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Interactive comment

Interactive comment on "Constraining Chemical Transport $PM_{2.5}$ Modeling Using Surface Monitor Measurements and Satellite Retrievals: Application over the San Joaquin Valley" *by* Mariel D. Friberg et al.

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Author Comments (AC) to Referee Comments (RC) 2 – Anonymous Referee 1

RC2_0. The paper provided a rigorous and detailed analysis of using satellite data (MISR, MODIS), surface observations (AERONET, $PM_{2.5}$ and aerosol speciation), and CMAQ to derive surface $PM_{2.5}$ and surface PM speciation. The novelty of this paper, as pointed by the authors, is the use of aerosol type information retrieved from

MISR research algorithm. This, however, is really not new, which is also acknowledged in the paper - past work by Liu et al. has used MSIR aerosol type already. The paper also developed several methods for data gap filling, data fusion, and reconstruction of surface $PM_{2.5}$ and total AOD from CMAQ. To this reviewer, the most interesting part is indeed the latter, as it has been vague in past studies on how $PM_{2.5}$ mass is indeed computed with CTM outputs.

AC2_0. We thank the reviewer for the encouragement and the valuable comments. All the comments have been addressed in the revised manuscript. Please see our itemized responses below.

The approach here is fundamentally different – Liu et al. used a statistical approach, whereas we present here a complementary, physical approach. The underlying model being refined here is the CTM (CMAQ) rather than a regression model. Furthermore, we use as model constraints the particle size and light-absorption information from MISR, in addition to the particle shape, in a novel manner consistent with the limitations of the data. This is now emphasized in the Introduction and Conclusions of the paper.

The paper has done an excellent job in organizing its structure and presenting the detailed analysis. The paper, however, can be further improved by acknowledging other work done in the past that used satellite observations and CTM together to improve estimate of surface $PM_{2.5}$. In various places, simplification and summary of the results (from the supplements) can make the paper more easier to read, keep the text flow smoother, improve the clarity, and ultimately enable more readability. The paper can be published after the following concerns/comments are fully addressed.

General concerns/comments:

RC2_1. The title of the paper. The work of this paper in essence is data fusion and statistical analysis by combining data from various sources. While CTM outputs are used, the satellite data here really didn't provide any constraint for improving CTM

MODELING that entails emissions, meteorology, different atmospheric processes, and data assimilation. It is recommended to add ‘outputs’ after ‘modeling’ in the tittle to avoid confusion, or change the title to emphasize the data fusion part. This paper didn’t improve any components in CTM modeling; instead, it belongs to research of “model output statistics” (MOS) to postprocess model outputs.
AC2_1. We have added the word “outputs” as recommended.

RC2_2. P2, L3. not sure what ‘a systematic and practical approach’ means here. As pointed by the first reviewer, there have been much work that combine satellite and ground-based observations already. Please see the summary paper by Hoff and Christopher (2010) prior to 2010 and many other works afterwards. Indeed, the study here is demonstrated for the days and locations that have field campaign data and fewer clouds (compared to many other regions that studied). So, further discussion of the application of the method here in other places is needed.
AC2_2. Please see the responses AC1_1, AC1_2, and AC2_0. There are fundamental differences with our approach that provide certain advantages. We have made a larger point of the differences and advantages in the revised text.

RC2_3. Overall, in what percentage spatially, the AOD values are filled based on MAIA AOD (and scaling factor based on MISR/MODIS AOD ratio)?
AC2_3. We gap-fill using results from the MODIS Multi-Angle Implementation of Atmospheric Correction advanced algorithm (MAIAC; Lyapustin et al., 2018). The MISR AOD case study retrievals had 70% or greater spatial coverage of the SJV boundary delineated in Figure 1 and AOD approximately above the 0.15 threshold. Thus, MAIAC (not MAIA) AOD was used to gap-fill between 0 to 30% of the MISR AOD scene for each case. This information is on Page 8 Line 17) in the text.

Specific concerns/comments:

RC2_4. P1, L25. This is a bit confusing. AOD is at 2 km resolution, while aerosol mass type can be retrieved at 275 m resolution? why not AOD at 275 m?
AC2_4. We have removed the phrase "2 km resolution", which referred to the CTM output.

RC2_5. P1, L30. R2 is only one of the measures for agreement. How about mean bias and RMSE?
AC2_5. We have added RMSE to the abstract. The remaining statistics are reported in Table S8.

RC2_6. P2, L26. Also emissions and parametrization schemes, especially for CTM. See Ge et al., JGR, 2017.
AC2_6. We revised the sentence as "The accuracy of the simulated fields is also affected by the accuracy of the simulated meteorology, emissions, and of the physical and chemical parameterization schemes specified in the model (Cooke et al., 1999; Tong and Mauzerall, 2006; Monks et al., 2009)" and added citations.

RC2_7. P3, L4, it is worth mentioning that early studies, while neglecting these factors (speciation and vertical profile), indeed acknowledge the importance of these factors such as in Wang and Christopher (2003). The current writing gives readers an impression that these early studies didn't recognize the importance of these factors, which in not true. These factors have been recognized since the beginning (Wang and Christopher, 2003).
AC2_7. We revised the sentence as "Early space-based $PM_{2.5}$ air quality studies directly correlated satellite-derived AOD from the MODerate resolution Imaging Spectroradiometer (MODIS) instruments and ground-level $PM_{2.5}$ concentrations acknowledged, but did not account for, particle vertical distribution, day-to-day variations,

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and/or aerosol speciation (Chu et al., 2003;Wang and Christopher, 2003;Engel-Cox et al., 2004;Chu, 2006;Gupta and Christopher, 2009;Wallace and Kanaroglou, 2007;Schaap et al., 2009;Zhang et al., 2009;Hu and Rao, 2009;Tsai et al., 2011;Hu et al., 2014)" and added citations.

RC2_8. P3, L10. It is worth mentioning that all the work cited here has inconsistence of aerosol optical properties between models and satellite retrieval algorithms. Work has been done that uses CTMs to inform aerosol types for the retrieval from satellites, which in turn improve the estimate of surface $PM_{2.5}$ from CTM. References include Drury et al. (2010, JGR), Wang et al. (2010, RSE), and van Donkelaar et al., 2013.
AC2_8. We added the sentence "Work has been done to improve estimates of surface $PM_{2.5}$ from CTM by improving the consistency of aerosol optical properties between models and satellite retrieval algorithms, as well as, using CTMs to inform satellite-retrieved aerosol types (Drury et al., 2010; Wang et al., 2010; Donkelaar et al., 2013). However, we map the MISR RA constraints on spherical light-absorbing, spherical non-absorbing, and non-spherical particles to the appropriate aerosol chemical species in the CTM, which is different from previous work." and added citations.

RC2_9. P5, L5. How long is the DISCOVR-AQ time period? In average, what are the percentage of days that MISR AOD has good spatial converge and AOD is higher than 0.15?
AC2_9. The DISCOVER-AQ SJV deployment ran from 16 January through 08 February 2013. Approximately half of the MISR retrievals met the case requirements of 70% or greater spatial coverage of the SJV boundary delineated in Figure 1 and AOD approximately above the 0.15 threshold. This information has been added to Page 6 Line 3 in the text.

RC2_10. P6, L10-20. How many layers in the vertical and in the boundary layer? What is fire emission inventory used? Is CTM outputs data saved at every hour?

AC2_10. The CMAQ domain consisted of 35 vertical layers with varying thickness extending from the surface to 50 hPa and an approximately 10 m midpoint for the lowest (surface) model layer. CMAQ outputs are saved hourly. This information has been added to the text. We used U.S. EPA 2011 NEI emissions data with 2013 updates to fire sources. The wildfire emissions used came from SMARTFIRE v2 (https://www.airfire.org/smartfire/).

RC2_11. P7, section 2.5.1. MISR-RA. How does MISR-RA AOD compare with MISR operational AOD? Does MSIR operational product offer the aerosol type retrievals? Using MISR operational product would seem more practical. It will be nice to have some justification here.

AC2_11. The current 4.4 km x 4.4 km MISR Standard Algorithm (SA) AOD product was not available at the time of the evaluation and is not available at higher resolution. The SA has greater inconsistencies in aerosol particle retrievals due to limitations in the aerosol climatology included in the algorithm (74 mixtures for the SA vs. over 700 for the RA), poorer surface-reflectance assumptions, issues with the radiometric calibration critical for aerosol-type retrievals that are corrected in the RA, details of the acceptance criteria, and the spatial resolution at which the algorithm is run. For more details, please see the series of papers by Limbacher and Kahn (2014; 2016; 2017; 2018). For particle-type retrievals, the RA performs considerably better than the SA. The information has been added to the text.

RC2_12. P11, equation 1. Does CMAQ offer concentration of Al, Si, Ca, Ti, etc? if not, please give the exact equation used in reconstructing CMAQ $PM_{2.5}$ in this research, so readers don't have to refer to the supplement often.

AC2_12. Yes, CMAQ does offer these and other dust related concentrations. The aerosol group equations used in this study are included in the supplement for brevity and are specific to CMAQ v5.0.2.

RC2_13. P11, equation 2. How are the values for negative and positive terms in right-hand side of equation obtained in this study?
AC2_13. The equation 2 terms are calculated using CMAQ and WRF outputs. These equations are discussed in detail elsewhere (Frank, 2006;Chow et al., 2015) and are referenced appropriately in our paper.

RC2_14. P12, equation 2. fRH (upper case) in equation 3, but frh (lower case) in L15
AC2_14. We revised the hygroscopic growth factor parameter to f_{rh}.

RC2_15. P12, L24. This is not correct. The extinction per unit length is called extinction coefficient, and it is inversely proportional to visibility; see details in Kessner et al., Atmospheric Environment, 2013.
AC2_15. The sentences were revised as follows:
"The ambient particle extinction as a function of height is the sum of the ambient scattering and absorption with respect to altitude (z), which are the two terms in Eq. (3). When integrated over a horizontal path, the extinction per unit length is sometimes called the visibility, typically reported in Mm-1. From Eq. 3, the dimensionless extinction AOD is obtained by multiplying the ambient particle extinction by the vertical atmospheric path height of each CMAQ layer."

RC2_16. P13, and P14; AOD gap filling using MODIS. How to scale MAIA AOD exactly? In cases where both Terra and Aqua MODIS have AOD, is it only Terra MODIS AOD used? Some details are needed here, including when the method works best and when may not work well (such as with large cloud cover).
AC2_16. We gap-fill using results from the MODIS Multi-Angle Implementation of Atmospheric Correction advanced algorithm (MAIAC; Lyapustin et al., 2018). Please

see response AC1_6, as Section 3.3 has been revised for clarity.

RC2_17. P14, L20-25. it will be good to show a scatter plot that summarizes the comparison for all days in one plot? Also, a plot showing the comparison for data filling only (e.g., in places/times that has no MISR AOD, but filled with MODIS AOD and through scaling/interpolation) can be good to show the improvement by combining both MODIS and MISR.
AC2_17. Please see Figures 3, S1, and S2. Aerosol airmass types and spatial distribution change over time. It is not clear to the authors what a scatterplot of all the days in one plot would contribute to the focus of this paper. The individual density scatter plots comparing AERONET, MISR, MAIAC, gap-filled MISR, and CMAQ are shown in Figures S1 and S2.

RC2_18. P15, L12. What happens in hours that have cloud? Daily AOD from AERONET has a clear-sky bias.
AC2_18. The AERONET clear-sky bias is a limitation of the satellite-based and AERONET AOD comparison. In the optimized dataset the pixels within the domain of study with no satellite-based retrievals rely on the fused CMAQ and ground observations. See also our response to RC1_1.

RC2_19. P15, L31 . not sure what 'sufficient' mean here?
AC2_19. We have removed the word "sufficient."

RC2_20. P15, L11. There are papers talking about diurnal variation of AOD. for example Kaufman et al. in GRL. Are the results here consistent with previous findings?
AC2_20. The context of diurnal variation of AOD in the Kaufman et al. (2000) paper is with respect to climate changes and thus compares annual aerosol measurements. The conclusion that a 10:30 AM AOD represents the diurnal average applies to

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specific location and/or scenarios. Fire events are some examples of situations where this conclusion does not apply. In our paper, we are interested in capturing diurnal variations with respect to short-term changes (please see Figures 4 and S2). Furthermore, it is difficult to compare diurnal variation conclusions from other study sites due to: (1) the unique weather pattern and pollution transport characteristic of the SJV (i.e., persistent inversion and very low PBL height), (2) differences in product version uncertainty (i.e., AERONET versions between this and earlier studies), and (3) disparity in satellite-retrieved spatial resolution (i.e., biases in earlier studies due to coarser spatial resolution).

RC2_21. equation 4. This equation is not correct. equation 3 won't give equation 4 as beta, fRH all depends on Z, and C(z) varies with Z.
AC2_21. It is correct that equation 4 depends on altitude. Therefore, we specifically use the height-stratified hygroscopic growth and specific dry extinction efficiency factors from Step 2 for equation 4 in Step 4. Equations 4 through 6 and their descriptions have been updated to make clear these are column-average dry particle concentrations.

RC2_22. for the results. It will be good to show the summary as several scatter plots respectively for $PM_{2.5}$ and speciation in all days and sites in the main manuscript. Having summary statistics (such as R, RMSE, and mean bias) in figure. Are the results or improvement by MISR statistically significant?
AC2_22. A limitation mentioned in the paper is that the study domain and timeframe did not offer a substantial quantity of suborbital observations for assessing the results statistically. Statistical power is a known issue in this study. Yet, we performed three separate statistical tests to establish as best we could the significance of the results. The comprehensive set of the various summary statistics can be found in the supplemental material.

RC2_23. P24, L5. Worthy mentioning recent studies that used VIIRS DNB to derive surface $PM_{2.5}$ at night. see Wang et al., AE, 2016; Fu et al., 2018.

AC2_23. The following sentence has been added to the diurnal sampling segment of the conclusion:

"Future research assessing diurnal sampling could benefit from the inclusion of Visible Infrared Imaging Radiometer Suite (VIIRS) instrument datasets, such as daylight-retrieved AOD (Jackson et al., 2013) and Day/Night Band as an estimate of $PM_{2.5}$ surface change (Wang et al., 2016)."