



# WRF-Chem simulation of aerosol seasonal variability in the San Joaquin Valley

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18 Highlights:

19 1. The WRF-Chem simulation successfully captures aerosol variations in cold season in the San  
20 Joaquin Valley (SJV), but has poor performance in warm season.

21 2. High resolution model simulation can better resolve inhomogeneous distribution of  
22 anthropogenic emissions in urban areas, resulting in better simulation of aerosols in cold  
23 season in the SJV.

24 3. Observations show that dust is a major component of aerosols in the SJV, especially in warm  
25 season. Poor performance of the WRF-Chem model in warm season in the SJV is mainly due  
26 to misrepresentation of dust emission and vertical mixing.



27 **Abstract**

28 WRF-Chem simulations of aerosol seasonal variability in the San Joaquin Valley (SJV),  
29 California are evaluated by satellite and in-situ observations. Results show that the WRF-Chem  
30 model successfully captures the distribution, magnitude and variation of SJV aerosols in cold  
31 season. However, the aerosols are not well represented in warm season. Aerosol simulations in  
32 urban areas during the cold season are sensitive to model horizontal resolution, with better  
33 simulations at 4 km resolution than at 20 km resolution, mainly due to inhomogeneous  
34 distribution of anthropogenic emissions. In rural areas, the model sensitivity to grid size is rather  
35 small. Our observational analysis show that dust is a primary contributor to aerosols in the SJV,  
36 especially in the warm season. Aerosol simulations in the warm season are sensitive to  
37 parameterization of dust emission in the WRF-Chem model. The GOCART (Goddard Global  
38 Ozone Chemistry Aerosol Radiation and Transport) dust scheme produces very little dust in the  
39 SJV while the DUSTTRAN (DUST TRANsport model) scheme overestimates dust emission.  
40 Vertical mixing of aerosols is not adequately represented in the model comparing to CALIPSO  
41 (Cloud-Aerosol Lidar and Infrared pathfinder Satellite Observation) aerosol extinction profiles.  
42 Improved representation of dust emission and vertical mixing are needed for better simulations  
43 of aerosols in warm season in the SJV. Aerosols generated by wild fires are not captured in the  
44 simulations with climatological fire emissions, underscoring the need of fire emission  
45 observations for operational usage.

46



47 **1. Introduction**

48 The San Joaquin Valley (SJV) in the southern portion of the California Central Valley is  
49 surrounded by coastal mountain range to the west and the Sierra Nevada range to the east. With  
50 cool wet winters and hot dry summers, the unique natural environment makes SJV one of the  
51 most productive agricultural regions in the world (SJV APCD, 2012 and references therein).  
52 However, SJV is also one of the most polluted regions in US due to its unique geographical  
53 location. Frequent stagnant weather systems are conducive to air pollution formation while the  
54 surrounding mountains block air flow and trap pollutions. Large seasonal and spatial variations  
55 of aerosols are observed in the SJV. Although significant progress at improving local air quality  
56 in past decades has been made through strong emission controls, the PM2.5 (particulate matter  
57 with diameter  $\leq 2.5 \mu\text{m}$ ) concentrations in the SJV remain well above the national ambient air  
58 quality standards (NAAQS) threshold of  $12 \mu\text{g m}^{-3}$  on annual basis and  $35 \mu\text{g m}^{-3}$  on daily basis,  
59 mainly during cold season. Improved understanding of the aerosol variabilities and their impact  
60 are needed to provide further guidance for emission control strategies in the SJV.

61 Air quality models are a critical tool to understand the formation and evolution of  
62 aerosols and their impacts on air quality and climate. However, it is still quite a challenge to  
63 accurately simulate aerosol properties (Fast et al., 2014). Fast et al. (2014) summarized the  
64 factors contributing to the errors in region-scale modeling of aerosol properties, including 1)  
65 emission sources; 2) meteorological parameterizations; 3) representation of aerosol chemistry; 4)  
66 limited understanding of the formation processes of secondary organic aerosol (SOA); 5) spatial  
67 resolution; and 6) boundary conditions.

68 As one of the advanced regional air quality models, the Weather Research and  
69 Forecasting model with Chemistry (WRF-Chem) has been widely used to study aerosols and



70 their impacts on regional air quality and climate (e.g., Misenis and Zhang, 2010; Zhang et al.,  
71 2010; Zhao et al., 2010; 2013; 2014; Wu et al., 2011a, 2011b, 2013; Fast et al., 2012, 2014;  
72 Scarino et al., 2014; Tessum et al., 2015; Campbell et al., 2016; Hu et al., 2016). Fast et al.  
73 (2014) showed that WRF-Chem simulations at 4 km horizontal resolution captured the observed  
74 meteorology and boundary layer structure over California in May and June of 2010. The model  
75 reasonably simulated the spatial and temporal variation of aerosols. Aerosol simulations by  
76 WRF-Chem are usually sensitive to both local emission and long-range transport of aerosols  
77 from the boundary conditions provided by the global Model for Ozone and Related chemical  
78 Tracers, version 4 (MOZART-4). Similarly, in a one-year simulation at 12 km horizontal  
79 resolution, Zhao et al. (2013) showed that the WRF-Chem model represented the observed  
80 seasonal and spatial variation of surface particulate matter (PM) concentration over California.  
81 However, underestimation of elemental carbon (EC) and organic matter were noticed in the  
82 model simulation, with no sensitivity to horizontal model resolution.

83 In this study, we extend the studies by Fast et al. (2014) and Zhao et al. (2013) by  
84 focusing on simulating aerosol seasonal variability in the most polluted SJV in California. This  
85 paper serves as the first step for future investigation of the aerosol impact on regional climate  
86 and the water cycle in California. Previous studies have demonstrated that aerosols are better  
87 simulated at higher model resolution (Misenis and Zhang et al., 2010; Qian et al., 2010; Stroud  
88 et al., 2011; Fountoukis et al., 2013). However, most regional climate studies are still limited to  
89 coarse model resolutions (on the order of 10 km) due to the availability of computational  
90 resources. This study will investigate the sensitivity of aerosol simulations to horizontal  
91 resolution and identify suitable model resolution for regional climate study in the SJV.



92 Another application of air quality modeling is to provide initial *a priori* input for remote  
93 sensing retrievals. The WRF-Chem model has been proposed as an input for retrieval algorithms  
94 to be developed for the recently-selected NASA (National Aeronautics and Space  
95 Administration) MAIA (Multi-Angle Imager for Aerosols) mission, which aims to map PM  
96 component concentrations in major urban areas (including the SJV). A reasonable initial estimate  
97 of aerosol speciation from WRF-Chem is critical to ensure the retrieval speed and quality.  
98 Considering the sensitivity of WRF-Chem simulations to various factors such as initial and  
99 boundary conditions, model parameterizations and emission sources (e.g., Wu and Petty, 2010;  
100 Zhao et al., 2010, 2013; Wu et al., 2011a, 2015; Fast et al., 2014; Campbell et al., 2016;  
101 Morabito et al., 2016), careful model evaluations are needed before the simulations can be used  
102 for remote sensing retrievals. This study also serves as an evaluation for WRF-Chem aerosol  
103 simulations in the SJV, which will provide important information for utilizing WRF-Chem for  
104 MAIA retrieval algorithms, critical to the success of the MAIA mission.

105 This paper is organized as follows. Section 2 describes observational datasets used for  
106 model evaluation. Section 3 provides the description of the WRF-Chem model and experiment  
107 setup. Model simulations and their comparison with observations are discussed in section 4.  
108 Section 5 presents the conclusions.

## 109 **2. Observations**

### 110 **2.1 Aerosol Optical Depth**

111 Aerosol optical depth (AOD) is a measure of column-integrated light extinction by  
112 aerosols and a proxy for total aerosol loading in the atmospheric column. The Aerosol Robotic  
113 Network (AERONET) provides ground measurements of AOD every 15 minutes during daytime  
114 (Holben et al., 1998), with an accuracy of  $\pm 0.01$  (Eck et al., 1999; Holben et al., 2001). The



115 monthly level 2.0 product with cloud screening and quality control is used in this study.  
116 AERONET AOD is interpolated to  $0.55\mu\text{m}$  using the Ångström exponent. In the SJV, only one  
117 AERONET station at Fresno, CA has regular observations throughout the California water year  
118 2013 (WY2013; i.e., from October 2012 to September 2013).

119 The Multiangle Imaging Spectroradiometer (MISR) (Diner et al., 1998) instrument  
120 onboard the Terra satellite has provided global coverage of AOD once a week since December  
121 1999. The standard MISR retrieval algorithm provides AOD observations at 17.6 km resolution  
122 using  $16 \times 16$  pixels of 1.1 km each. About 70% of MISR AOD retrievals are within 20% of the  
123 paired AERONET AOD, and about 50% of MISR AOD falls within 10% of the AERONET  
124 AOD, except in the dusty and hybrid (smoke+dust) sites (Kahn et al., 2010). We use version 22  
125 of Level 3 monthly AOD product at  $0.5^\circ$  resolution in this study.

## 126 **2.2 Surface Mass Concentration**

127 Surface PM2.5 speciation and PM10 (particulate matter with diameter  $\leq 10 \mu\text{m}$ ) data are  
128 routinely collected by two national chemical speciation monitoring networks: Interagency  
129 Monitoring of Protected Visual Environments (IMPROVE) and the PM2.5 National Chemical  
130 Speciation Network (CSN) operated by Environmental Protection Agency (EPA) (Hand et al.  
131 2011; Solomon et al., 2014). IMPROVE collects 24-h aerosol speciation every third day at  
132 mostly rural sites since 1988. The same frequency of aerosol speciation data was collected at  
133 EPA CSN sites in urban and suburban areas since 2000. Selected IMPROVE and EPA CSN sites  
134 used in this study are shown in Figure 1a.

## 135 **2.3 Aerosol Extinction Profile**

136 The aerosol extinction coefficient profile reflects the attenuation of the light passing  
137 through the atmosphere due to the scattering and absorption by aerosol particles as a function of



138 range. Version 3 Level 2 532 nm aerosol extinction profiles derived from Cloud-Aerosol Lidar  
139 with Orthogonal Polarization (CALIOP) backscatter profiles collected onboard the Cloud-  
140 Aerosol Lidar and Infrared pathfinder Satellite Observation (CALIPSO) satellite are used (Omar  
141 et al., 2009; Young and Vaughan, 2009). Seasonal mean profiles are derived for WY2013 based  
142 on the methodology outlined in Campbell et al. (2012), whereby quality-assurance protocols are  
143 applied to individual profiles before aggregating and averaging the data. We highlight that no  
144 individual profiles are included in the averages if the CALIOP Level 2 retrieval failed to resolve  
145 any extinction within the column, a potential biasing issue that has recently been described by  
146 Toth et al. (2016). Level 2 532 nm aerosol extinction is speciated, with algorithms resolving  
147 aerosol type present for clean marine, dust, polluted continental, clean continental, polluted dust  
148 and smoke. Dust and polluted dust are specifically distinguished in the averages applied below  
149 for their contribution to total extinction and the vertical profile seasonally in the SJV.

#### 150 **2.4 Equivalent Potential Temperature**

151 Equivalent potential temperature ( $\theta_e$ ) is a quantity relevant to the stability of the air. The  
152  $\theta_e$  profiles used in this study are derived from temperature and moisture profiles observed by AIRS  
153 (Atmospheric Infrared Sounder) onboard the Aqua satellite (Susskind et al., 2003; Divakarla et al.,  
154 2006). AIRS has provided global coverage of the tropospheric atmosphere at approximately 01:30  
155 and 13:30 local time since 2002. AIRS retrievals have root-mean-squared (RMS) difference of  $\sim 1$   
156 K for temperature and  $\sim 15\%$  for water vapor (Divakarla et al., 2006). Level 3 monthly temperature  
157 and moisture retrievals (version 6) at  $1^\circ \times 1^\circ$  grid are used in this study.

#### 158 **3. Model Description and Experiment Setup**

159 The WRF-Chem model Version 3.5.1 (Grell et al., 2005) updated by Pacific Northwest  
160 National Laboratory (PNNL) is used in this study (Zhao et al., 2014). Similar to the chemical



161 parameterizations used in the Zhao et al. (2014), this study uses the CBM-Z (carbon bond  
162 mechanism) photochemical mechanism coupled with the four-sectional-bin MOSAIC (Model for  
163 Simulating Aerosol Interactions and Chemistry) aerosol scheme as the chemical driver. The major  
164 components of aerosols (nitrate, ammonium, EC, organic carbon, sulfate, sea salt, dust, etc.) as  
165 well as their physical and chemical processes are simulated in the model. More details of the  
166 chemical settings used in this study can be found in Zhao et al. (2014) and references therein.

167 The model simulations start on 1 September 2012 and run continuously for 13 months.  
168 With the first month as spin-up, our analysis focuses on WY2013 from October 2012 to September  
169 2013. The model is configured with 40 vertical levels and a model top at 50 hPa. The model center  
170 is placed at 38°N, 121°W, with 250 x 350 grids at 4 km horizontal resolution (referred to as “4km”  
171 hereafter; Table 1), covering California and the surrounding area. To test the sensitivity of aerosol  
172 simulations on horizontal resolution, one simulation with the same model settings and domain  
173 coverage is conducted at 20 km horizontal resolution (referred to as “20km” hereafter).

174 The physics parameterizations used in the simulations include the Morrison double-  
175 moment microphysics scheme (Morrison et al., 2009), Rapid Radiative Transfer Model for General  
176 circulation model (RRTMG) shortwave and longwave radiation schemes (Iacono et al., 2008),  
177 Yonsei University (YSU) planetary boundary layer scheme (Hong et al., 2006), Community Land  
178 Model (CLM) Version 4 land surface scheme (Lawrence et al., 2011). Grell 3D ensemble cumulus  
179 scheme (Grell and Devenyi, 2002) is used in the 20km simulation while the 4km simulation does  
180 not use cumulus parameterization. The ERA-Interim reanalysis data (Dee et al., 2011) provides  
181 meteorological initial and boundary conditions for the WRF-Chem. The MOZART-4 global  
182 chemical transport model (Emmons et al., 2010) is used for the chemical initial and boundary  
183 conditions. Fast et al. (2014) found that the MOZART-4 model has overestimation of aerosols in



184 the free troposphere over California. Following Fast et al. (2014), the chemical initial and boundary  
185 conditions from MOZART-4 are divided by two in all simulations.

186 Anthropogenic emissions are provided by US EPA 2005 National Emissions Inventory  
187 (NEI05), with area-type emissions on a structured 4-km grid and point type emissions at latitude  
188 and longitude locations (US EPA, 2010). Anthropogenic emissions are updated every hour to  
189 account for diurnal variability, while its seasonal variation is not considered in the simulations.

190 Biogenic emissions are calculated online using the Model of Emissions of Gases and Aerosols  
191 from Nature (MEGAN) model (Guenther et al., 2006). Biomass burning emissions are obtained  
192 from the Global Fire Emissions Database, version 2.1 with eight-day temporal resolution  
193 (Randerson et al., 2007). Sea salt emissions use the PNNL-updated sea salt emission scheme that  
194 includes the correction of particles with radius less than 0.2  $\mu\text{m}$  (Gong et al., 2003) and dependence  
195 on sea surface temperature (Jaeglé et al., 2011).

196 Following Zhao et al. (2013), dust emission is computed from the GOCART (Goddard  
197 Global Ozone Chemistry Aerosol Radiation and Transport) dust scheme (Ginoux et al., 2001) in  
198 the 20km and 4km simulations. As shown later, a significant amount of dust is observed in the  
199 SJV while the GOCART dust scheme produces little dust. One sensitivity experiment at 4 km  
200 horizontal resolution (referred to as “4km\_D2” hereafter) is conducted by switching dust emission  
201 scheme to the DUST TRANsport model (DUSTTRAN) scheme (Shaw et al., 2008). Detailed  
202 descriptions of the two dust emission schemes can be found in Zhao et al. (2010).

#### 203 **4. Model Simulation Results**

204 WRF-Chem model simulation results and their evaluations are in this section. We start the  
205 discussions with a focus on the polluted urban areas. Because aerosols properties and model  
206 performance are similar at all urban sites, our discussion is focused on the results at Fresno, CA



207 while those at other urban sites are provided in supplementary materials. Model simulations in  
208 rural areas are presented in the last subsection.

209 **4.1 Sensitivity to Horizontal Resolution**

210 Figure 1 shows daily mean anthropogenic PM2.5 emission rates used in the 20km and 4km  
211 simulations, respectively. Although both of the PM2.5 emission rates are derived from the 4 km  
212 NEI05 dataset, localized high emission rates with sharp gradients are evident at urban areas in the  
213 4km simulation (Figure 1b). The 20km simulation has lower emission rates with smoother features  
214 due to the averaging process (Figure 1a).

215 Consistent with the emission rate differences, higher AOD is simulated at 4km than 20km,  
216 mainly in cold season (OND and JFM in Figure 2). The 4km simulation reproduces the distribution  
217 and magnitude of AOD observed by MISR well in the cold season. The AOD difference between  
218 20km and 4km is small in the warm season (AMJ and JAS in Figure 2). Both the 20km and 4km  
219 runs underestimate AOD in the warm season compared with MISR. Model performance identified  
220 in Figure 2, including the sensitivity to horizontal resolution in cold season and underestimation  
221 of AOD in warm season, are further confirmed by comparing to AERONET observations at Fresno,  
222 CA (Figure 3). In cold season at Fresno, the AOD in the 20km simulation is 23% lower than the  
223 AOD in the 4km simulation. The different model sensitivities to horizontal resolution from the  
224 cold to the warm season suggest that the dominant aerosol sources are different through the two  
225 seasons. We will elaborate upon the aerosol composition in the following section. AERONET  
226 shows small seasonal variation of AOD in the SJV, which is not well represented in the 20km and  
227 4km simulations (Figure 2 and 3).

228 Aside from AOD, significant seasonal variability of PM2.5 is observed in the SJV urban  
229 areas (Figure 4a and Supplementary Figure 1a and 2a). PM2.5 at Fresno peaks in January (26.18



230  $\mu\text{g m}^{-3}$ ) and has minimum of  $7.03 \mu\text{g m}^{-3}$  in June, with an annual nonattainment value of  $12.64 \mu\text{g}$   
231  $\text{m}^{-3}$  in total (Figure 4a). All WRF-Chem simulations successfully capture the seasonal variability  
232 of PM2.5 observed in the SJV.

233 In the cold season, the 4km simulation overestimates PM2.5 by 27% while the 20km  
234 simulation exhibits a low bias of 19% compared with IMPROVE observations at Fresno (Table 2).  
235 High PM2.5 concentrations are primarily nitrate. Both simulations produce seasonal variability of  
236 nitrate, but with high biases of 17% in 20km and 75% in 4km in the cold season (Figure 4c). It  
237 suggests that the NEI05 dataset may have a high bias in nitrate emissions, which was also found  
238 in Texas (Kim et al., 2011). OC, the second largest contributor of cold season PM2.5 in the SJV,  
239 is significantly underestimated by 76% in the 20km simulation (Figure 4f). The 4km simulation  
240 produces more OC than the 20km simulation, but it is still lower than IMPROVE by 46%. Fast et  
241 al. (2014) suggested that the low bias in the WRF-Chem simulation is primarily due to incomplete  
242 understanding of SOA processes.

243 Significant underestimation of EC and sulfate in the cold season are also shown in the  
244 20km simulation, while the 4km simulation exhibits good agreement with IMPROVE (Figure 4d  
245 and 4e). Sulfate in both simulations exhibits a low bias of ~45% in the warm season. Low bias of  
246 simulated sulfate, with a failure of capturing the peaks during late afternoon, was also shown at  
247 Bakersfield in Fast et al. (2014). It suggests that improvement in understanding the photochemical  
248 processes involving sulfate is needed to reproduce seasonal variability of sulfate in the SJV. The  
249 4km simulation of PM10 has good agreement with IMPROVE in winter (December, January and  
250 February), but a large low bias is found in other months (Figure 4b). The 20km simulation  
251 underestimates PM10 throughout WY2013.



252 Overall, the 4km simulation produce higher AOD and surface PM than the 20km  
253 simulation in urban areas of the SJV, especially in the cold season. The 4km simulation has better  
254 agreement with satellite and surface observations than the 20km simulation. The 4km simulation  
255 captures seasonal variability of PM2.5 and its speciation. However, significant underestimation of  
256 AOD and PM10 are shown during the warm season in both 4km and 20 km simulations. The  
257 underestimation also exists in a sensitivity experiment initialized in April (not shown). The  
258 relatively good performance in simulating PM2.5 but PM10 suggests that coarse aerosol particle  
259 mass (CM;  $10 \mu\text{m} \geq$  particulate matter with diameter  $> 2.5 \mu\text{m}$ ), mainly dust in the SJV, is not  
260 represented well in the simulations. The impact of dust parameterizations is investigated in the  
261 4km\_D2 experiment.

262 **4.2 Sensitivity to Dust Scheme**

263 Limited amounts of PM2.5\_dust (dust with diameter  $\leq 2.5 \mu\text{m}$ ) are observed in the SJV  
264 cold season, with a minimum in December (Figure 5c). The amount of PM2.5\_dust increases in  
265 the warm season, with a peak in September. The 4km simulation produces comparable PM2.5\_dust  
266 to IMPROVE in the winter, but almost no dust in other months. The 4km\_D2 simulation represents  
267 well the magnitude of PM2.5\_dust in cold season. However, too much PM2.5\_dust is simulated  
268 in warm season, resulting in an overestimation of PM2.5 by 52% (Figure 5b and Table 2). Both  
269 the 4km and 4km\_D2 simulations capture seasonal variability of PM2.5, but not for PM10 (Figure  
270 5a). The magnitude of PM10 in the 4km\_D2 is larger than the 4km simulation. PM10 in the  
271 4km\_D2 is overestimated in AMJ but underestimated in JAS, leading to comparable season mean  
272 with IMPROVE observations.

273 On the relative contribution of different aerosol species, IMPROVE observations at Fresno  
274 show that nitrate is the primary contributor (32.3%) to PM2.5 while only 5.3% of PM2.5 is dust



275 in the cold season (panel 1 of Figure 6). Both 4km and 4km\_D2 roughly reproduce the relative  
276 contributions to PM2.5 in the cold season, with an overestimation of nitrate and underestimation  
277 of OC found in Figure 4. Relative contributions of dust to PM2.5 are better simulated in 4km\_D2  
278 than in 4km. IMPROVE shows that 46.6% of PM10 is in the cold season (panel 2 of Figure 6).  
279 Both 4km (6.3%) and 4km\_D2 (20.6%) underestimate the contribution of CM to PM10. In the  
280 warm season, dust (24.6%) becomes the primary contributor to PM2.5 while the contribution from  
281 nitrate decreases to 9.9% as observed by IMPROVE (panel 3 of Figure 6). Almost no PM2.5\_dust  
282 is simulated in 4km while too much PM2.5\_dust is produced in 4km\_D2 in the warm season. The  
283 relative contribution of CM to PM10 is too small (27.6%) in 4km while 4km\_D2 has better relative  
284 contribution of 66.3% comparing to IMPROVE observed 75.8% (panel 4 of Figure 6).

285 AOD simulations are improved in the 4km\_D2 experiment (Figure 7), with better  
286 agreement with MISR (Figure 2). AOD in 4km\_D2 is comparable to observations in AMJ, but still  
287 underestimated in JAS. Consistent with AOD, the vertical distribution of aerosol extinction is  
288 reasonably simulated in cold season in the WRF-Chem simulations while large discrepancies are  
289 shown in warm season (Figure 8). As observed by CALIOP at 532 nm, aerosols are mainly  
290 confined below 1 km above the surface in the cold season. Model simulations reasonably capture  
291 the vertical distribution of aerosol extinction observed by CALIOP, with low biases in the  
292 boundary layer and high biases in the free atmosphere. Similar discrepancy between the model  
293 simulations and CALIOP is shown in other studies (Wu et al., 2011a; Hu et al., 2016). The  
294 difference between 4km and 4km\_D2 is small in cold season.

295 Dust in the boundary layer is a primary factor contributing to aerosol extinction in the SJV,  
296 as illustrated by the differences between the bulk seasonal CALIOP mean profile and those  
297 excluding the contributions of the dust and polluted dust species (CALIOP\_nodust) profiles



298 (Figure 8). The simulated aerosol extinctions fall between the two in all seasons, suggesting  
299 relatively good performance of simulating aerosols except for dust. Although a small portion of  
300 PM2.5 is dust in the cold season, dust contributes to about 50% of total aerosol extinction (Figure  
301 8a and 8b). A predominate portion of aerosol extinction in the boundary layer is contributed to by  
302 dust in the warm season (Figure 8c and 8d). There, the 4km\_D2 simulation produces higher aerosol  
303 extinction in the boundary layer than the 4km simulation, though it is still lower than CALIOP.

304 Overall, poor simulations of dust play the dominant role in the bias of aerosols, especially  
305 in warm season. Both the GOCART and DUSTTRAN dust emission schemes used in this study  
306 have problems in reproducing dust emission in the SJV, with underestimation in GOCART and  
307 overestimation in DUSTTRAN (Figure 5c). Improvement on dust emission is required for correctly  
308 simulating seasonal variability of aerosols in the SJV.

### 309 **4.3 The Role of Meteorology**

310 In the warm season, more aerosols are observed at higher altitude than during the cold  
311 season (Figure 8). A well-mixed layer of aerosols is observed below 1.5 km in AMJ (Figure 8c),  
312 consistent with the large instability below 1.5 km observed by AIRS (Figure 9c). Both simulations  
313 fail to capture this mixed layer of aerosols (Figure 8c) due to weak vertical mixing as evidenced  
314 by relatively small instability in the simulations (Figure 9c). Aerosol extinction gradually  
315 decreases with height in the simulations (Figure 8c). Similar biases of aerosol and instability in the  
316 boundary layer are also shown in JAS (Figure 8d and 9d). Weak instability in the simulation, which  
317 limits vertical mixing of aerosols, likely enhances the low bias of JAS AOD (Figure 7). Although  
318 the 4km\_D2 experiment produces comparable AOD and surface mass in AMJ (Figure 5 and Figure  
319 7), the vertical distribution of aerosols is not well represented (Figure 8). The comparable AOD in  
320 4km\_D2 results from the low bias in the boundary layer and high bias in the free atmosphere. The



321 high bias in the free atmosphere suggests that the low bias in AOD are not due to the halved  
322 chemical boundary conditions from MOZART-4. The stability biases in cold season are relatively  
323 small (Figure 9a and 9b), consistent with good performance of aerosol simulation in the cold  
324 season. These results highlight that the vertical mixing of dust must be correctly represented in  
325 order to resolve the aerosol extinction profile correctly. Improved simulation of boundary layer  
326 physics and dynamics during the warm season in the SJV warrants future investigation.

#### 327 **4.4 Results in Rural Areas**

328 In general, low values of PM concentration are observed in the rural areas, Pinnacles and  
329 Kaiser (Figure 10 and 11). The rural areas share some similar model performance with the urban  
330 areas, such as the overestimation of nitrate, reasonable simulation of EC, good representation of  
331 sulfate in cold season and underestimation of sulfate in warm season. However, the sensitivity to  
332 model resolution is not significant. It suggests that high model resolution is particularly important  
333 for heavily polluted areas due to the inhomogeneity of emission sources, but less important for  
334 relatively lightly polluted areas.

335 In late July/early August, MODIS (Moderate Resolution Imaging Spectroradiometer) fire  
336 data (not shown) observed active wild fires close to Kaiser, which resulted in high concentration  
337 of aerosols at Kaiser (Figure 11). Our model simulations with climatological fire emissions fail to  
338 reproduce these fire events. Based on fire locations from satellite observations, Wu et al. (2011a)  
339 has demonstrated that the WRF-Chem model can capture aerosols distributions from wild fires  
340 over South America. Campbell et al. (2016) further described the difficulties in both constraining  
341 total aerosol mass from operational satellite fire observations and the time necessary within the  
342 model for diffusion within the near-surface layers to render both reasonable AOD and vertical



343 profiles of aerosol extinction. For operational application of the WRF-Chem model in MAIA  
344 retrievals, the observations of fire events need to be considered.

345 **5. Summary**

346 The WRF-Chem model is applied to simulate seasonal variability of aerosols in WY2013  
347 (water year 2013) in the SJV (San Joaquin Valley). Model simulations are evaluated using satellite  
348 and in-situ observations. In general, the model simulations at 4 km resolution reproduce the spatial  
349 and temporal variations of aerosols in cold season, when aerosols are mainly contributed by  
350 anthropogenic emissions in the SJV. The magnitude of simulated aerosols in the cold season,  
351 especially in the urban areas, is sensitive to model horizontal resolution. The 4km simulation has  
352 comparable magnitude to the observations while the 20km simulation underestimates aerosols.  
353 The differences of aerosol simulations between different model resolutions are mainly due to the  
354 difference in aerosol emissions. Emissions at higher resolution can better resolve the  
355 inhomogeneity of anthropogenic emissions in the SJV than at lower resolution. The sensitivity to  
356 horizontal resolution is small in the rural areas and in warm season, when the contribution of  
357 anthropogenic emissions is small.

358 Previous studies in the SJV are mainly focused on PM2.5 (particulate matter with diameter  
359  $\leq 2.5 \mu\text{m}$ ) and during cold season (e.g. Chow et al., 2006; Herner et al., 2006; Pun et al., 2009;  
360 Ying and Kleeman, 2009; Zhang et al., 2010; Chen et al., 2014; Hasheminassab et al., 2014; Kelly  
361 et al., 2014; Baker et al., 2015; Brown et al., 2016). CALIOP (Cloud-Aerosol Lidar with  
362 Orthogonal Polarization) and IMPROVE (Interagency Monitoring of Protected Visual  
363 Environments) observations show that dust is a primary contributor to aerosols in the SJV in warm  
364 season. Dust contributes 24.6% to PM2.5 while more than 75.8% to PM10 (particulate matter with  
365 diameter  $\leq 10 \mu\text{m}$ ) in warm season. For all seasons, the major component of aerosol extinction in



366 the boundary layer is dust as observed by CALIOP, consistent with Kassianov et al. (2012). For a  
367 complete understanding of aerosol impact on air quality and regional climate, the full spectrum of  
368 aerosols should be considered during all seasons.

369 All the model simulations fail to capture aerosol distribution and variability in the SJV  
370 warm season, largely due to the misrepresentation of dust emission and vertical mixing. The  
371 GOCART (Goddard Global Ozone Chemistry Aerosol Radiation and Transport) dust emission  
372 scheme significant underestimates dust while the DUSTTRAN (DUST TRANsport model) scheme  
373 may overestimate dust emission in the SJV. Along with the bias in dust emissions, our simulations  
374 produce weak atmospheric instability in warm season, leading to weak vertical mixing. Improved  
375 dust emission and better simulations of boundary layer properties are needed for correct simulation  
376 of aerosols in warm season in the SJV.

377 Other biases are also identified in the model simulations. Nitrate in the cold season is  
378 overestimated in the model, possibly due to the overestimation of emissions. Incomplete  
379 understanding of SOA (secondary organic aerosol) could contribute to the underestimation of OC  
380 (organic carbon). Underestimation of sulfate in the warm season may be due to incorrect  
381 photochemical processes of sulfate in the model. Aerosols from wild fires are not captured in the  
382 simulations with climatological fire emissions. Further investigations are needed to improve model  
383 simulations in the SJV for both scientific and operational applications. The evaluation framework  
384 used in this study can be used to other polluted regions to ensure that aerosols are simulated  
385 correctly for the right reasons.

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611 **List of Table**

612 Table 1. Experiment description

Experiment ID	Experiment description
20km	Simulation with the GOCART dust scheme at 20 km horizontal resolution.
4km	Same as 20km, but at 4 km horizontal resolution.
4km_D2	Same as 4km, but with the DUSTTRAN dust scheme.

613



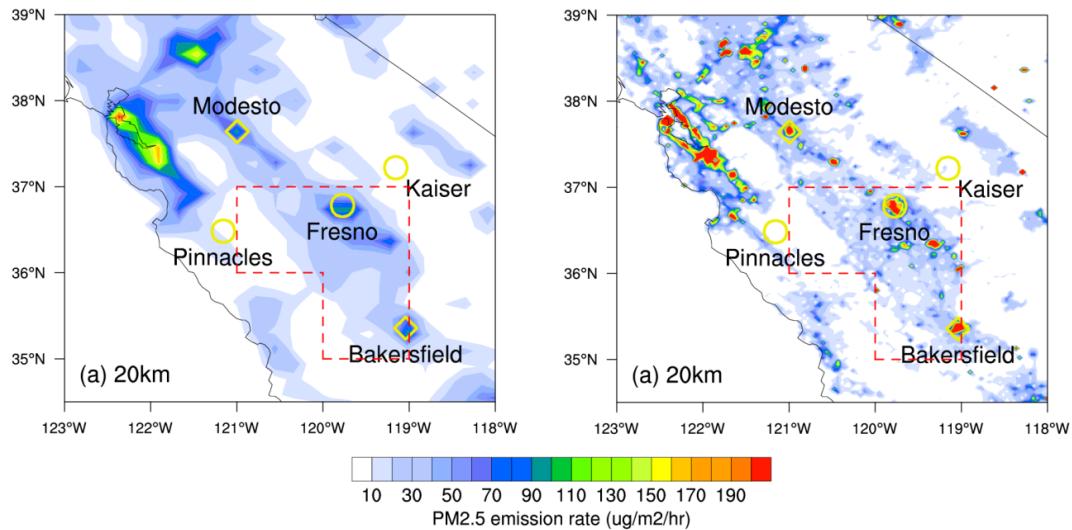
614 Table 2. Surface aerosol mass ( $\mu\text{g m}^{-3}$ ) for different species at Fresno, CA

Species	Cold season				Warm season			
	IMPROVE	20km	4km	4km_D2	IMPROVE	20km	4km	4km_D2
PM2.5	16.84	13.71	21.38	22.48	8.44	4.91	6.29	12.85
PM2.5_NO <sub>3</sub>	5.43	6.36	9.54	9.22	0.84	0.55	0.69	0.79
PM2.5_OC	3.85	0.92	2.07	2.07	1.76	0.49	0.87	0.87
PM2.5_EC	1.08	0.52	1.12	1.13	0.32	0.27	0.49	0.49
PM2.5_SO <sub>4</sub>	0.87	0.53	0.82	0.81	1.04	0.54	0.61	0.60
PM2.5_dust	0.90	0.11	0.11	1.65	2.08	0.04	0.03	6.49
PM10	31.55	14.93	22.81	28.32	34.82	7.08	8.69	38.12

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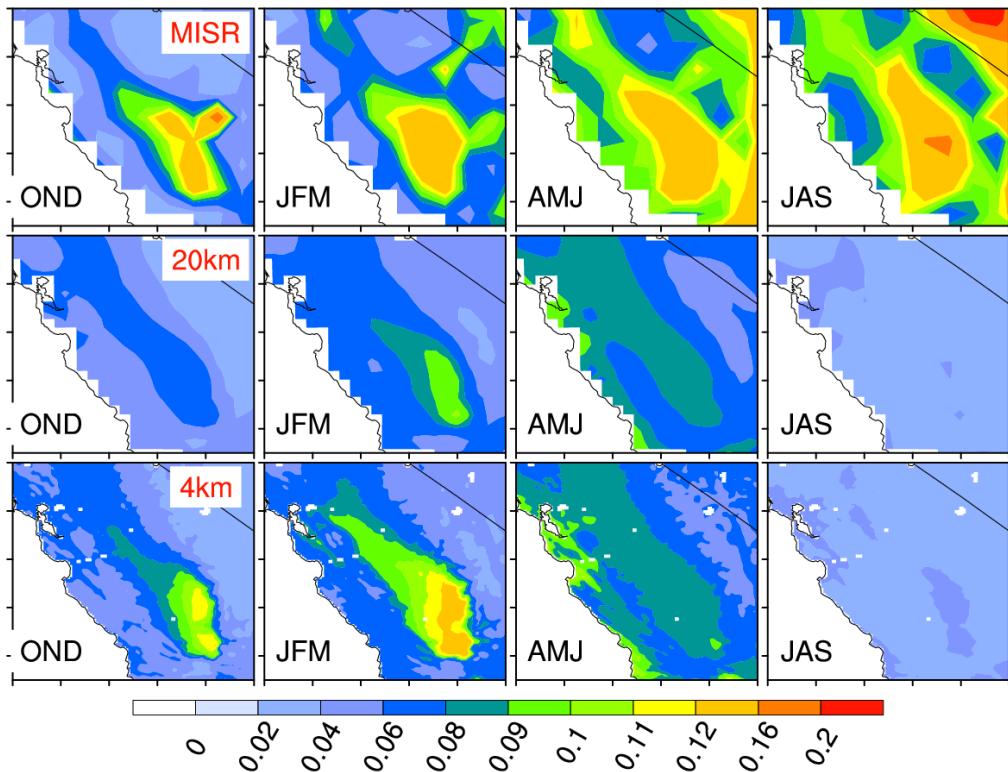


616 **List of Figures**



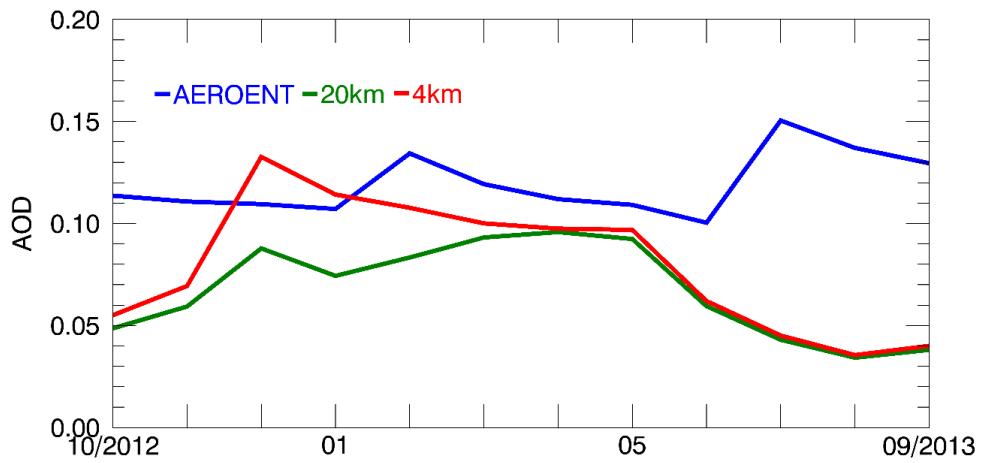
617

618 Figure 1. Daily mean anthropogenic PM2.5 emission rate ( $\mu\text{g m}^{-2} \text{s}^{-1}$ ) at (a) 20km and (b) 4km  
619 simulation. Red dashed lines in Figure 1a represent the region used for domain averages in Figure  
620 8 and 9. Yellow circle: IMPROVE site; yellow diamond: EPA CSN site. Three urban sites: Fresno,  
621 Bakersfield and Modesto; two rural sites: Pinnacles and Kaiser.



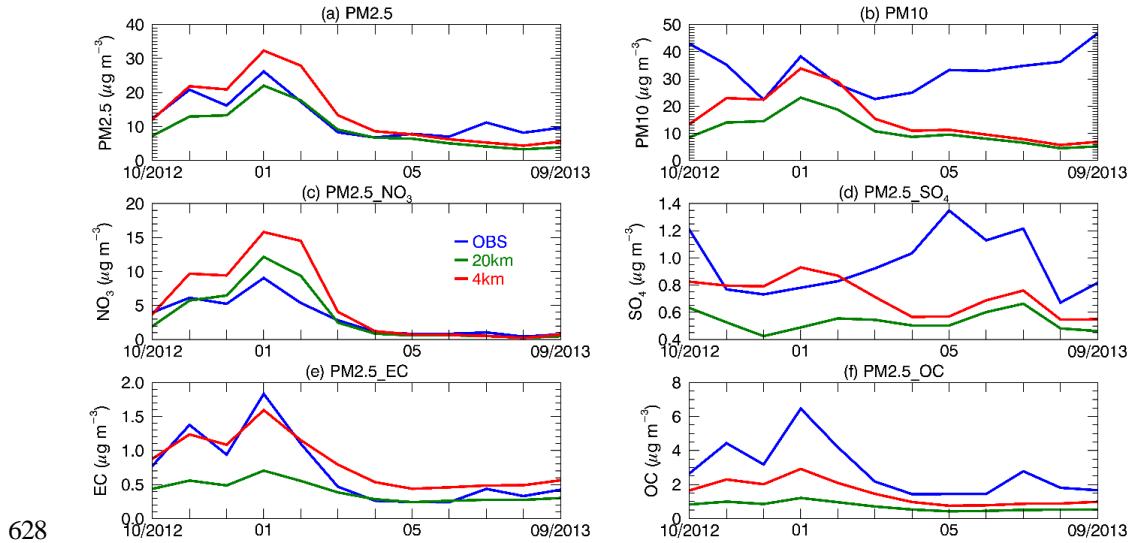
622

623 Figure 2. Spatial distribution of seasonal mean 550 nm AOD from MISR and the WRF-Chem  
624 (20km and 4km) simulations in WY2013. OND: October, November and December; JFM: January,  
625 February and March; AMJ: April, May and June; JAS: July, August and September.

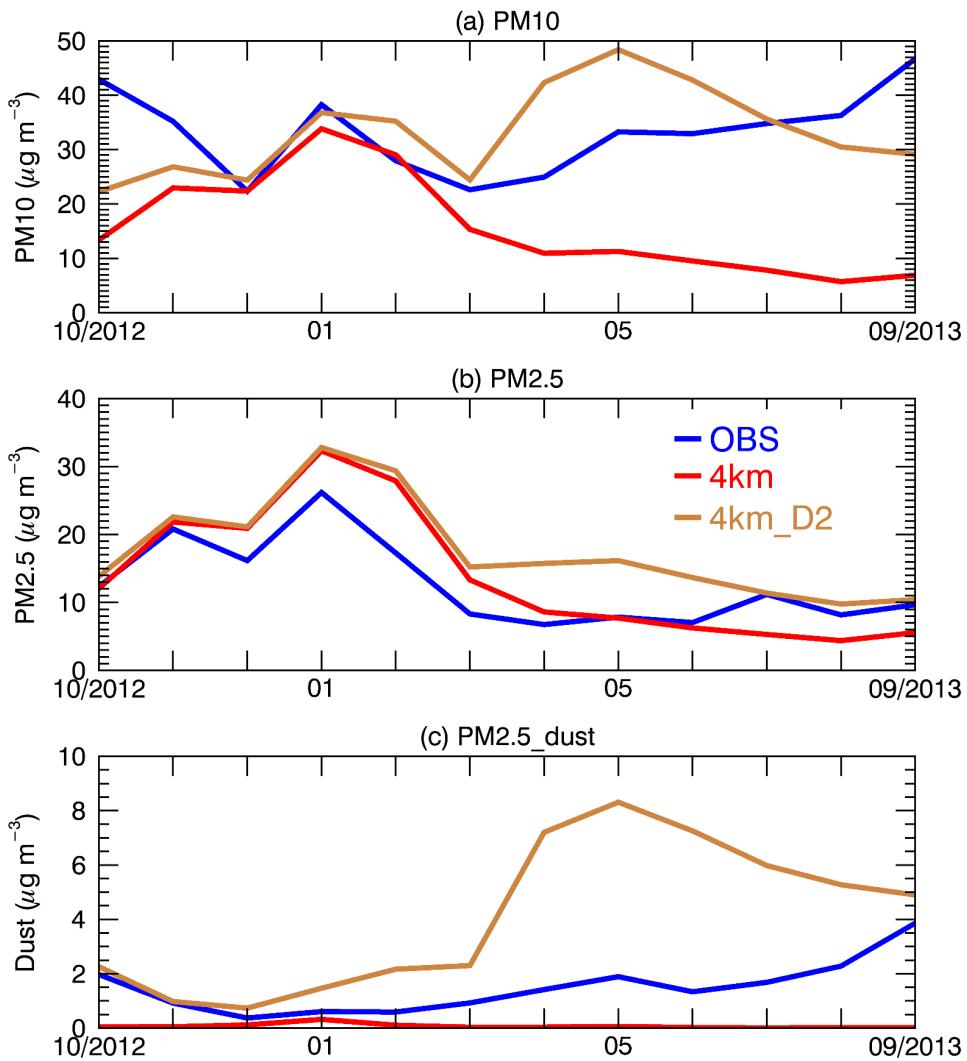


626

627 Figure 3. Monthly mean 550 nm AOD at Fresno, CA from October 2012 to September 2013.

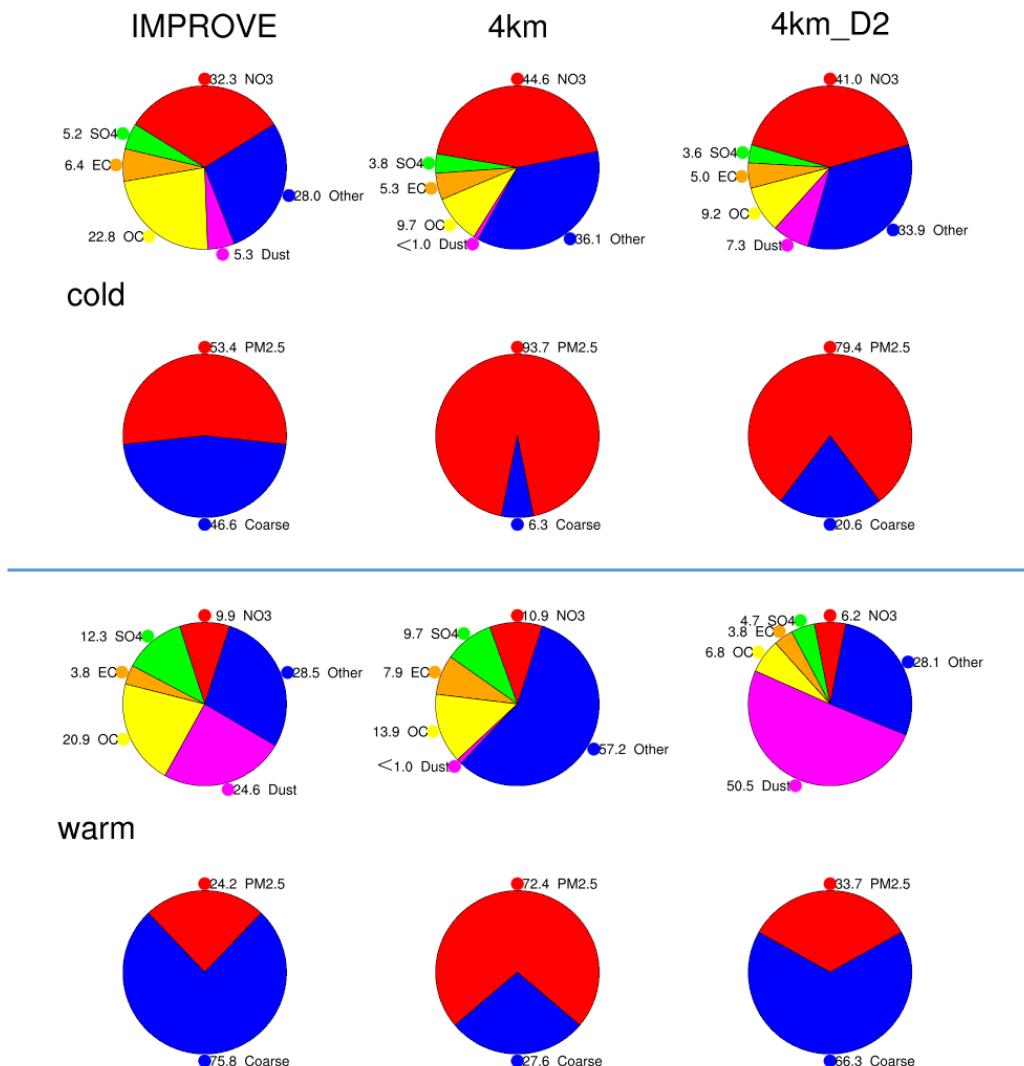


628  
629 Figure 4. Aerosol mass ( $\mu\text{g m}^{-3}$ ) for different species from IMPROVE (OBS), 20km and 4km  
630 simulations at Fresno, CA. PM2.5\_NO<sub>3</sub> represents NO<sub>3</sub> with diameter  $\leq 2.5 \mu\text{m}$ . Similar definition  
631 for SO<sub>4</sub>, EC and OC in the figures.



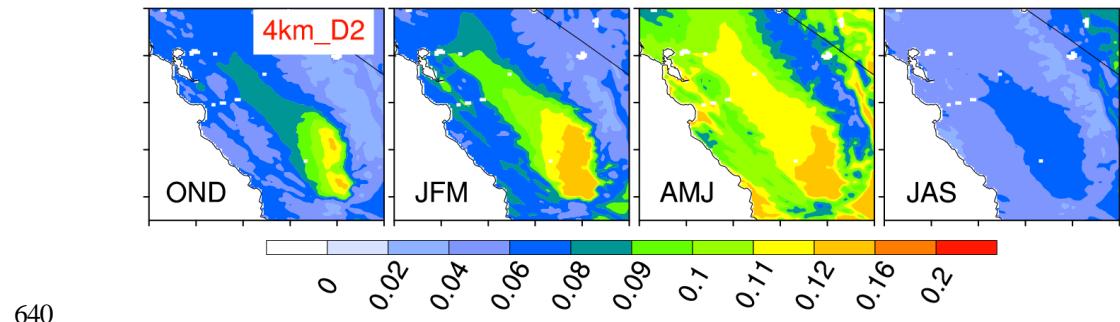
632

633 Figure 5. (a) PM10; (b) PM2.5; (c) PM2.5\_dust from IMPROVE (OBS), 4km and 4km\_D2  
634 simulations at Fresno, CA.

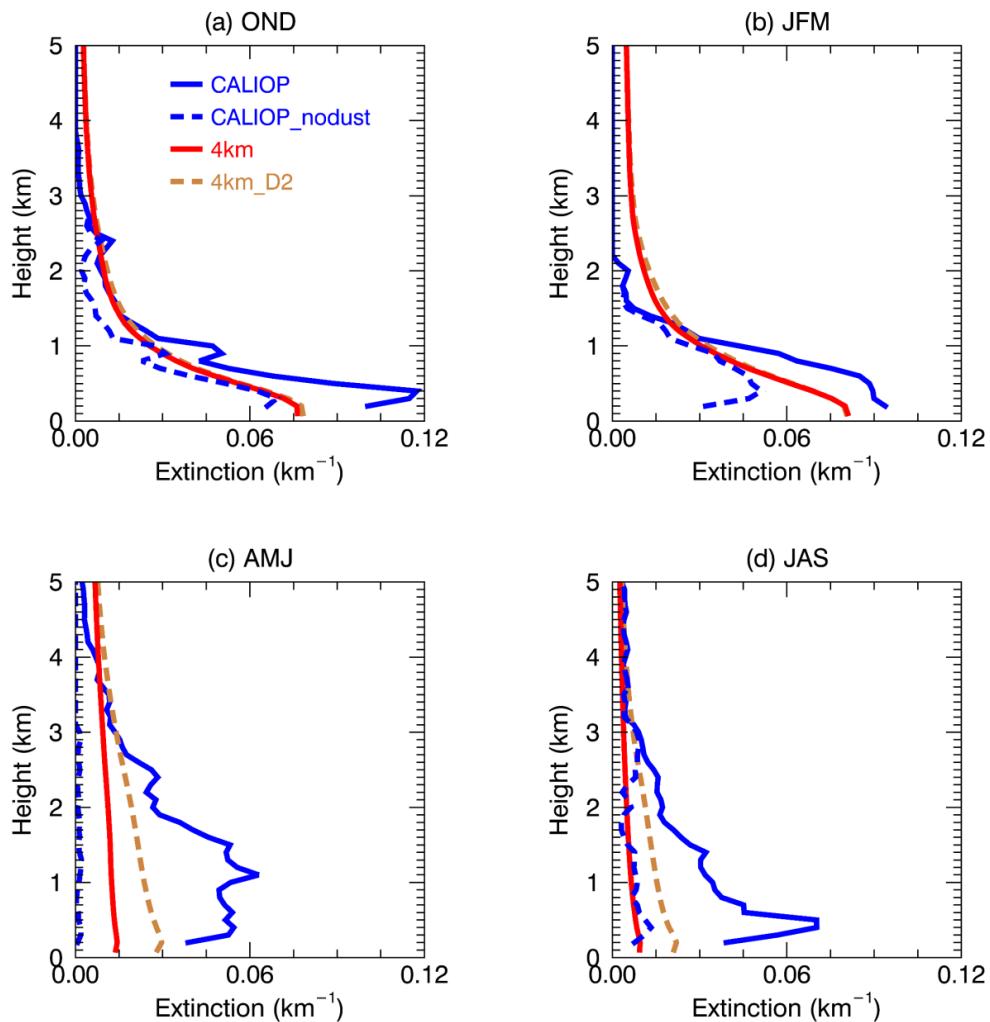


635

636 Figure 6. Relative contribution (%) of aerosol species from IMPROVE and the WRF-Chem  
637 simulations (4km and 4km\_D2) at Fresno, CA in WY2013. (Panel 1) Contribution to PM2.5 in  
638 cold season; (Panel 2) relative contribution of PM2.5 and coarse mass to PM10 in cold season;  
639 (Panel 3) same as Panel 1 but in warm season; (Panel 4) same as Panel 2 but in warm season.

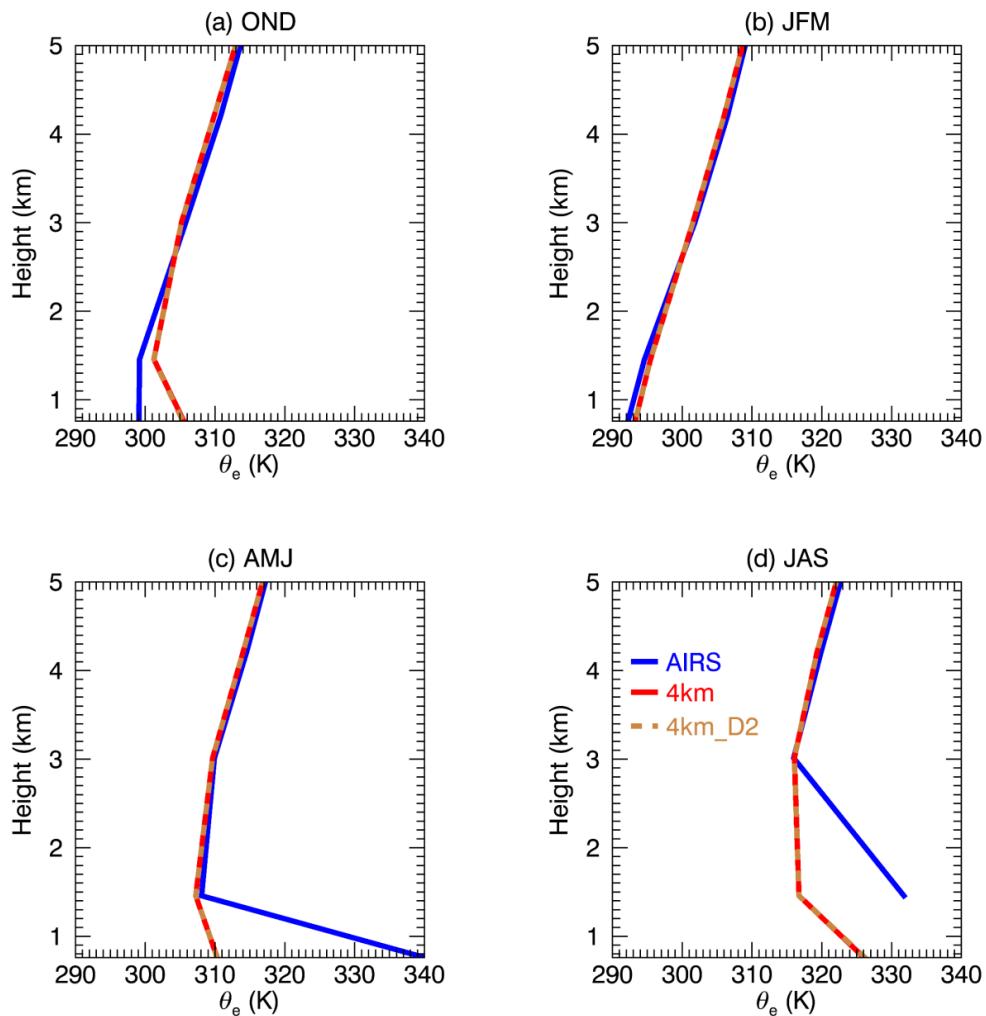


641 Figure 7. Spatial distribution of seasonal mean 550 nm AOD from 4km\_D2 in WY2013.



642

643 Figure 8. Vertical distribution of seasonal mean 532 nm aerosol extinction coefficient ( $\text{km}^{-1}$ )  
644 from CALIOP (blue) and the WRF-Chem (4km and 4km\_D2) simulations over the red box  
645 region in Figure 1a) in WY2013. Blue dashed lines (CALIOP\_nodust) represent the CALIOP  
646 profiles without dust (dust and polluted dust).

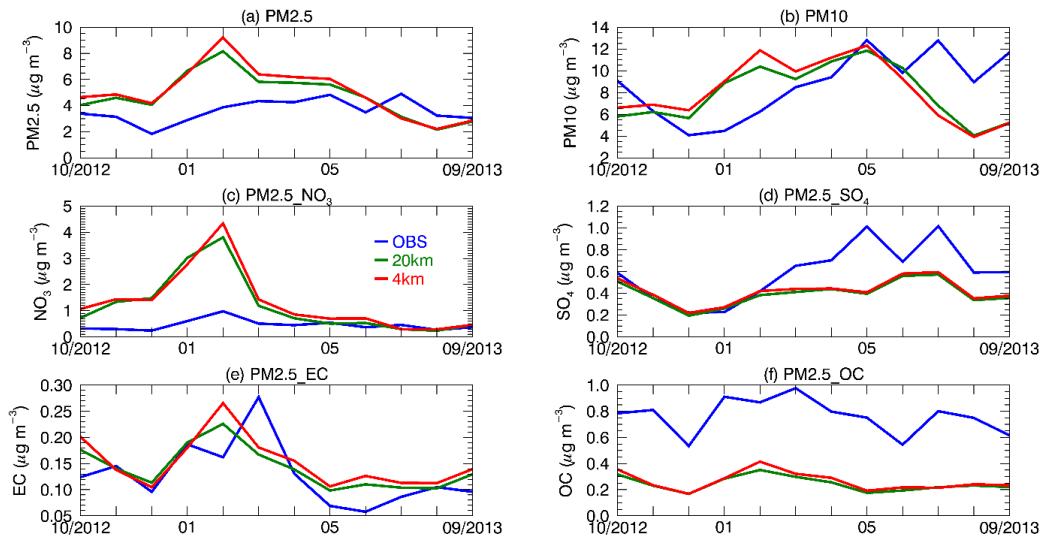


647

648 Figure 9. Vertical distribution of season mean equivalent potential temperature ( $\theta_e$ ; K) from AIRS  
649 and the WRF-Chem (4km and 4km\_D2) simulations over the red box region in Figure 1a in  
650 WY2013.

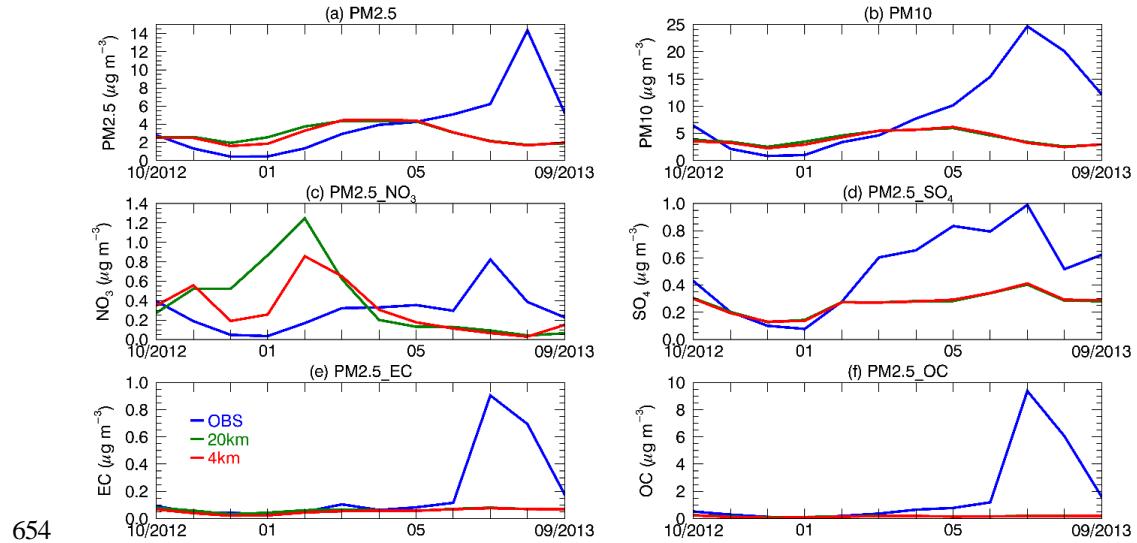


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Figure 10. Aerosol mass ( $\mu\text{g m}^{-3}$ ) for different species from IMPROVE (OBS), 20km and 4km simulations at Pinnacles, CA.



655 Figure 11. Aerosol mass ( $\mu\text{g m}^{-3}$ ) for different species from IMPROVE (OBS, blue), 20km and 4km  
656 simulations at Kaiser, CA.