the report to provide the user confidence in the model.

What was the basis for the assumption "that effects for fuels and temperature are independent and multiplicative."

4.2.3. Appropriateness of Technical Approach

Are the methods and procedures employed technically appropriate and reasonable, with respect to the relevant disciplines, including physics, chemistry, engineering, mathematics and statistics? Are you able to suggest or recommend alternate approaches that might better achieve the goal of developing accurate and representative model inputs? In making recommendations please distinguish between cases involving reasonable disagreement in adoption of methods as opposed to cases where you conclude that current methods involve specific technical errors.

4.2.3.1. Dr. Tom Durbin

The equations for this report appear to trace back to methods used and reviewed previously. The current application of these methods appears to be appropriate in that context. Comments to consider on the presentation of the methods are provided above.

Its difficult to determine how recent the Predictive/Complex model are. In another document that discusses fuel effects for sulfur its seems to rely heavily on studies conducted in the early 1990s by CRC and EPA and then goes to the EPAct Study with almost no consideration of anything done in between. CARB, on the other hand, considered a number of additional and robust dataset in its 2007 update of its predictive model.

4.2.3.2. Dr. Allen Robinson

This sort of statistical fitting is commonly done to create "models" to describe fuel effects. The parameters included in the model are known to influence emissions. However, I am not aware of any

scientific basis for the underlying mathematical form of the model. If there is one the report would benefit from a description of it. In addition, without the information on goodness of fit and evaluation of model with independent data as described in the previous section it is impossible to answer these questions.

Beyond a description of the goodness of fit, the major shortcoming of the model is there is no treatment of uncertainty. I would advocate that the model should provide uncertainty estimates (confidence intervals) for every output/prediction. One simple way to provide an estimate would be to use the statistical uncertainty of the fit. This is reasonably straightforward. A more robust approach would also be to try to account for the limitations in the underlying dataset (e.g. lack of GDI). Providing a robust treatment of uncertainty is not easy but it seems essential to ensure that the data are used appropriately. Including uncertainty estimates would be a major upgrade of the model, which may not be possible for this release of MOVES. However, I would strongly encourage EPA to make starting implementing uncertainty a high priority for future releases.

4.2.4. Appropriateness of Assumptions

In areas where EPA has concluded that applicable data is meager or unavailable, and consequently has made assumptions to frame approaches and arrive at solutions, do you agree that the assumptions made are appropriate and reasonable? If not, and you are so able, please suggest alternative sets of assumptions that might lead to more reasonable or accurate model inputs while allowing a reasonable margin of environmental protection.

4.2.4.1. Dr. Tom Durbin

This report does not deal extensively on data sets where data is meager. On the other hand, the data set being used does not contain any GDI vehicles, which will represent a growing and important segment of the in-use fleet going into the future.

4.2.4.2. Dr. Allen Robinson

I don't think that there are any statements about data limitations in this section. However, there are some critical data gaps, such as for GDI, higher mileage vehicles, and malfunctioning (gross emitting) Tier2 emitting vehicles. It would be good to at least specifically mention these gaps.

4.2.5. Consistency with Existing Body of Data and Literature

Are the resulting model inputs appropriate, and to the best of your knowledge and experience, reasonably consistent with physical and chemical processes involved in emissions formation and control? Are the resulting model inputs empirically consistent with the body of data and literature that has come to your attention?

4.2.5.1. Dr. Tom Durbin

The paragraph at the bottom of page 8 provides some sense of what the model outputs would be and how fuel properties would influence emission rates. Interpreting these results in terms of natural log of the emissions is not necessarily straightforward to a more casual reader.

4.2.5.2. Dr. Allen Robinson

This is not covered in this chapter. The trends as report in the EPAct final report seem consistent with expectations.

4.2.6. General/Catch-All Reviewer Comments

Please provide any additional thoughts or review of the material you feel important to note that is not captured by the preceding questions.

4.2.6.1. Dr. Tom Durbin

- p. 6 . The description of the LA92 should explicitly note that is has a cold start phase, since this is one of the process categories included in the modeling, and how the start emissions are obtained.
- The abbreviations CO, THC, are given on page 4, instead of when they are first use in the 1st paragraph of the document.
- There are lots of extra spaces in the text. P. 3 last paragraph 2nd sentence was launched; p. 4 "EPAct Test Program Report" 2 and (fueltypeID = 1) .; p 8 1st sentence etOHxArom interaction
- Superscripted numbers are used for both references and footnotes, which takes away from the presentation.
- Introduction – 3rd sentence is very long. Suggest splitting into 3 sentences.
- p. 4 3rd full paragraph "The analysis involved several iterations between analysis and additional physical and chemical review of data." The part about physical and chemical review of data is unclear. Same paragraph add commas ", including subsets of terms,"
- page 5 Emissions Process: add evap reference.
- page 8 1st full paragraph "while the impacts of fuel properties on running isare dictated …1st and second part of sentence should match

4.2.6.2. Dr. Allen Robinson

Section 2.1

- It would be good to list the fuel properties that are used in the model (or at least considered in the modeling, since some were dropped out in the analysis) in section 2.1 so that it is clear to the reader what they are. The properties are listed in the intro but it was not clear those were the properties used in the model.

- Readers may not know what you mean by second-order and linear terms as these are never defined.

Table 2

- Units this is % by vol or mass. Same comment for aromatics.
- The terms like "etOH x etOH" terms are not defined. Presumably this is the ZZetOHxetOH listed in Equation 3. If so then the table should use the same nomenclature. If not then these terms need to be defined.
- The document frequently uses the term "start." Presumably this is actually "cold start" (bag 1) as opposed to "hot start" (bag 3). The term start should always be defined

Section 3. Fuel effect adjustments

- It seems like the key here is equation 6 because that is what is actually used by MOVES. You are calculating a scaling factor (equation 6) to apply to the base MOVES emission rate. If that is correct then that should be explicitly stated.
- Equations 5 -- I think that it would be useful to list out all the terms.
- Equation 6—X (bold) and Beta_in-use are not defined. These are some sort of vector?

Table 3

- It would be helpful if you included a column that had the actual model nomenclature (e.g. ZetOH) as opposed to what you currently list as model terms. Right now the reader may be confused trying to relate the information in Table 3 with the equation (this applies especially to the cross terms).
- Why are the variance values in Table 3 different than those in the EPAct report for the same set of model parameters? (This is based on comparing with values in Tables ES-1 and ES2 in EPAct report).
- Some discussion of the meaning of the values in Table 3 would be useful to provide the reader some understanding of the actual model. From reading the EPAct report it appears that the sign on the coefficient indicates that it is positively or negatively correlated. The magnitude indicates the size of the dependence?

Section 4

- This table only defines selective values of parameters. It would be useful to have a footnote to a reference where all of the values of each parameter are defined (this would include report and page number).

Table 6

- When you write something like ETOHVolume presumably this actual the Z value for this parameter. Should probably try to make this clear in the table in comments column?
- Fuel sulfur – ppm volume or mass?

Section 4.1 example

- I really like including an example because it can help people understand the model. In this particular chapter, it would be very useful if you actually complete the sample calculation. Provide the reader

with a table of input values (actual fuel values and then presumably the Z values for each parameter calculated using the parameters Table 2 -- my understanding is the Z values are what is actually used in the model) and the numerical value of what the model predicts. Having the answer will allow the reader to verify that they understand how to use the model. I would encourage EPA to include this sort of calculation in each of the documents.

- There are few places in report where the text is not complete e.g. “add reference to evap report” “Chapter X.X”

4.3. MOVES2014 Sulfate and Sulfur Dioxide Emissions Calculator

This section provides a verbatim list of peer reviewer comments submitted in response to the charge questions for the chapter MOVES2014 Sulfate and Sulfur Dioxide Emissions Calculator, IN: *Modelling Effects of Fuel Properties in the Motor Vehicle Emissions Simulator (MOVES2014)*.

4.3.1. Adequacy of Selected Data Sources

Does the presentation give a description of selected data sources sufficient to allow the reader to form a general view of the quantity, quality and representativeness of data used in the development of emission rates? Are you able to recommend alternate data sources might better allow the model to estimate national or regional default values?

4.3.1.1. Dr. Tom Durbin

Refer to response to All Documents Reviewed in Section 4.1.1.1.

4.3.1.2. Dr. Allen Robinson

I think that the paper gives a good description of the underlying datasets used to derive the model (in fact I think that these descriptions are better in this document then in some of the other documents).

The models (gas, old diesel, new diesel, CNG) are based on a relatively limited amount of data (one or two studies). The selected studies are relevant because some of them systematically varied key parameters such as fuel sulfur levels (e.g. FUL and DECSE). I am not aware of other studies that have systematically varied these properties.

It seems concerning that some of the core studies (e.g. the KCVES) used gasoline with much higher sulfur content gasoline compare to Tier 2 gas. This means the model has to extrapolate a long way from the reference case. I understand the FUL dataset help do this extrapolation, but it seems strange to have the reference be so far from the current norm on fuel sulfur content.

A major shortcoming of this report is that they show no model evaluation and only limited discussion of goodness of fit. This sort of quality assurance seems essential in an application like MOVES. The model can be evaluated by the many other studies have measured sulfate emissions (e.g. PM characterization by Kleeman group, gasoline component of the gasoline diesel split study, etc.). If some of the parameters are not available in these studies (e.g. fuel sulfur content) the comparison will still provide insight into the suitability of default values. The model should be tested against at least some of these other data to evaluate its robustness. This analysis should be performed and described in the report to provide the user confidence in the model.

4.3.2. Clarity of Analytical Methods and Procedures

Is the description of analytic methods and procedures clear and detailed enough to allow the reader to develop an adequate understanding of the steps taken and assumptions made by EPA to develop the

model inputs? Are examples selected for tables and figures well chosen and designed to assist the reader in understanding approaches and methods?

4.3.2.1. Dr. Tom Durbin

The description of the methods and procedures is reasonable. The following are some suggestions in this area.

As equations 1 and 2 are described, it should be noted that the derivation of these formulas is provided in Appendix 1.

What are typical value for $(H_2O)_B$?

Were any measurements made of the oil sulfur levels in the Kansas City study. Can EPA provide an estimate of what the oil sulfur levels might have been in Kansas City based on typical levels in oils of the time.

Pre-2007 Vehicles section. It would be worth noting how many samples the 172 ppm is based on.

The examples in the Appendices provide a good description of how the sulfate contribution is determined for each of the different vehicle/engine categories. They are a nice contribution to the report.

4.3.2.2. Dr. Allen Robinson

The basic approach is reasonably well described. I also think that the basic approach of linking sulfate emissions to nonECPM makes sense (and is an improvement from the old approach of linking to fuel S) because it avoids the potentially absurd result if you make assumptions about fuel sulfur content conversion to SO4.

Equation 1 is the core of the model. It was not totally clear how this is implemented in practice. It appears that NonECPM is an output from another part of MOVES2014 and that this model simply scales that fraction using the actual fuel sulfur concentration. Therefore the only independent input into the model is the fuel sulfur concentration (x). All of the rest of the parameters are determined by the reference (listed in Table 1 of main text). If this is the case then it should be clarified in the text.

Presumably there is a default value for this if the user does not know the fuel sulfur content. It would be good to define that value.

There seems to be two assumptions from the It seems like a key assumption is sulfate emission rate from lube oil (SO4o) is fixed for different types of vehicles. Is there evidence to support this assumption? If so it was not adequately discussed in the report. The second assumption is the parameter that describes the conversion of fuel sulfur to sulfate.

I do not understand the treatment of particulate water (Appendix 1 equation 2). Aerosol water depends on the composition of the aerosol and the relative humidity of the exhaust. This can be easily calculated

using thermodynamic model such as ISOROPIA. I am not sure how this equation relates to the underlying theory.

A table of variables and definitions would be useful. This is general comment that applies to all chapters.

4.3.3. Appropriateness of Technical Approach

Are the methods and procedures employed technically appropriate and reasonable, with respect to the relevant disciplines, including physics, chemistry, engineering, mathematics and statistics? Are you able to suggest or recommend alternate approaches that might better achieve the goal of developing accurate and representative model inputs? In making recommendations please distinguish between cases involving reasonable disagreement in adoption of methods as opposed to cases where you conclude that current methods involve specific technical errors.

4.3.3.1. Dr. Tom Durbin

The inclusion of both sulfur for fuel and lubricating oil is an important advancement, especially as fuel sulfur level have been reduced. Overall, the methodology appears to be reasonable based on the data available.

Data for pre-2007 heavy-duty engines/vehicles appears to be lacking. One consideration with sulfate emissions for diesel engines equipped with such DPFs is that the formation of sulfate emissions is highly nonlinear. Nucleation particles comprised of sulfate increase substantially above a certain temperature threshold (~350°C). This phenomena is likely too complex to incorporate into the current model, but is worth considering in future versions of the model.

For the light-duty gasoline vehicle, the expanded use of gasoline direct injection engine is an important consideration in model future fleets. Little data on sulfate emissions is available for these types of vehicles, but EPA should keep this in mind in the development of future versions of the model. UC Riverside is collected some data that might be of interest as part of a mixed alcohol program being funded by the California Energy Commission.

4.3.3.2. Dr. Allen Robinson

The model is empirical with the constraint of conservation of mass. This seems like a reasonable approach given the complexity of the system.

4.3.4. Appropriateness of Assumptions

In areas where EPA has concluded that applicable data is meager or unavailable, and consequently has made assumptions to frame approaches and arrive at solutions, do you agree that the assumptions made are appropriate and reasonable? If not, and you are so able, please suggest alternative sets of

assumptions that might lead to more reasonable or accurate model inputs while allowing a reasonable margin of environmental protection.

4.3.4.1. Dr. Tom Durbin

Page 7 2nd paragraph – It indicates that fuel consumption data was not available for E55/59. If the CO_2, CO, and THC emissions are available using standard carbon balance equations using assumptions for the properties of typical diesel fuel.

For the CNG measurements, EPA should consider data from CARB's latest round of studies on CNG vehicles.

4.3.4.2. Dr. Allen Robinson

A limitation that is not discussed is that the sulfur levels of the fuels used in the KCVES are much higher than they are in current Tier 2 gasoline.

Another limitation is the lack of GDI vehicles – as the report states the sulfate emissions depend on sulfur content of the oil/fuel but also combustion conditions. Presumably the differences between combustion in a GDI versus PFI may influence sulfate emission rates.

The major shortcoming of the model is there is no treatment of uncertainty. I would advocate that the model should provide uncertainty estimates (confidence intervals) for every output/prediction. One simple way to provide an estimate would be to use the statistical uncertainty of the fit. This is reasonably straightforward. It appears to have been done in Figures 3-1 and 3-3, which shows the results for the conventional diesel. This needs to be transferred into the core model. Uncertainties should be listed for each of the parameters in Table 1.

A more robust approach would also be to try to account for the limitations in the underlying dataset (e.g. lack of GDI). Providing a robust treatment of uncertainty is not easy but it seems essential to ensure that the data are used appropriately. One way to define this uncertainty would be to challenge the model with additional data that were not used to derive the parameters listed in Table 1. Including uncertainty estimates would be a major upgrade of the model, which may not be possible for this release of MOVES. However, I would strongly encourage EPA to make starting implementing uncertainty a high priority for future releases.

4.3.5. Consistency with Existing Body of Data and Literature

Are the resulting model inputs appropriate, and to the best of your knowledge and experience, reasonably consistent with physical and chemical processes involved in emissions formation and control? Are the resulting model inputs empirically consistent with the body of data and literature that has come to your attention?

4.3.5.1. Dr. Tom Durbin

It would be useful to bring some of the information from the Appendix into the main part of the text. In particular, it would be useful to provide oil and fuel contributions in mg/mi and oil and fuel sulfate contributions for both the fuel sulfur = 0 case and for the fuel sulfur = reference level. This would immediately give the reader a feel for what the model inputs would be.

4.3.5.2. Dr. Allen Robinson

There were not sample calculations presented in the chapter. Adding a simple figure that plots sulfate fraction of non-ECPM for a range of reasonable fuel sulfur contents would help the reader understand the model predictions. I suspect that the results will be reasonable a few percent of the PM is sulfate.

4.3.6. General/Catch-All Reviewer Comments

Please provide any additional thoughts or review of the material you feel important to note that is not captured by the preceding questions.

4.3.6.1. Dr. Tom Durbin

- Document needs page numbers.
- Page 1 paragraph 1 final sentence – change "consist of" to "make up".
- Page 2 1st paragraph - 1st sentence …shown in schematically in Figure 1.; 2nd sentence …~~has~~ support~~ed~~s; 3rd sentence ….treated that the; 4th sentence ….engines decreases
- page 3 1st paragraph – last sentence "If included in the PM2.5 speciation profile…" is somewhat unclear.
- Several sentences begin with a number; page 5 1st paragraph 11 ppm; Appendix 2 2nd paragraph 171; Appendix 3 3rd page 11 ppm and 172 ppm; Appendix 4 page 1 15 ppm and 11 ppm.
- Appendix 2 2nd paragraph – mean sulfur level is significantly ~~smaller~~lower in the summer,; 2nd page of Appendix 2 last sentence – need space before last sentence; 3rd page of Appendix 2 last sentence ~~has~~have
- Appendix 1 – 5th line – eliminate space ….reference case . x_B

4.3.6.2. Dr. Allen Robinson

Table 1 –

- In headers I would add the word "reference" to the last three columns. For example, xB is the reference fuel sulfur level not just the fuel sulfur level.

Table 2-1

- Units for sulfur content

- Definition of SES variable – sulfur emitted as sulfate suggests that this is ratio or fraction. However this appears to be an absolute emission rate. Why not just call it a sulfate emission rate?
- Equations before Table 2-2 – It seems like the Beta1 and Beta2 parameters in this equation are test specific (KC or FUL) and then you make the assumption that they are equivalent.

Table 2-2

- Did FUL use FTP or UDDS? In text I thought you said UDDS.

4.4. Calculating the Effects of Gasoline Sulfur on Exhaust Emissions

This section provides a verbatim list of peer reviewer comments submitted in response to the charge questions for the chapter Calculating the Effects of Gasoline Sulfur on Exhaust Emissions, *IN: Modelling Effects of Fuel Properties in the Motor Vehicle Emissions Simulator (MOVES2014)*.

4.4.1. Adequacy of Selected Data Sources

Does the presentation give a description of selected data sources sufficient to allow the reader to form a general view of the quantity, quality and representativeness of data used in the development of emission rates? Are you able to recommend alternate data sources might better allow the model to estimate national or regional default values?

4.4.1.1. Dr. Tom Durbin

Refer to response to All Documents Reviewed in Section 4.1.1.1.

4.4.1.2. Dr. Allen Robinson

The data sources for the Tier 2 models are poorly described. They seem to be contained in references 10-12. Were all these data weighted equally for the modeling? How were the data from different studies that had different sulfur contents included in the interpolation? It is not clear which study the paragraph starting with "The study .." refers to. I assume study 12.

4.4.2. Clarity of Analytical Methods and Procedures

Is the description of analytic methods and procedures clear and detailed enough to allow the reader to develop an adequate understanding of the steps taken and assumptions made by EPA to develop the model inputs? Are examples selected for tables and figures well chosen and designed to assist the reader in understanding approaches and methods?

4.4.2.1. Dr. Tom Durbin

The description of the methods and procedures is reasonable. The following are some suggestions in this area.

Top of page 2. Would like to see some explanation as to why the weighting of high and normal emitters is 50/50.

There should be some discussion of why the Tier 2 Low Sulfur Model applies to 2001 and later vehicles, and how this relates to the NLEV and other phase in transitions.

Section 2.1 – This section could be improved in terms of provided an overview of the model. A table should be added defining the elements in the table structure. There should be an explanation as to why the model in the log-log form or log-linear form is applied in one case but not the other. Why is log-log

used for Tier 0 and LEV+ vehicles, whereas log-linear is used for the in between Tier 1 vehicles? Beta is not defined.

Section 2.2 – This section says even less than section 2.1. Does this use the same table structure as for the short term fuel effects? What is the basis of the different factors for HC, CO, and NOx and what is the source of their derivations (maybe a couple sentences).

Section 2.3.1 – Would be useful to add a sentence on why w_{IR} is 0.425 or where it came from.

Section 2.4 – Would be useful to add a sentence on why the numerator is multiplied by 0.608 for high NOx emitters. Is this not applied for other pollutants.

Section 2.6 – Last sentence – Would the calculation be greater than 1 for 90 ppm.

It should be noted somewhere in section 2 examples of the model output are provided in section 4.

Section 3 – The coefficients in Table 2 represent the slope but not sure how to interpret them without understanding the intercept.

Section 4 – The graphs in section 4 are very informative.

4.4.2.2. Dr. Allen Robinson

The model is based on statistical analysis of emission testing performed with gasoline that had two different sulfur levels. The report refers to this analysis as "mixed-model analysis." I am not sure what that means – presumably this is some sort of multivariate model. The chapter needs to describe what the mixed model analysis is. On page 8 the document states that details "can be found in the report." There is not reference provided for this report.

Presumably the mixed model analysis is used to derive the beta values in equation 17? The report discussing using interpolation for this analysis?

Equation 17 – This needs to be much better described.

- What is A? A scaling factor? How is it used? Presumably there are different values of A for different pollutants (e.g. NOx, CO, THC)?
- I do not understand how the betaS were derived. The text says they were developed by linearly interpolating? However you have many vehicles so presumably you get a whole bunch of betaS values (one for each vehicle tested at the two fuel S levels). In addition the different studies used different fuel S levels? How do you combine the betaS values for different vehicles and different studies? Lumping them together and then averaging? Presumably the data are stratified by pollutant, model year? What is the uncertainty in these values? How did the values of betaS vary across the vehicle fleet?
- What is listed in Table 2? The BetaS values?

4.4.3. Appropriateness of Technical Approach

Are the methods and procedures employed technically appropriate and reasonable, with respect to the relevant disciplines, including physics, chemistry, engineering, mathematics and statistics? Are you able to suggest or recommend alternate approaches that might better achieve the goal of developing accurate and representative model inputs? In making recommendations please distinguish between cases involving reasonable disagreement in adoption of methods as opposed to cases where you conclude that current methods involve specific technical errors.

4.4.3.1. Dr. Tom Durbin

The methods and procedures for the M6Sulf is an already developed model, with developed methods, so most of the comments in this regard are related to the presentation of the model methodology and if it is clear, as discussed under point 2.

The discussion on the Tier Low Sulfur Model is somewhat short, but appears to be sufficient based on the fact that the data sources and analysis have been reviewed as part of another report.

4.4.3.2. Dr. Allen Robinson

I do not understand the methods or analysis ("mixed model analysis"). This appears to be a purely statistical model as opposed to something based on the underlying physics and chemistry.

Uncertainty is a key issue that is completely neglected in this chapter. For example, table 1 lists sulfur reduction with 3 significant figures. These values need uncertainty estimates. Uncertainty estimates on these parameters can be derived from the statistical analysis. A better approach would be to challenge the model by performing leave one out cross validation. Ideally both of these approaches would be taken. The complete lack of uncertainty seems like a major weakness of the entire report.

4.4.4. Appropriateness of Assumptions

In areas where EPA has concluded that applicable data is meager or unavailable, and consequently has made assumptions to frame approaches and arrive at solutions, do you agree that the assumptions made are appropriate and reasonable? If not, and you are so able, please suggest alternative sets of assumptions that might lead to more reasonable or accurate model inputs while allowing a reasonable margin of environmental protection.

4.4.4.1. Dr. Tom Durbin

Even though M6Sulf is supposed to model Tier 1, LEV, and ULEV vehicles, the majority of the datasets listed are from studies conducted in the early 1990s. Given that early 1990s technologies are not very representative of Tier 1, LEV, and ULEV vehicles, consideration should be given to incorporating more data here. Example data sets include the CRC E-60 program.

The assumption on page 9 under Table 1 that NLEV vehicles are more similar to upcoming Tier 2 vehicles than Tier 1 vehicles is reasonable. This detail and how it related to the 2001+ vehicles should be discussed earlier, however.

4.4.4.2. Dr. Allen Robinson

The data seem reasonable. I am not aware of other data.

4.4.5. Consistency with Existing Body of Data and Literature

Are the resulting model inputs appropriate, and to the best of your knowledge and experience, reasonably consistent with physical and chemical processes involved in emissions formation and control? Are the resulting model inputs empirically consistent with the body of data and literature that has come to your attention?

4.4.5.1. Dr. Tom Durbin

The presentation of model results in section 4 provide good information on how sulfur effects are implemented in MOVES. The results appear to be reasonably representative of sulfur effects over the range of different vehicle technologies being evaluated.

4.4.5.2. Dr. Allen Robinson

The chapter presents no data that demonstrates the model provides reasonable results. For example data could be added to Figures 1-4 to help the reader evaluate the model.

4.4.6. General/Catch-All Reviewer Comments

Please provide any additional thoughts or review of the material you feel important to note that is not captured by the preceding questions.

4.4.6.1. Dr. Tom Durbin

- The "x" in NOx should be subscripted.
- Page 1 paragraph 2 – impair the effectiveness of the catalyst int~~o~~ converting the products of combustion, leading to increases; last sentence …as though they are independent
- Page 1 paragraph 5 – Add section number for Tier 2 gasoline vehicles
- page 4 Section 2.3 1st paragraph – …represent the long-term.. only to target fuel sulfur levels
- page 9 paragraph below Table 1 2nd sentence – model years as early as ..
- there is an extra space… bottom of page 6 Equation 14; section 2.6 Equation 16; Last paragraph section 3 Equation 17; section 4 Equation 1 to Equation 16)

- section 3 – 1st sentence greater 30 ppm, and for all vehicles older than 2001. 2nd sentence ..For sulfur contents; 2nd paragraph catalytic convert~~or~~er; 4th paragraph 29 ppm, the higher level was…
- Appendix 1 – 5th line – eliminate extra space ….reference case . x_B

4.4.6.2. Dr. Allen Robinson

I found this document to be very difficult to follow. The model was poorly described with many variables not even defined. It was also not clear how the model would be used. It would be impossible for the reader to reproduce the calculations shown in Figures 1-4.

Figures 1-4. These appear to summarize the output from the sulfur model. What is the "fuel sulfur adjustment" (which variable, some version of A?)? How is it used? Simply as a scaling parameter on the base emissions? These details need to be clarified.

The review is focusing on the Tier 2 model which applies up to fuel sulfur level of 30 ppmv. It is hard to see the predictions of this model in Figure 1-4 because the x-axis scale goes to 600 ppm. Less than 30 ppmv is less than 5% of this scale. Given the Tier 2 standard for fuel sulfur the report should focus more on the model behavior at current and future sulfur levels (< 30 ppm). For retrospective analyses showing such high fuel sulfur levels may be useful (how long ago were fuel-S levels greater than 400 ppm?). Bottomline is that these figures or a comparable set such focus on performance of the models over the range of current fuel-S levels. Does it even make sense to plot MY 2017 vehicle out at such high fuel S levels?

Although I realize we were not supposed to review the older M6Sulf model, I found the description of the model to be impossible to follow. It is clear that the model is simply a curve fit of the underlying dataset. However, many of the variables in this section are not defined. For example what is A? What do the M6SulfurCoeff values listed on the bottom of page 3 represent? Without more description it is essentially impossible to understand how to apply the model.

It would be useful if this chapter listed the parameterization developed for the M6Sulf model. Presumably these are the wIR, betas's etc. A table defining each variable and listing its value would be very helpful.

You need to define all variables – a short table would be very helpful. What is A2, As,short, As,long, As,Irr ϕ, etc. A is clearly an important symbol. What does it represent? It appears to be some sort of adjustment factor. Is this multiplied with the base emissions to estimate the effects of sulfur? In order for someone to figure out the model, these details need to be much more clearly spelled out. Equation 8??? I have no idea of the basis for this equation. It is doing some sort of weighting of undefined terms. What is the basis for the irreversibility factor (a sentence to help the reader so that they don't have to look up that grey literature reference).

30 ppmv is the boundary between the two models (Mobile and new Tier 2). Do the two models predict the same effect at 30 ppm? Figures 1-4 suggests that the models link up. What is the basis for the 30 ppm cut – just that it is the tier 2 fuel standard?

4.5. TOG and PM Speciation in MOVES for Air Quality Modeling

This section provides a verbatim list of peer reviewer comments submitted in response to the charge questions for the report *TOG and PM Speciation in MOVES for Air-Quality Modeling*.

4.5.1. Adequacy of Selected Data Sources

Does the presentation give a description of selected data sources sufficient to allow the reader to form a general view of the quantity, quality and representativeness of data used in the development of emission rates? Are you able to recommend alternate data sources might better allow the model to estimate national or regional default values?

4.5.1.1. Dr. Tom Durbin

Refer to response to All Documents Reviewed in Section 4.1.1.1.

4.5.1.2. Dr. Allen Robinson

The report provides some description of data sources. For example Table 12 points the reader to different EPA reports. That is valuable, but it is not clear that the information in the Table is sufficient if a reader wanted to truly understand where the source profile came from. I have been frustrated in the past trying to track down the source data for speciation profiles used in EPA models. Sometimes there are no references (not a problem here), but other times the references point to a large report (the case here). However, these reports can be massive documents that describe lots of data, but the reader has no idea which specific data were actually used to develop the input for the model (or how they were used). Maybe that is not an issue here (I have not gone and looked at the underlying reports), but I would encourage the authors to make sure the reader truly can figure out where the source profiles came from so that can start with the actual data and recreate the actual profiles. For example, the report could refer to specific emissions data form the underlying report.

The report seems to do a better on the PM side of things (PM speciation appendix, which is built upon this unpublished paper). It is very helpful that the PM appendix includes the actual profiles. I would encourage EPA to write a similar Appendix for the TOG speciation.

I was surprised that there modeling assumes that a constant EC/PM emission ratio for LDGV. This may be because the KCVES did not test many Tier 2/LEV2 vehicles. The CRC A74/E96 project found a pretty significant increase in the EC/PM for newer Tier 2/LEV2 vehicles. This has been presented in project reports and will be published shortly.

It also seems like default LDGV EC/PM ratio is not appropriate for GDI, which are becoming a larger part of the fleet. ARB has been doing a fair bit of testing of GDI – presumably those data are available. This will be critical for MOVES to be able to predict emissions from future fleets.

4.5.2. Clarity of Analytical Methods and Procedures

Is the description of analytic methods and procedures clear and detailed enough to allow the reader to develop an adequate understanding of the steps taken and assumptions made by EPA to develop the model inputs? Are examples selected for tables and figures well chosen and designed to assist the reader in understanding approaches and methods?

4.5.2.1. Dr. Tom Durbin

Sections 3.1 to 3.5 – The description here is not clear. In equation 1, defines a "speciation factor". Then later on the page there is a "speciationConstant" that is not defined. Similarly, "oxySpeciation" does not appear to be defined. The equations above table 4 are also not clear. Does this mean that the speciation is defined separately for the pure gasoline as opposed to the oxygenate part of the fuel. What is the voltowtpercentoxy term?

Table 13 is useful, providing a link with other models, as our Figure 2 and Figure 3.

Section 5.1 step 1 – It would be useful to provide a one sentence explanation as to why the EC/PM2.5 ratios vary across operating modes.

Step 2 – last sentence "the nonECnonSO4PM as a whole…. (potential suggestion)

Step 4 – It would be useful to give a simple example of a basis temperature effect (effect on catalyst temp, for example).

Step 5 – For the crankcase emissions for the pre-2007 diesel, there are some important factors that are left out that would be useful in interpreting Table 14. In particular, from the MOVES2014 Heavy-duty Emissions Rate Report it indicates that "The crankcase emission factors shown in Table 51 are derived such that the crankcase PM2.5 emissions are 20% of the PM2.5 exhaust measurements, and have an EC/PM split of 1.57%."

Top of page 28 – refers to Table 7, but this deals with VOC/NMHC not PM.

Step 8 – It seems like since there are only 7 categories that a table could actually be included with the speciation profiles used for each of the categories.

4.5.2.2. Dr. Allen Robinson

No response.

4.5.3. Appropriateness of Technical Approach

Are the methods and procedures employed technically appropriate and reasonable, with respect to the relevant disciplines, including physics, chemistry, engineering, mathematics and statistics? Are you able to suggest or recommend alternate approaches that might better achieve the goal of developing

accurate and representative model inputs? In making recommendations please distinguish between cases involving reasonable disagreement in adoption of methods as opposed to cases where you conclude that current methods involve specific technical errors.

4.5.3.1. Dr. Tom Durbin

The methods and procedures appear to be reasonable for this document. The bigger question is probably the description of the methods and the evaluation of the data sets, as described above. One major category that is missing is pre-2007 retrofit heavy-duty diesel engines and how these are modeled. Also, GDI vehicles for future years.

4.5.3.2. Dr. Allen Robinson

I like the approach of defining nonECPM because EC is refractory while other components, in particular OC, are semivolatile. This addition is an important step towards implementing a more physically realistic treatment of OC. However, I am concerned that the model continues to treat OC as an inert, non-volatile component of the exhaust. Presumably MOVES is supposed to estimate the PM emissions at typical atmospheric conditions (not those in CVS). The problem is that the low levels of dilution commonly often used in vehicle testing campaigns such as the KCVES create high PM concentrations in the CVS. This bias the gas-particle partitioning of the OC. Few studies have quantified the behavior, but the recent CRC A74/E96 project demonstrates the issues with fleet of 60+ LDGV and MDDV/HDDV vehicles (see May et al. dx.doi.org/10.1021/es400782j | Environ. Sci. Technol. 2013, 47, 8288−8296, May et al. Atmospheric Environment 77 (2013) 128e139). At a minimum the report should point out this limitation that the emission rates may be overestimated because of partitioning biases. I would encourage EPA to start explicating accounting for these biases in both the MOVES emission rates and source profiles. This can be done using the volatility distributions in the May et al. papers and the measured CVS concentrations.

I was confused with section 3 which describes the method for converting between different classes of gas phase organics (NMOG, TOG, THC, etc.).

- First, Title of section 3. Hydrocarbon speciation. I found this confusing. Hydrocarbons are organic compounds that contain carbon and hydrogen. This is a subset of the organic, which can contain compounds in addition to C and H. This should be called total organic gas speciation.
- Second I am concerned with defining the THC emissions based on what is measured by the FID. I realize that this is standard definition but it is not scientifically correct. The FID measures carbon. A problem is that the measurement efficiency is species dependent (as mentioned in the document). The FID quantitatively measure carbons in hydrocarbons (organic compounds comprised of carbon and hydrogen) and the standard propane calibration works well. However, the FID can also measure some of the carbon in oxygenated organics (especially carbons not associated with oxygen atoms) so some of the signal in the FID comes from oxygenated organics, which are not hydrocarbons. Therefore, there is no straightforward interpretation of the FID signal, but it does detect more than just the hydrocarbon emissions.

- Third, I could not follow the equations used to convert between the different classes of organic gases (NMOG to NMHC, etc. – e.g. section 3.2). This correction seems to be relatively straightforward – it appears that you are simply using different ratios of, e.g. NMOG to FID defined THC. Not surprisingly, these ratios depend on vehicle MY and type of fuel.
- I will focus my comments on section 3.2 but the same comments to apply to the other sections (e.g. 3.3) that perform the same analysis. What is the basis of equation (1)? Some underlying physical or chemistry principle? How is equation (1) used? Is equation (1) used to derive un-numbered equations later on page 9? What is the definition CF is molar or mass carbon fraction? MPC is mass of what? per carbon? Where is FIDx defined – give table or reference? Is the speciation constant listed in Table 5 the same as the speciation factor defined by equation 1? If so then you need to reconcile the names. I tried played with equation with equation (1) but could not figure out some of the inputs. It should be clear that I found this whole section pretty confusing and do not have a basic understanding of what MOVES is doing, never mind being able to reproduce the calculations.
- It seems that the key to calculating the needed ratios is not equation (1) but the un-numbered equations listed on page 9. The inputs for these equations appear to be given in Table 4 and 5. I assume that these values are fixed (or can the user input a difference volume to weight percent oxygen)? Where did these values come from? Derived from fuel analyses? Derived from fitting experimental data? If they are fixed, then it seems like one could get rid of Table 4 and simply replace Table 5 with the actual ratios used to convert between NMHC and NMOG for the different model year groups. That would be much simpler. I think that the equations make it appear that what is being done is more sophisticated then it is.

Page 25 "Step 2" states that sulfate and particular water emissions were obtained by speciation profiles. However, I thought these were calculated with the sulfate model?

The report should define what is meant by the ratios of means (or mass weighted means) used to create average profiles. Right now the report assumes the reader can knows this.

4.5.4. Appropriateness of Assumptions

In areas where EPA has concluded that applicable data is meager or unavailable, and consequently has made assumptions to frame approaches and arrive at solutions, do you agree that the assumptions made are appropriate and reasonable? If not, and you are so able, please suggest alternative sets of assumptions that might lead to more reasonable or accurate model inputs while allowing a reasonable margin of environmental protection.

4.5.4.1. Dr. Tom Durbin

Again, the most critical assumption appears to be where the datasets sufficiently cover the vehicle categories that are needed for the model. Additional categories that could be added include pre-2007 retrofit heavy-duty diesel engines and GDI vehicles for future years, as well as some of the data sets described above.

4.5.4.2. Dr. Allen Robinson

Limited data for GDI. This is not mentioned in report. ARB has been doing some work on this.

Limited data for CNG. This is acknowledged in the report. Not clear how critical a gap that is given the limited number of CNG vehicles (maybe important in places like LA or NYC with lots of CNG buses?).

Limited data for post-2007 diesels, especially on long-term performance on aftertreatment devices.

These limitations are expensive to address. They should be pointed out in the report.

4.5.5. Consistency with Existing Body of Data and Literature

Are the resulting model inputs appropriate, and to the best of your knowledge and experience, reasonably consistent with physical and chemical processes involved in emissions formation and control? Are the resulting model inputs empirically consistent with the body of data and literature that has come to your attention?

4.5.5.1. Dr. Tom Durbin

The resulting model inputs appear to be consistent with exhaust emissions formation and the associated literature.

4.5.5.2. Dr. Allen Robinson

The PM profiles were weighted using Kansas City MSA VMT data. How sensitive are the profiles to that assumption? If they are sensitive then that potentially creates a number of concerns. How representative is that of other areas in the country? How representative are they of future vehicle fleets?

Section 4.2 – "But they are the major species by mass and reactivity" I am concerned about the gaps between speciated and total emissions. The standard approach (adopted here), assumes that the unspeciated portion of the NMOG behaves the same as the speciated. This likely is not the case when it comes to secondary organic aerosol (SOA) formation. The unspeciated emissions are likely a complex mixture of higher molecular weight species – these species contribute disproportionately to SOA formation relative to lighter species (e.g. propane).

"while assuring that the PM2.5 species achieved a 100% mass balance" I find these sorts of statements very concerning, especially given that these sorts of renormalizations are often poorly documented resulting in users not being aware of these assumptions. It is important to document if there are significant mass balance discrepancies, not just normalize them away. I realize that the profiles don't have a PM_unkown species, but enforcing mass balance may create other problems.

Other studies with diesel (e.g. Schauer et al. 1999 EST, Subramanian et al. 2009 EST) show a pretty significant gap in PM mass balance for diesels (sum of speciated low).

4.5.6. General/Catch-All Reviewer Comments

Please provide any additional thoughts or review of the material you feel important to note that is not captured by the preceding questions.

4.5.6.1. Dr. Tom Durbin

- extra space – page 3 1st sentence (THC) ,; page 4 elemental carbon " 5; Page 7 last sentence 1 ." might be extra space; page 8 under table 3 (field meanbase rate in..; page 14 section heading …for Evaporative
- add space – page 8 (TOG): h;
- add comma – page 3 3rd sentence , such as; page 6 nonECPM, such as; page 28 2nd full paragraph (i.e., ;
- page 3 sentence 4 add "to make TOG" to end of sentence.
- page 3 last sentence first paragraph ..seems to be missing something
- page 3 second paragraph 3rd sentence – under different measurement
- page 4 elemental carbon – can a reference to the TOR method be provided?
- page 4 chemical mechanism – to speed up the atmospheric…
- page 5 integrated species – 3rd sentence CM-speciate is unclear
- page 8 Table 4 not centered – some headings are centered but not others throughout
- page 12 and 13 – there is an issue with the paging
- page 14 & 15– issue with section numbering should be 3.4 and 3.5
- page 15– section 4.1 1st sentence – MOVES2014 produces an or the output
- page 28– 3rd full paragraph there is a reference in (EPA, 2014) and not number format
- page 28– last paragraph "capability"

4.5.6.2. Dr. Allen Robinson

Page 5 Intermediate PM section -- EC is not a "real" species in that it is not a distinct chemical substance but something that is operational defined. Although not defined, I assumed a real species was an actual chemical species like CO.

Page 7 Real speciation profile – A key shortcoming is that these real profiles are incomplete – they are typically missing around a quarter of the TOG mass. This point is mentioned later but should be mentioned here as well.

Page 7 – I am concerned with defining the THC emissions based on what is measured by the FID. I realize that this is standard definition but it is not scientifically correct. The FID measures carbon. A problem is that the measurement efficiency is species dependent (as discussed in the document). For

FID quantitatively measure carbons in hydrocarbons (organic compounds comprised of carbon and hydrogen) and the standard propane calibration works well. However, the FID will also measure some oxygenated organics (especially carbons not associated with oxygen atoms) so some of the signal in the FID comes from oxygenated organics, which are not hydrocarbons.

The qualifier "start" is often used to characterize the emissions. Every instance of that should be further classified as cold or hot start, as that can make a big difference on emissions. Many times it was not clear what type of start the text was referring too.

Page 3 defined **by** discrete – missing by

Page 3 although "county"? Not sure what county is

Page 9 "as the all" delete the

Page 14 – "3.1 NMHC and VOC calculations …" this section heading is misnumbered.

PM fractions of median profile greater than 1 → how much greater than 1?

4.6. PM2.5 Speciation in MOVES

This section provides a verbatim list of peer reviewer comments submitted in response to the charge questions for the appendix PM2.5 Speciation in MOVES.

4.6.1. Adequacy of Selected Data Sources

Does the presentation give a description of selected data sources sufficient to allow the reader to form a general view of the quantity, quality and representativeness of data used in the development of emission rates? Are you able to recommend alternate data sources might better allow the model to estimate national or regional default values?

4.6.1.1. Dr. Tom Durbin

Refer to response to All Documents Reviewed in Section 4.1.1.1.

4.6.1.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.1.2.

4.6.2. Clarity of Analytical Methods and Procedures

Is the description of analytic methods and procedures clear and detailed enough to allow the reader to develop an adequate understanding of the steps taken and assumptions made by EPA to develop the model inputs? Are examples selected for tables and figures well chosen and designed to assist the reader in understanding approaches and methods?

4.6.2.1. Dr. Tom Durbin

p. 3 Why was EC measured for considerably more vehicles for the KCVES than OC. What method was used for the EC?

The comparisons in Table A-8 and the associated discussion is valuable in that it ties the current estimates to earlier model estimates and data in the literature.

Under Table A-4. The discussion needs to be clarified about how OM is split into organic carbon and non-carbon organic matter using the relationship: OM = 1.2 * OC. The table seems to show that the OC is scaled down and then renamed OM, which is subsequently modified by the 1.2 factor. It seems that it would be best to start out by saying that the initial OC includes organic carbon, a positive artifact, and other non-carbon species associated with the organic carbon (such as hydrogen, oxygen, etc.).

4.6.2.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.2.2.

4.6.3. Appropriateness of Technical Approach

Are the methods and procedures employed technically appropriate and reasonable, with respect to the relevant disciplines, including physics, chemistry, engineering, mathematics and statistics? Are you able to suggest or recommend alternate approaches that might better achieve the goal of developing accurate and representative model inputs? In making recommendations please distinguish between cases involving reasonable disagreement in adoption of methods as opposed to cases where you conclude that current methods involve specific technical errors.

4.6.3.1. Dr. Tom Durbin

Although the silicone contamination from the connecting pieces from the transfer line can be removed, is it possible that some other PM species relating the transfer line heating/burning. I see in another section that there is some compensation for other species, but it reinforces the idea that EPA should consider a broader range of data sources in its modeling.

Although the Kansas City study is one of the more recent comprehensive studies of gasoline PM, it is not obvious that fleet average composition profiles would be representative of the fleet going into the future. On page 2, it does indicate that there were differences in PM2.5 composition that between different model year groups. If there are differences between Tier 0, Tier 1, and NLEV/Tier 2 vehicles, will a fleet average profile be adequate for the fleet going into the future. Of course, future generations of the model will need to include GDI vehicles, as more information on their PM species profiles become more available. Additionally, how are light-duty diesel vehicles accounted for in the model?

4.6.3.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.3.2.

4.6.4. Appropriateness of Assumptions

In areas where EPA has concluded that applicable data is meager or unavailable, and consequently has made assumptions to frame approaches and arrive at solutions, do you agree that the assumptions made are appropriate and reasonable? If not, and you are so able, please suggest alternative sets of assumptions that might lead to more reasonable or accurate model inputs while allowing a reasonable margin of environmental protection.

4.6.4.1. Dr. Tom Durbin

Although the silicone contamination from the connecting pieces from the transfer line can be removed, is it possible that some other PM species relating the transfer line heating/burning.

It seems reasonable that the sample size might be too high to capture high emitters in each of the model years groups, and especially for newer model years. It would be interesting to know if the population of high emitters in the KCVES was comparable to that found in previous studies of high emitters, although many of those estimates were made in older studies.

How different is the PM2.5 composition by model year groups? As this would be an important consideration in terms of using the fleet average approach.

There are some differences between the cruise and transient OC/PM factors. How was it determined that the transient cycle is more representative than the cruise for heavy-duty vehicles. Is this based on more urban driving?

For the 2007+ heavy-duty vehicles, while it is understandable to utilize measurements that are not background corrected and the associated negative numbers. It should be noted and understood that this would likely overestimate the contributions of different individual species. Nevertheless, the breakdown in Table A-9, with a predominantly sulfate contribution and minimal contribution from minor species seems reasonable.

The discussion relating to the exclusion of sulfate-bound water provides a good basis for this assumption and is adequately described.

4.6.4.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.4.2.

4.6.5. Consistency with Existing Body of Data and Literature

Are the resulting model inputs appropriate, and to the best of your knowledge and experience, reasonably consistent with physical and chemical processes involved in emissions formation and control? Are the resulting model inputs empirically consistent with the body of data and literature that has come to your attention?

4.6.5.1. Dr. Tom Durbin

The intercomparisons between the model inputs and the available data for the pre-2007 heavy-duty vehicles indicate that the model inputs are reasonably representative. The relatively low sulfate contribution in these profiles may not be appropriate for retrofit heavy-duty diesel vehicles, however.

4.6.5.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.5.2.

4.6.6. General/Catch-All Reviewer Comments

Please provide any additional thoughts or review of the material you feel important to note that is not captured by the preceding questions.

4.6.6.1. Dr. Tom Durbin

- p. 2. Missing high emitter study
- page 1 2nd paragraph – updated speciation profiles changes

- the references are numbered in the main document, but use the name/year format in the Appendix
- add comma – page 3 (effective beginning 2006-2008),;
- page 3 3rd paragraph. Missing period after …..161.2 ppm. Fuel sulfur….
- page 3 2nd to last sentence. i~~m~~nput**e**
- page 5 The CRC E-55/59 is listed three different was ….E55/59, -55/59, E-55/59
- page 6 first sentence – extra space 2010). [1]; and 1st full sentence begins with number; 2nd to last full sentence on page beings with a number
- page 7 2nd paragraph "Instead we used calculated"; last sentence in paragraph impact~~ed~~ing
- page 8 last sentence – the adjusted OC speciation factors are
- page 5 integrated species – 3rd sentence CM-speciate is unclear
- page 8 Table 4 not centered – some headings are centered but not others throughout
- page 12 and 13 – there is an issue with the paging
- page 14 & 15– issue with section numbering should be 3.4 and 3.5
- page 15– section 4.1 1st sentence – MOVES2014 produces an or the output
- page 28– 3rd full paragraph there is a reference in (EPA, 2014) and not number format
- page 28– last paragraph "capability"

4.6.6.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.6.2.

4.7. Estimating Elemental Carbon Factions

This section provides a verbatim list of peer reviewer comments submitted in response to the charge questions for section 2.3 Estimating Elemental Carbon Fractions, IN: *Development of Emission Rates for Light-duty Vehicles in the Motor Vehicle Emissions Simulator (MOVES2014)*.

4.7.1. Adequacy of Selected Data Sources

Does the presentation give a description of selected data sources sufficient to allow the reader to form a general view of the quantity, quality and representativeness of data used in the development of emission rates? Are you able to recommend alternate data sources might better allow the model to estimate national or regional default values?

4.7.1.1. Dr. Tom Durbin

Refer to response to All Documents Reviewed in Section 4.1.1.1.

4.7.1.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.1.2.

4.7.2. Clarity of Analytical Methods and Procedures

Is the description of analytic methods and procedures clear and detailed enough to allow the reader to develop an adequate understanding of the steps taken and assumptions made by EPA to develop the model inputs? Are examples selected for tables and figures well chosen and designed to assist the reader in understanding approaches and methods?

4.7.2.1. Dr. Tom Durbin

No response.

4.7.2.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.2.2.

4.7.3. Appropriateness of Technical Approach

Are the methods and procedures employed technically appropriate and reasonable, with respect to the relevant disciplines, including physics, chemistry, engineering, mathematics and statistics? Are you able to suggest or recommend alternate approaches that might better achieve the goal of developing accurate and representative model inputs? In making recommendations please distinguish between cases involving reasonable disagreement in adoption of methods as opposed to cases where you conclude that current methods involve specific technical errors.

4.7.3.1. Dr. Tom Durbin

No response.

4.7.3.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.3.2.

4.7.4. Appropriateness of Assumptions

In areas where EPA has concluded that applicable data is meager or unavailable, and consequently has made assumptions to frame approaches and arrive at solutions, do you agree that the assumptions made are appropriate and reasonable? If not, and you are so able, please suggest alternative sets of assumptions that might lead to more reasonable or accurate model inputs while allowing a reasonable margin of environmental protection.

4.7.4.1. Dr. Tom Durbin

No response.

4.7.4.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.4.2.

4.7.5. Consistency with Existing Body of Data and Literature

Are the resulting model inputs appropriate, and to the best of your knowledge and experience, reasonably consistent with physical and chemical processes involved in emissions formation and control? Are the resulting model inputs empirically consistent with the body of data and literature that has come to your attention?

4.7.5.1. Dr. Tom Durbin

No response.

4.7.5.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.5.2.

4.7.6. General/Catch-All Reviewer Comments

Please provide any additional thoughts or review of the material you feel important to note that is not captured by the preceding questions.

4.7.6.1. Dr. Tom Durbin

The photoacoustic instrument should provide relatively good measurements for EC over a range of concentrations. The 2.4 mg/mi differences between the TOR and the photoacoustic seems a bit high. How due these two measurements compare to the total PM mass on the filter would be a good question to address here. Also, how high are the PM mass emission rates, where the 2.4 mg/mi offset would be small considered to be a small fraction of. Seems like 2.4 mg/mi would be a big number in comparison to emission rates of typical modern vehicles.

1st sentence – extra space (PM2.5)
Final sentence in first paragraph – speciation is misspelled

4.7.6.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.6.2.

4.8. Updates to PM2.5 Emission Rates in MOVES2014

This section provides a verbatim list of peer reviewer comments submitted in response to the charge questions for section 2.5 Updates to PM2.5 Emission Rates in MOVES2014, IN: *Development of Emission Rates for Light-duty Vehicles in the Motor Vehicle Emissions Simulator (MOVES2014)*.

4.8.1. Adequacy of Selected Data Sources

Does the presentation give a description of selected data sources sufficient to allow the reader to form a general view of the quantity, quality and representativeness of data used in the development of emission rates? Are you able to recommend alternate data sources might better allow the model to estimate national or regional default values?

4.8.1.1. Dr. Tom Durbin

Refer to response to All Documents Reviewed in Section 4.1.1.1.

4.8.1.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.1.2.

4.8.2. Clarity of Analytical Methods and Procedures

Is the description of analytic methods and procedures clear and detailed enough to allow the reader to develop an adequate understanding of the steps taken and assumptions made by EPA to develop the model inputs? Are examples selected for tables and figures well chosen and designed to assist the reader in understanding approaches and methods?

4.8.2.1. Dr. Tom Durbin

No response.

4.8.2.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.2.2.

4.8.3. Appropriateness of Technical Approach

Are the methods and procedures employed technically appropriate and reasonable, with respect to the relevant disciplines, including physics, chemistry, engineering, mathematics and statistics? Are you able to suggest or recommend alternate approaches that might better achieve the goal of developing accurate and representative model inputs? In making recommendations please distinguish between cases involving reasonable disagreement in adoption of methods as opposed to cases where you conclude that current methods involve specific technical errors.

4.8.3.1. Dr. Tom Durbin

No response.

4.8.3.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.3.2.

4.8.4. Appropriateness of Assumptions

In areas where EPA has concluded that applicable data is meager or unavailable, and consequently has made assumptions to frame approaches and arrive at solutions, do you agree that the assumptions made are appropriate and reasonable? If not, and you are so able, please suggest alternative sets of assumptions that might lead to more reasonable or accurate model inputs while allowing a reasonable margin of environmental protection.

4.8.4.1. Dr. Tom Durbin

No response.

4.8.4.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.4.2.

4.8.5. Consistency with Existing Body of Data and Literature

Are the resulting model inputs appropriate, and to the best of your knowledge and experience, reasonably consistent with physical and chemical processes involved in emissions formation and control? Are the resulting model inputs empirically consistent with the body of data and literature that has come to your attention?

4.8.5.1. Dr. Tom Durbin

No response.

4.8.5.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.5.2.

4.8.6. General/Catch-All Reviewer Comments

Please provide any additional thoughts or review of the material you feel important to note that is not captured by the preceding questions.

4.8.6.1. Dr. Tom Durbin

The issue of silicone contamination is probably something that needs further consideration. I think that some rational should be given in this description as to where the 4.075 factor comes from. In fact, I looked through the referenced ES&T paper and did not find anything either, unless there was a error with the reference numbering. This issue further emphasizes points raised above that EPA probably is using too narrow a focus in the data sets that it considers.

2nd paragraph – 4th sentence – add comma ….rates**,** as documented…

4.8.6.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.6.2.

4.9. Computation of Elemental Carbon and Non-Elemental Carbon Emission Factors

This section provides a verbatim list of peer reviewer comments submitted in response to the charge questions for sub-section 2.1.3.5 Computation of Elemental Carbon and Non-Elemental Carbon Emission Factors, IN: *Development of Emission Rates for Heavy-Duty Vehicles in the Motor Vehicle Emissions Simulator (MOVES2014)*.

4.9.1. Adequacy of Selected Data Sources

Does the presentation give a description of selected data sources sufficient to allow the reader to form a general view of the quantity, quality and representativeness of data used in the development of emission rates? Are you able to recommend alternate data sources might better allow the model to estimate national or regional default values?

4.9.1.1. Dr. Tom Durbin

Refer to response to All Documents Reviewed in Section 4.1.1.1.

4.9.1.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.1.2.

4.9.2. Clarity of Analytical Methods and Procedures

Is the description of analytic methods and procedures clear and detailed enough to allow the reader to develop an adequate understanding of the steps taken and assumptions made by EPA to develop the model inputs? Are examples selected for tables and figures well chosen and designed to assist the reader in understanding approaches and methods?

4.9.2.1. Dr. Tom Durbin

No response.

4.9.2.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.2.2.

4.9.3. Appropriateness of Technical Approach

Are the methods and procedures employed technically appropriate and reasonable, with respect to the relevant disciplines, including physics, chemistry, engineering, mathematics and statistics? Are you able to suggest or recommend alternate approaches that might better achieve the goal of developing accurate and representative model inputs? In making recommendations please distinguish between

cases involving reasonable disagreement in adoption of methods as opposed to cases where you conclude that current methods involve specific technical errors.

4.9.3.1. Dr. Tom Durbin

No response.

4.9.3.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.3.2.

4.9.4. Appropriateness of Assumptions

In areas where EPA has concluded that applicable data is meager or unavailable, and consequently has made assumptions to frame approaches and arrive at solutions, do you agree that the assumptions made are appropriate and reasonable? If not, and you are so able, please suggest alternative sets of assumptions that might lead to more reasonable or accurate model inputs while allowing a reasonable margin of environmental protection.

4.9.4.1. Dr. Tom Durbin

No response.

4.9.4.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.4.2.

4.9.5. Consistency with Existing Body of Data and Literature

Are the resulting model inputs appropriate, and to the best of your knowledge and experience, reasonably consistent with physical and chemical processes involved in emissions formation and control? Are the resulting model inputs empirically consistent with the body of data and literature that has come to your attention?

4.9.5.1. Dr. Tom Durbin

No response.

4.9.5.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.5.2.

4.9.6. General/Catch-All Reviewer Comments

Please provide any additional thoughts or review of the material you feel important to note that is not captured by the preceding questions.

4.9.6.1. Dr. Tom Durbin

It would be interesting to see how the EC fractions developed based on Kweon et al. compare to those of other should, which could be evaluated by looking at cycles such as cruise cycles, or idle, vs. transient cycles. Comparisons could be made against E-55/59 or studies by CARB.

Last paragraph on 1st page – 1st sentence add comma after i.e., ; and also the reference for Kweon is given in the author/year format, whereas the references in the back are listed by number.

4.9.6.2. Dr. Allen Robinson

Refer to response to TOG and PM Speciation in MOVES for Air Quality Modeling in Section 4.5.6.2.

4.10. Estimation of Air-Toxic Emissions from Highway Vehicles in the Motor Vehicle Emissions Simulator (MOVES 2014)

This section provides a verbatim list of peer reviewer comments submitted in response to the charge questions for the report *Estimation of Air-Toxic Emissions from Highway Vehicles in the Motor Vehicle Emissions Simulator (MOVES 2014)*.

4.10.1. Adequacy of Selected Data Sources

Does the presentation give a description of selected data sources sufficient to allow the reader to form a general view of the quantity, quality and representativeness of data used in the development of emission rates? Are you able to recommend alternate data sources might better allow the model to estimate national or regional default values?

4.10.1.1. Dr. Tom Durbin

Refer to response to All Documents Reviewed in Section 4.1.1.1.

4.10.1.2. Dr. Allen Robinson

I thought that the report did not do a good job of providing in text citations to the data sources. Often when the report referred to a data source there was not an in text citation. For example, on page 14 -- they were taken directly from the Complex Model Spreadsheet "*CM Final.xls*". Need a reference for this spreadsheet. This is just on example.

Pre2000 vehicles (Section 2.1) This model is based on old Tier 0 data, which is applied to a large fraction of Tier1 vehicles. There is alot of speciated data for Tier 1 vehicles from the KCVES. Why was a model not developed based on that data? The proposed model should be tested against the KCVES Tier 1 data to demonstrate that it is applicable to those vehicles. At a minimum this needs to be discussed.

4.10.2. Clarity of Analytical Methods and Procedures

Is the description of analytic methods and procedures clear and detailed enough to allow the reader to develop an adequate understanding of the steps taken and assumptions made by EPA to develop the model inputs? Are examples selected for tables and figures well chosen and designed to assist the reader in understanding approaches and methods?

4.10.2.1. Dr. Tom Durbin

p. 6 – 2nd paragraph discusses pre-2001 vehicles and 2004+ vehicles, but does not address 2001-2004 vehicles. 4th paragraph – what two fuel properties are used for evaporative emissions.

p. 15 – its not clear what is meant by the phrase that "relations of air toxic emissions to changes in fuel properties has remained stable from Tier 0 to Tier 1"

p. 17 – There is a reference to modeling 2000 and earlier vehicles on E15-E20, but not discussion on factors that would be used for such fuels. It would be useful to at least reference the section where this will be discussed.

For section 2.2.1 see suggestions for the report "Gasoline Fuel Effects for Vehicles Certified to Tier-2 Standards". Then on page 32, it talks about the "full" vs. "reduced" design. The fact that the reduced design represents 5 vehicles and 11 fuels (as opposed to 5 vehicles by 27 fuels) should be discussed in the 1st paragraph, rather than the 2nd. Then the 2nd paragraph talks about Table 30 and 31 before these tables are introduced in the 3rd paragraph, so the 2nd paragraph seems out of place. It should at least be mentioned here that acrolein, benzene, and 1,3 butadiene are not modeled for hot running emissions in this section (even though it is discussed in the next section). The approach using "information parity" appears to the reasonable for NMOG and ethane.

Section 2.1.3 – It should be mentioned at the start of the paragraph that metals are represented both with these metals and the metals presented in the PM2.5 emission profile. Also, "conservative" is probably too weak a term to describe using the bag 2 emission rates, since its actually more of an upper limit estimate (although this only appears to be the case for manganese).

p. 42 – A recent study by CARB/UC Riverside/UC Davis should provide some information related to biodiesel emission factors.

p. 42/43 seems like final paragraph on 42 and 1st paragraph on 43 could be combined, since the three different references to Table 39 in these paragraphs is a little confusing.

p. 46 – section 2.3.4 – It seems like dioxin emissions might be overestimated using a data set with such older vehicles. This might be worth mentioning in the text.

p. 47 – section 2.4.2 – Its not clear what the basis of the particulate to gaseous phase split is for the PAHs. If it is discussed previously, it should be reiterated here.

p. 53 – 3rd paragraph on 20% ethanol. Its unclear what fuel speciation data was used here. Was this from in-use fuels? Since the test fuels were not necessary representative of average fuels, but rather represent the extremes of in-use fuels. Table 51 is useful.

4.10.2.2. Dr. Allen Robinson

The report commonly uses the word "fraction" or "toxic fraction". You need to define fraction of what – VOC, NMOG, THC, etc (presumably each of these is defined using standard EPA definitions). For tables actually defining in header as was done for Table 20 is useful. Also is this a mass or a mole fraction.

Please make sure that all variables are defined – a nomenclature table with units should be added to the report.

Centering data (page 10) – It appears that you are using a different centering approach for older data than for the new model (e.g. eqn 8). Why were different approaches used?

What is meant by model year specific weightings (page 10)? What do these weights represent? Fraction of vehicles for a given year?

Equation 1 – what are the units of the different variables?

Table 8 – Complex model coefficients – these are beta's in equation (1).

Page 13 "For each compound, the model equations as shown in **Error! Reference source not found.**, are evaluated for a "base" and a "target" fuel." This base fuel resides in MOVES? Is this the same as the average fuel listed in Table 7?

Page 14 – equation 3. It was not clear how the weights are being applied. You are trying to derive one adjustment factor for all pre2000 vehicles? Are you driving a separate factor for the 10 different technology classes? This needs to be clarified.

Table 12 -- According to the text these weights represent prevalence for a given technology year. Prevelance means what? Fraction of vehicles based on number, VMT? I am confused that Table 12 lists weights based on "age" as opposed to model years? Is this age relative to 2000? It would be clear to define a base year to calculate age.

Equation 6 -- What is I_{VOC}? Where does the value come from? The standard moves code.

Post2000 organic emissions are based on models derived from the EPAct data. It was not clear if these models are the same as those in the EPAct report. I assumed that they were. If so, the Toxic report needs to specifically acknowledge that. In addition, it should provide specific references to which models are being used as the EPAct report describes a whole bunch of models. Please provide in text citations for the EPAct report.

Table 1 – Are all these hydrocarbons? There are compounds that contain elements other H and C, which I don't consider to be hydrocarbons.

When you use the term "start" please define it as either cold (e.g. bag 1 of LA92 with appropriate preconditioning) or hot start (bag 3 of LA92).

Page 6 "algorithms" –are these really curve fits as opposed to algorithms?

Page 8 "Toxics inputs for MOVES are not explicitly designed to vary by temperature." Not sure what this means? The outputs do not vary with temperature? What does temperature refer to? Ambient? Cold versus hot start?

"In addition, while MOBILE6.2 relied on very limited data from heavy-duty gasoline vehicles, MOVES applies Complex Model algorithms to both light-duty and heavy-duty gasoline vehicles" Is there a basis for this extensions. Have additional heavy duty gasoline vehicle data been obtained? If not why is MOVES being extended to heavy duty gas while MOBILE did not?

Page 16 (last sentence of first paragraph) Does MOVES have representative fuel data for different regions and simulations year? Given the focus of fuel dependence of emissions providing the user with a robust set of default fuel values (year and region) would be helpful.

Equation 7 – what is V and what are its units? Equation 7 and associated parameters in Table 13 were derived by fitting MOBILE output. Why not fit directly the original data or use the original parameterization in MOBILE? You claim this equation provides the best fit. What are statistics of fit?

Table 12 -- What do these weight represent? The distribution of different classes of vehicles in different model years? It seems like the minimum age of 2000 vehicle is 13 years (if running a present day simulation).

"It should be noted that the sulfur effects terms in the equations were not included; rather, sulfur effects on toxic emissions were assumed to be proportional to the sulfur impacts on total VOC estimated by MOVES." Sulfur effects in what equations? There is no sulfur in equation 7 (which is the equation that this sentence seems to refer to).

Table 16 exists in Pre-2000 section (2.1– in fact it is in section 2.1.1.1.3) but appears to apply more generally. Move into a more general section of the report?

Do you really want to call ethanol blends gasohol? When I hear gasohol I think of Brazil.

Page 31 "one set representing start emissions and a second set representing hot-running" start emissions is hot start (LA92 bag 3) or cold start (LA92 bag 1, with appropriate conditioning).

There are table reference problems (e.g. see page 32, 35, 38, 40, …). There are other instances of this.

Table 27, 28, etc. Are these parameters from the EPAct report. If so provide citation. Please cite the specific model from the EPAct report, not just the general report.

Page 40 What is OC2.5 VOC?

Page 41—dioxins and furans – "to be similar" You are assuming them to be the same not just similar. Seems like these estimates are very uncertain since they are based on very old vehicles.

The word "data" is plural. E.g. Data were not data was

Diesel PAH data – Similar problems with the partitioning estimates. Partitioning in Schauer study is biased compared to atmosphere. This needs to be explicitly noted in the report. There is a "higher concentration of particles in diesel exhaust" compared to gasoline exhaust in the CVS or plume, but not in the atmosphere. Concentrations in the atmosphere not exhaust is what matters for partitioning.

Table 49 – Particle phase naphthalene? That must be a measurement artifact.

4.10.3. Appropriateness of Technical Approach

Are the methods and procedures employed technically appropriate and reasonable, with respect to the relevant disciplines, including physics, chemistry, engineering, mathematics and statistics? Are you able to suggest or recommend alternate approaches that might better achieve the goal of developing accurate and representative model inputs? In making recommendations please distinguish between cases involving reasonable disagreement in adoption of methods as opposed to cases where you conclude that current methods involve specific technical errors.

4.10.3.1. Dr. Tom Durbin

Overall, the complex model provides a robust framework for modeling acetaldehyde, formaldehyde, benzene, and 1-3 butadiene, especially with its recent updates.

Table 7 – the mean value for centering the sulfur at 204 ppmw is relatively high compared to current sulfur levels. Will this potentially be modified going into the future.

Tables 8 to 11 – What do the dashes in the table represent? Is that where the data show no effect or are insufficient? For example, there is no sulfur effect on formaldehyde.

For MTBE, the model applied previously in MOBILE6.2 should be adequate, especially since MTBE use is essentially historical. Similarly, in section 2.2.2.1.1, the use of Tier 1 and earlier vehicles for Tier 2 vehicles appears reasonable.

Section 2.1.2 Its not clear what samples are being used to estimate the PAHs. It talks about a set of 99 samples being used for the fractions in the second paragraph and how the fractions are determined in terms of PAH/THC and PAH/OC2.5. Then it talks about the partitioning into gaseous and particulate phases in the 3rd and 4th paragraph that appears to be based on 2 vehicles in the medium emitter category, which was selected from 4 samples collected at two temperatures. Why was the "medium emitter" sample selected? How significant were the differences between the samples collected at 20°C and 47°C? If there were big differences wouldn't that make a big difference in the partitioning for the PAH/THC and PAH/OC2.5 for the other 99 samples? Then its unclear what Table 20 represents, since it is multiplying fractions (PAH/THC and PAH/OC2.5) by fractions (Table 19) in a seemingly strange was. Where do the absolute emission rates for the individual species play in here?

Page 37 - Although benzene can be a function of fuel benzene, it can also be a function of other low weight aromatics, especially toluene. In the EPA study on benzene, how did toluene levels vary between the fuels.

Section 2.3 – Developing the air toxics factors from the E-75 database appears to be a reasonable approach. Its unclear how these factors might account for states with low levels of aromatics, such as California. Also, its unclear why the partitioning for the PAHs was made based on a medium-duty diesel engine. Maybe just one sentence to clarify this.

The ACES study provides a good data set for the development of the air toxics factors for the 2007 and new engines. p. 49 section 2.4.4 – Would be interested to see how backgrounds were dealt with in this study. At such levels backgrounds would be important in terms of not overestimating emissions.

Section 2.6 – CNG emissions – For the PAHs, is there any consideration given to how the oxidation catalyst would reduce PAHs. It appears that the estimates were based on measurements without an oxidation catalyst, but that these are applied to both technology categories. p. 51– section 2.6.3 – By using the only the data where chromium and nickel were detected, this would presumably overestimate emissions. Were the metal rates from heavy-duty engines also considered before deciding to use the gasoline emission rates.

Section 3 – Some more details should be provided for why the hot soak and running loss algorithms from MOBILE6.2 are applied to MOVES for the non-permeation factors. The methodologies for the permeation factors appear reasonable.

Appendix A – the fleet of vehicles used for this study appears to be too heavily weighted towards older vehicles. Were the results for the different vehicles to provide a profile that was more representative of the modern fleet.

Using an average exhaust flow might tend to underestimate emissions, since often periods of higher emissions also can be periods with higher exhaust flow.

Last paragraph – by using only the first 715 seconds, would this over represent cold start emissions.

4.10.3.2. Dr. Allen Robinson

It is not clear why the demarcation for the gasoline vehicles is MY2000 – it seems like the years in which tier 1 or tier 2 vehicles were introduced would make alot more sense. In contrast, the MY2007 distinction for diesel vehicles makes alot more sense than the apparently arbitrary split for gasoline vehicles.

Page 19 section 2.1.1.2 It seems very problematic to be using emissions data from EPAct for a new Tier 2 vehicle to apply to these older vehicles to simulate emissions from high ethanol fuel operations from a pre2000 vehicle. The uncertainty must be very large. Can you run older vehicles on E85? There seems to be little basis for this extrapolation – it seems like you are simply trying to be comprehensive. Ideally a quantitative estimate of uncertainty should be provided for this estimate. At a minimum MOVES should flag the value as massively uncertain.

Phase partitioning of PAH (page 21). This applies to all vehicles (pre2000 and post2000). However it is in the pre2000 section. I found this confusing. Why not have one section that says PAH emissions of all gasoline vehicles estimated using this approach.

More PAH: There is a paragraph that provides the caveat that "gas-particle partitioning of PAHs emission in the atmosphere depends on particle and gas concentrations, exhaust temperature and other factors." It is good to state this. However, presumably the relevant temperature for atmosphere partitioning is atmospheric temperature (not exhaust). This paragraph implies, but does not specifically state, that the gas particle partitioning measured in source test is not representative of atmospheric conditions (or at least not all atmospheric conditions). I think that this caveat needs to be explicitly stated. "The gas particle partitioning of PAHs measured in source tests and implemented in MOVES is likely not representative of atmospheric partitioning."

More PAH: The model use results for composite class, "medium emitters," to estimate gas particle partitioning of all PAHs. Why was a medium-emitters class used? I also suspect that the conditions inside the CVS during the test of these old vehicles (esp. PAH concentrations, PM concentrations, BC concentrations) are not representative of atmospheric conditions (or the newer Tier 2 vehicles). This likely biases phase partitioning towards particle phase. EPA should choose a test in which the conditions concentration and temperature inside the CVS were within the envelope of conditions that likely occur in the atmosphere. This likely would be a test for a cleaner vehicles. An even better approach would be to review the literature of ambient gas-particle partitioning measurements of these compounds and use

those values (as opposed to values from a source test). Finally, if the phase partitioning of PAHs is an important output for some of MOVES uses then it is not difficult to implement a gas-particle partitioning model.

Table 20 –The same PAH emissions ratios appear to be applied to all vehicles, which are based on some sort of fleet average from the entire KCVES (or just the pre-2001 vehicles)? It is not clear why this approach was adopted. With this approach you are locking in the emissions based on a fleet that was 10 years old today. How constant were these ratios across the fleet? If they are not constant, why not stratified the emissions into classes (at least Tier1, Tier2) which will allow the model to better forecast future emissions?

4.10.4.Appropriateness of Assumptions

In areas where EPA has concluded that applicable data is meager or unavailable, and consequently has made assumptions to frame approaches and arrive at solutions, do you agree that the assumptions made are appropriate and reasonable? If not, and you are so able, please suggest alternative sets of assumptions that might lead to more reasonable or accurate model inputs while allowing a reasonable margin of environmental protection.

4.10.4.1. Dr. Tom Durbin

p. 9 at the top The EPA assumption that metals should be independent of temperature appears reasonable. It might be useful to examine metal emissions as a function of operation mode, however, for example, comparing more vs. less aggressive driving, although perhaps not for the metals included in Table 4.

Page 16 developing regressions for ETBE and TAME from algorithms for ethanol and MTBE appears to be a reasonable assumption, especially as these fuels are not at all prevalent.

p. 37 – When modeling 1,3 butadiene as 0.0 for hot-running operation, the impact of olefins should be considered. Later on the page – CRC E-83 can be considered for olefins, although these values were near background levels as well.

Section 2.2.2.2 – Overall, the assumptions used in this section appear to be reasonable, as E85 data are not available for some of the toxics being measured. The section does use a range of different descriptions of higher ethanol levels from E70 to E85 to 74% ethanol without clearly describing when all of these different conditions are applied. For example is the same factor used for E70 and E85? Also, on page 40, the approach that ethanol contributes no PAHs should be verified. A UC Riverside/CEC/SCAQMD study will be completed next year that will provide some data in that area.

Section 3 – For section 3.1.1, when using the fuel speciation from the EPAct study to make estimates for E15 and E20, was the volatility of the species considered? This would not necessarily be an essential change.

4.10.4.2. Dr. Allen Robinson

In this chapter/report there is wider range of data quality compared to other reports and chapters. Some of the models are based on pretty robust data sources (e.g. basic gaseous organic air toxics), but others are based on data that, at best, are loosely related to the source (Why should fraction of hexavalent chromium emissions from a stationary turbine be representative of onroad vehicles? Or why should emissions from a tier 2 E85 vehicle be representative of emissions from much older vehicle operating on high ethanol blends). I understand the desire for the model to be comprehensive as possible, but the uncertainty of the predictions will vary widely. It does not seem like the model user will have any idea about the quality of the predictions. Ideally each MOVES prediction would provide a quantitative estimate for every prediction. At a minimum the model should provide a grade (e.g. similar to AP42) for each pollutant. For pollutants with robust models, the grade will be high (e.g. A). For less robust models (e.g. hexavalent chromium), the grade would be poor (e.g. F).

In some cases there are important sources of data that have not been utilized (e.g. KCVES to estimate pre2000 vehicle air toxics emissions or PAH emissions for post2000 vehicles).

CNG buses – It seems like there is more data available. WVU has done a bunch of testing on transit buses. Aerodyne research also did a bunch of chase studies of CNG powered transit buses in which they measured high formaldehyde emissions.

Section 2.1.3 Metals –You assume constant emission rates across fleet (which seems plausible, much more so than for PAHs). However, if there were systematic variations in metals emission rates across the fleet why not stratify the model to capture them. What is the quality of the metal emissions? Presumably metal emissions will be sensitive to lube oil therefore it is not clear how widely applicable the data are.

Hexavalent chromium – The speciation is based on stationary combustion turbine testing. Is there any reason to think that is applicable to on-road vehicles? If not, why even report it. At best the results will be highly uncertain. I think this an example of where the model predictions are not supported by robust data.

Page 25 – Why are dioxins and furans expressed as TEQs as opposed to not mass. I am not familiar with dioxins but it struck me as strange. The quality of the dioxins data seemed low.

4.10.5. Consistency with Existing Body of Data and Literature

Are the resulting model inputs appropriate, and to the best of your knowledge and experience, reasonably consistent with physical and chemical processes involved in emissions formation and control? Are the resulting model inputs empirically consistent with the body of data and literature that has come to your attention?

4.10.5.1. Dr. Tom Durbin

Overall, the methodologies selected and applied for this report appear to be providing reasonable input to the MOVES model. As additional data sets become available, they should also be considered for incorporation into the model, as discussed above.

4.10.5.2. Dr. Allen Robinson

The report does not provide sufficient information to asses this.

4.10.6.General/Catch-All Reviewer Comments

Please provide any additional thoughts or review of the material you feel important to note that is not captured by the preceding questions.

4.10.6.1. Dr. Tom Durbin

- page 5 extra page
- p. 6 2nd paragraph used to calculated ~~d~~ toxic..; final sentence "persistent" is not a well defined word here.
- p. 9 1st sentence – make it two sentences ~~As~~ Metals… emission rates. T~~t~~hese rates ; 2nd paragraph look at indentation; final paragraph look at indentation
- page 10 1st paragraph don't capitalize Air injection; last sentence goes to next page
- page 11 1st sentence Table 8 to Table 11.
- page 13 last sentence 1st paragraph – last sentence signpost?
- page 16 2nd paragraph MTBE levels using a simple regression; 3rd to last paragraph MTBE …used for TAME blends; 2nd to last paragraph end of 1st sentence; last paragraph from the National County Database;
- page 17 3rd line 12 vol. % or more or tert.. extra space
- page 19 3rd sentence winter, or ~~and~~ blends
- page 21 PAH seems like it should be PAHs throughout page and in title; 2nd paragraph end of 1st sentence; 3rd paragraph last sentence particulates and hydrocarbons also differ… and heavy-duty vehicles, ; last sentence small ~~est~~er high ~~est~~er e.g., dibenzo..
- page 22 – 1st sentence table error; last sentence structure, which
- page 23– last paragraph 1st sentence end of sentence; page 24 include reference to 2005 EPA study; 1st paragraph 2nd to last sentence … differences … are
- page 25– end of 3rd sentence
- page 31– last sentence VOC emissions are ~~is~~
- page 32– several table reference errors; 3rd paragraph reverse order of second sentence; 4th paragraph 1st sentence VOCs; last sentence in this context,
- page 38– 20% ethanol, fractions; also switch the order of the last two sentences in the final paragraph. Also, eliminate "the" before Table 34 in the last sentence.

- page 40– Table error under 2.2.3.1; last sentence …fractions are …add period at end of sentence.
- page 42– section title should be pre-2007 or MY 2006 and earlier.
- page 43– table reference error in last paragraph
- page 50– 2nd sentence gasoline ~~of~~for diesel
- page 51– 1st paragraph under section 2.6.3, end of last sentence in paragraph has extra space?
- page 52– 1st paragraph after 3.1 (evaporative?); later <source>
- page 55– under eq. 18 linearlyinterpolated
- Appendix A – p. 61 2nd paragraph 1st sentence "in the raw exhaust"; p. 62 last paragraph the end of the 1st sentence is no clear, and should have a comma after power, "; p. 63 last sentence "The ~~E~~equation.."

4.10.6.2. Dr. Allen Robinson

Compared to the other reports there were more typos, broken links, placeholders like "???" in the text, and many typos (e.g. superscripts for references and on numbers, e.g. see Table 47) in this report.

Appendix A. Dr. Tom Durbin's Supporting Documentation

A.1. Reviewer's Delivery Email (i.e., Cover Letter)

See files: *Tom Durbin Review.msg.pdf*
Tom Durbin Review Cover Letter.pdf

A.2. Reviewer's CV

See file: *Durbin CV 2013.pdf*

A.3. Reviewer's COI Statement

See file: *COI_Disclosure_Durbin(FE)_Redacted.pdf*

Appendix B. Dr. Allen Robinson's Supporting Documentation

B.1. Reviewer's Delivery Email (i.e., Cover Letter)

See files: *Allen Robinson Review (1 of 2).msg.pdf*
Allen Robinson Review (2 of 2).msg.pdf

B.2. Reviewer's CV

See file: *ALR CV Current.pdf*

B.3. Reviewer's COI Statement

See file: *COI_Disclosure_Robinson(HD)_Redacted.pdf*

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