

1 **PM_{2.5} Assimilation within JEDI for NOAA's Regional Air**

2 **Quality Model (AQMv7): Application to the September 2020**

3 **Western U.S. Wildfires**

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19 **Abstract.** This paper describes efforts to establish aerosol data assimilation capabilities for NOAA's National Air
20 Quality Forecasting Capability (NAQFC), a regional online air quality modeling (AQM) system under NOAA's
21 Unified Forecast System (UFS), by assimilating measurements of fine particulate matter (PM_{2.5}, particles with
22 aerodynamic diameters less than 2.5 μm). PM_{2.5} assimilation is developed within the Joint Effort for Data
23 assimilation Integration (JEDI) framework and tested using its 3D-Var data assimilation (DA) component. The
24 PM_{2.5} observation operator is constructed by combining newly developed PM_{2.5} transformation recipes in the JEDI
25 Variable Derivation Repository (VADER) with a general spatial interpolation operator in the Unified Forward
26 Operator (UFO).

27 Cycled DA and forecast experiments were conducted from 1 to 21 September 2020, during a period of Western U.S.
28 wildfires, to assess the impact of assimilating PM_{2.5} observations from the AirNow and PurpleAir networks. The
29 control and analysis variables include individual aerosol species, with background error standard deviations
30 generated by scaling their respective background values. Prognostic variables such as aerosol particle number and
31 total particulate surface area are updated accordingly following each analysis update. All DA experiments use a
32 3-hourly cycling interval, with PM_{2.5} observations assimilated every 3 hours. The control experiment uses the same
33 configuration but without any data assimilation. Results show that assimilating either AirNow or PurpleAir PM_{2.5}

34 data reduces 1–24 h forecast errors in terms of mean absolute error (MAE) and root mean square error (RMSE)
35 compared to the control run over [Continental United States](#)(CONUS). [Substantial improvements are in regions](#)
36 [where fire events took place and largely affected by transported smoke](#). AirNow observations have a greater impact
37 overall, while PurpleAir shows its strongest impact over northern Utah, Colorado, and southwestern New Mexico.
38 Overall, the assimilation of PurpleAir observations in addition to AirNow data leads to a slight reduction in 3–24 h
39 MAE.

40 **1 Introduction**

41 Particulate matter with an aerodynamic diameter of 2.5 micrometers or smaller ($PM_{2.5}$) is a [key](#) contributor to poor
42 air quality in the United States, posing significant risks to public health and the environment, and contributing to
43 substantial loss of life (Cohen et al. 2017; Colmer et al. 2020; Huang et al., 2025). Over the past few decades, poor
44 air quality in the U.S. has contributed to over 100,000 premature deaths annually, far exceeding fatalities from all
45 other weather-related causes combined, which average around 500 per year (Huang et al., 2025). Given its public
46 health significance, $PM_{2.5}$ is one of the [important](#) pollutants used in calculating the Air Quality Index (AQI)—a
47 standardized system designed to communicate daily air pollution levels to the public [at the U.S. Environmental](#)
48 [Protection Agency \(EPA\)](#). Elevated $PM_{2.5}$ concentrations frequently result in "unhealthy" AQI ratings, triggering
49 health advisories and public warnings.

50 $PM_{2.5}$ in the United States originates from a range of both anthropogenic and natural sources. Anthropogenic
51 sources include agricultural activities and combustion processes, such as emissions from motor vehicles, power
52 plants, industrial facilities, and residential heating systems. Among natural sources, wildfires are a particularly
53 significant contributor, especially in the western United States, where their frequency and intensity have escalated
54 dramatically over the past two decades (Wen and Burke, 2021). According to the U.S. Environmental Protection
55 Agency (EPA), wildfires account for approximately 15% to 30% of total $PM_{2.5}$ emissions nationwide (EPA, 2017).
56 While national seasonal averages of $PM_{2.5}$ have generally declined, summer $PM_{2.5}$ concentrations in the western
57 U.S. have remained persistently high, primarily due to wildfire smoke (O'Dell et al., 2019). In addition to degrading
58 air quality, wildfires have caused widespread property loss. Since 2005, more than [129,000](#) homes, businesses, and
59 other structures have been destroyed by wildfire-related events
60 (<https://headwaterseconomics.org/natural-hazards/structures-destroyed-by-wildfire>, last access on [February 18,](#)
61 [2026](#)), underscoring the urgent need for more effective strategies in air quality monitoring, forecasting, and wildfire
62 management.

63 The National Oceanic and Atmospheric Administration (NOAA) has developed an advanced regional Air Quality
64 Modeling (AQM) prediction system within the Unified Forecast System (UFS) framework to enhance the accuracy
65 of air quality forecasts across the United States, particularly during wildfire events (Huang et al. 2025). The National
66 Air Quality Forecast Capability (NAQFC), operated by NOAA's National Weather Service (NWS), has been
67 providing operational air quality forecast guidance for over 20 years, with continuous inclusion of new capabilities.

68 Under NAQFC, the AQM version 7 was implemented and became operational on May 14, 2024. The system
69 features online coupling of atmospheric and chemical models, allowing dynamic interactions between meteorology
70 and atmospheric chemistry. This integration improves the representation of emissions and ensures real-time
71 feedback of meteorological fields that influence chemical transformations and the transport of pollutants in the
72 atmosphere. The UFS-AQM online system has consistently shown improved performance in simulating major
73 wildfire events, including the significant wildfires in the northwestern coastal regions of the U.S. in September
74 2020, and widespread smoke transport from Canadian wildfires in the summer of 2023. This system was officially
75 implemented on May 14, 2024 as NOAA's operational air quality prediction system (AQMv7), replacing the
76 previous offline-coupled Global Forecast System using the Finite Volume Cube-Sphere dynamical core (GFS-FV3)
77 version 15 with the Community Multiscale Air Quality modeling system (CMAQv5.0.2)(Chen et al. 2021).

78 PM_{2.5} data assimilation (DA) has proven effective in reducing errors in air quality forecasts (e.g., Pagowski et al.
79 2010, 2012; Schwartz et al. 2012; Wu et al. 2015; Robichaud 2017; Lee et al. 2021; Chen et al. 2022, Ha 2022;
80 Vogel et al. 2025, among others). Pagowski et al. (2010) demonstrated that fine aerosol forecasts benefit from
81 AirNow PM_{2.5} DA, showing improved verification scores for a period of at least 24 hours. Schwartz et al. (2012)
82 found that assimilating AirNow PM_{2.5} observations significantly improved surface PM_{2.5} forecasts over the
83 CONUS compared to forecasts without DA. Wu et al. (2015) reported that incorporating ground-based PM_{2.5}
84 observations notably enhanced 24-hour forecasts during a severe pollution episode in Shanghai. Similarly, Chen et
85 al. (2022) showed that assimilating multi-source PM_{2.5} data significantly improved WRF-Chem PM_{2.5} forecasts
86 with benefits lasting up to 48 hours. Lee et al. (2021) highlighted the effectiveness of assimilating ground in-situ
87 surface PM_{2.5} observations in improving the short-term PM_{2.5} predictions in Northeast Asia.

88 Many operational regional air quality prediction systems around the world use some form of data assimilation to
89 initialize the forecasts. These approaches vary in complexity, ranging from simple optimal interpolation to full
90 variational or ensemble Kalman filter methods (e.g. Robichaud et al. 2016; Wei et al. 2024; Colette et al. 2024). In
91 NOAA's current regional air quality model (AQM) operations, aerosol and chemical initial conditions are
92 "warm-started" using 6-hour forecasts from the previous model cycle. The implementation of an aerosol data
93 assimilation system can further enhance short-term air quality forecasts by providing more accurate spatial analyses
94 of initial aerosol distributions.

95 To establish aerosol data assimilation capabilities for NOAA's regional operational AQM system, we employ the
96 Joint Effort for Data assimilation Integration (JEDI) (Trémolet and Auligné, 2020). JEDI is a flexible, agnostic, and
97 modern data assimilation system applicable to a wide range of forecasting systems (e.g. Liu et al. 2023; Huang et al.
98 2023; Sluka, 2024). JEDI offers a platform that supports efficient scientific development and facilitates the transition
99 from research to operations. As part of a broader strategic shift, NOAA and partner agencies are transitioning their
100 data assimilation systems to JEDI, opening the door for rapid integration of new scientific advancements, greater
101 consistency across modeling systems, and enhanced collaboration across research communities and operational
102 centers.

103 This study aims to develop and evaluate an initial aerosol analysis capability for the NOAA’s regional AQM system
104 by assimilating PM_{2.5} observations using the JEDI three-dimensional variational (3D-Var) data assimilation
105 framework. Compared to previous PM_{2.5} data assimilation studies, this research adopts the NOAA’s
106 regional operational AQMv7 system and incorporates a new PM_{2.5} transform in JEDI for assimilating
107 PM_{2.5} observations. In addition to evaluating the impact of assimilating AirNow PM_{2.5} measurements on
108 air quality prediction, this study also examines the impact of assimilating low-cost PurpleAir
109 observations. Although PurpleAir data are valuable for real-time air quality monitoring, their impact on
110 numerical air quality prediction has not been thoroughly investigated. To the authors’ best knowledge,
111 this is the first study to demonstrate the value of PurpleAir observations for air quality prediction during a
112 major fire event using the AQMv7 system.

113 The paper is organized as follows: section 2 provides a description of Methodology including the NOAA’s AQM
114 system, 3D-Var approach, and JEDI PM_{2.5} assimilation. Experimental setup is presented in section 3 including case
115 description, AQM configuration, AirNow and PurpleAir PM_{2.5} observations and background errors setup. Results
116 are described in section 4. A summary and [discussion](#) are presented in the final section.

117 **2 Methodology**

118 **2.1 AQMv7 overview**

119 The NOAA’s regional operational AQMv7 system was developed through the online coupling of the Finite-Volume
120 version 3 (FV3) dynamical core-based atmospheric model (Black et al 2021) with the EPA’s Community Multiscale
121 Air Quality (CMAQ) model v5.2.0 within the UFS framework (Huang et al., 2025). In this UFS-AQM online
122 system, CMAQ is treated as an atmospheric chemistry column model to simulate atmospheric chemistry reactions
123 that govern concentrations of chemical species including gas- and aerosol-phase species. The transport terms of
124 chemical species are handled by the FV3 dynamical core in the same way as other physics tracers (Huang et al.,
125 2025). Aerosol module version 6 (AERO6) (Zhang et al. 2018) is utilized by CMAQ to simulate aerosol processes.

126 **2.2 PM_{2.5} assimilation within JEDI 3D-Var**

127 In the JEDI framework, a series of components are provided to create a flexible, comprehensive data assimilation
128 system (Trémolet. and Auligné, 2020). The [JEDI 3D-Var component](#) is used to assimilate PM_{2.5} for AQMv7.
129 The 3D-Var method is chosen for its operational feasibility, primarily due to its low computational cost and the fact
130 that it does not require an ensemble prediction system, [as is needed in \(hybrid\) ensemble–variational data](#)
131 [assimilation](#).

132 In practice, a 3D-Var data assimilation system typically uses an incremental approach to minimize a quadratic cost
 133 function which is defined in terms of the analysis increment δx relative to the guess state x_g :

$$134 J(\delta x) = \frac{1}{2} (\delta x - \delta x_g) B^{-1} (\delta x - \delta x_g)^T + \frac{1}{2} (\mathbf{H}[\delta x] - d) R^{-1} (\mathbf{H}[\delta x] - d)^T \quad (1)$$

135 Where:

- 136 • $\delta x_g = x_b - x_g$ is the guess state departure from background state x_b , which is usually taken from a
 137 previous short-term forecast.
- 138 • \mathbf{H} is the linearized observation operator of nonlinear observation operator H .
- 139 • \mathbf{B} and \mathbf{R} are the background and observation error covariance matrices, respectively.
- 140 • d is the innovation vector, defined as:

$$141 d = y - H(x_g) \quad (2)$$

142 with y representing the observation vector.

143 Once the increment δx is obtained, the analysis state x^a is reconstructed as:

$$144 x^a = x_g + \delta x \quad (3)$$

145 2.2.1 PM_{2.5} observation operator

146 To assimilate PM_{2.5} data, a PM_{2.5} transform that builds relationships between the model aerosol variables and the
 147 observed PM_{2.5} needs to be developed. In AQMv7, the modal approach taken in the CMAQ model represents
 148 aerosol particle size distributions as the superposition of three lognormal modes: Aitken (I), accumulation (J), and
 149 coarse (K). It predicts only three integral properties of the size distribution for each mode: the total particle number
 150 concentration, the total surface area concentration, and the total mass concentration of the individual chemical
 151 components.

152 The total PM_{2.5} concentration is calculated as a weighted sum of the individual aerosol concentration across these
 153 three modes:

$$154 PM_{2.5} = ATOTI \cdot PM25AT + ATOTJ \cdot PM25AC + ATOTK \cdot PM25CO \quad (4)$$

155 Here, ATOTI, ATOTJ, and ATOTK represent the total aerosol mass concentrations in the Aitken, accumulation, and
 156 coarse modes, respectively. For example, ATOTI is the combined mass of 14 prognostic aerosol variables in the
 157 Aitken mode from the AERO6 aerosol module. Similarly, ATOTJ and ATOTK are the aggregated mass
 158 concentrations of 49 and 7 aerosol variables in the accumulation and coarse modes, respectively. PM25AT,
 159 PM25AC, and PM25CO are mass scaling factors for the three modes that vary by location and time. The aerosol
 160 variables within the same mode share the same mass scaling factor.

161 The $PM_{2.5}$ observation operator is constructed by combining the newly developed $PM_{2.5}$ transformation recipes in
162 the JEDI Variable Derivation Repository (VADER) with an existing general spatial interpolation operator in the
163 Unified Forward Operator (UFO). VADER is responsible for transforming model variables using user-defined
164 “recipes” to generate new variables in model space. For $PM_{2.5}$ assimilation, VADER computes $PM_{2.5}$ from
165 individual aerosol species using model-specific transformation, specifically using the equation 4 for this application.
166 Since $PM_{2.5}$ composition varies by model, these transforms are implemented within VADER to match the specific
167 structure of the regional air quality model AQMv7. Once $PM_{2.5}$ is derived in model space, UFO applies a generic
168 spatial interpolation operator to map the model-simulated values to the observation locations, enabling computation
169 of the observed minus forecast values.

170 The input for the $PM_{2.5}$ transformation are mixing ratio of the 70 aerosol variables wrt dry air in unit ug/kg, the
171 three mass scaling factors in the three modes, and dry air density for unit conversion. The output product is the
172 $PM_{2.5}$ in unit ug/m³. It is noted that a new recipe to derive dry air density from temperature, surface
173 pressure, and delta pressure has been added to VADER for cases where the dry air density is not provided.

174 The new JEDI/VADER $PM_{2.5}$ recipe provides nonlinear (NL), tangent linear (TL), and adjoint (AD) transforms of
175 $PM_{2.5}$ that keeps the output products in the same grid space as the input variables. Hence, the generic interpolation
176 operator in UFO is used to connect the model-derived $PM_{2.5}$ fields with observed surface $PM_{2.5}$ measurements.
177 This respects the JEDI paradigm of keeping the UFO part of the JEDI model independent.

178 2.2.2 Background error covariance modeling

179 In a 3D-Var system, the background error covariance (BEC) determines both the spatial spreading of information
180 from observations and the magnitude of the analysis increments along with the observation error variance.

181 The background error covariance matrix B can be decomposed into a standard deviation matrix (Σ) and a correlation
182 matrix (C), as follows:

$$183 B = \Sigma C \Sigma \quad (5)$$

184 The correlation matrix C is generally non-diagonal. Σ is a diagonal matrix, with the standard deviations of the
185 background errors for each variable on the diagonal.

186 The error modeling of the correlation matrix and standard deviations usually apply to control variables. In the first
187 implementation of aerosol data assimilation in JEDI for AQMv7, the control variables are defined as individual
188 forecast aerosol variables, resulting in 70 control variables for AQMv7 with the AERO6 aerosol mechanism. The
189 setup of background error standard deviation and correlation modeling will be described in Section 3: Experimental
190 setup.

191 2.2.3 Minimization Algorithm (DRIPCG)

192 JEDI provides several minimization algorithm options. In this paper, we use the Derber–Rosati Inexact
193 Preconditioned Conjugate Gradient (DRIPCG) algorithm (Derber and Rosati, 1989), as implemented in the JEDI's
194 OOPS (Object-Oriented Prediction System) framework. DRIPCG has been extensively tested and is chosen here for
195 stability and convergence efficiency.

196 **3 Experimental setup**

197 **3.1 The September 2020 fire event and AQMv7 system setup**

198 The wildfires of September 2020 ranked among the most intense in the U.S. in recent years. These fires produced
199 dense smoke that initially moved westward over the Willamette Valley in western Oregon and eventually blanketed
200 the broader region. As a result, air quality rapidly across Oregon, Washington, and Idaho deteriorated to hazardous
201 levels, marking one of the worst air quality periods in recent decades (Mass et al., 2021). Wildfire smoke originating
202 from California, Oregon, and Washington was injected into the free troposphere and transported across the country
203 by prevailing winds, leading to hazy conditions in several states. According to Li et al. (2021), from August to
204 October 2020, wildfires in the western U.S. contributed 23% of surface $PM_{2.5}$ across CONUS, with higher
205 contributions observed along the Pacific Coast (43%) and in mountain region (42%). This study focuses on the peak
206 fire activity occurring between September 1 and 21.

207 In this research, the model configuration is almost the same as the operational AQMv7 setup except for running over
208 the CONUS domain with a 3 hourly cycling interval. The AQMv7 system is configured over the CONUS domain
209 with a grid-spacing of 13 km and 65 vertical levels, extending up to 0.2 hPa. The system uses the Global Forecast
210 System version 16 (GFSv16) physics package within the Common Community Physics Package (CCPP) framework
211 to generate the meteorological fields driving air quality predictions. Meteorological initial conditions and lateral
212 boundary conditions are generated using GFS forecast outputs with lead times up to 30 hours at 3-hour intervals
213 from the previous GFS cycle. Fire-related emissions are represented using real-time Regional hourly Advanced
214 Baseline Imager (ABI) and Visible Infrared Imaging Radiometer Suite (VIIRS) Emissions (RAVE) data at 0.03°
215 spatial resolution. Anthropogenic emissions are based on the 2016 U.S. EPA NEI Collaborative (NEIC2016v1)
216 modeling platform. Gas-phase chemistry is simulated using the Carbon Bond Mechanism version 6 (CB6r3) with
217 updated isoprene chemistry and revised photolysis rates. More detailed information including physics, chemistry
218 options, anthropogenic emissions, and fire emissions about the model configuration can be found in Huang et al.
219 (2025).

220 **3.2 $PM_{2.5}$ observations**

221 In this study, surface $PM_{2.5}$ observations were obtained from two sources: AirNow and PurpleAir observing
222 networks. These datasets differ in sensor type, spatial coverage, and quality control (QC) requirements. AirNow
223 provides regulatory-grade measurements from federal, state, and local monitoring stations, while PurpleAir is a
224 low-cost, community-based network of air quality sensors. PurpleAir sensors are widely deployed by individuals

225 and communities, providing real-time data on PM_{2.5} concentrations as well as meteorological variables such as
226 temperature, pressure, and relative humidity. Only the data reported from outdoor PM_{2.5} sensors are used in this
227 study. The PurpleAir data were available for registered users through the PurpleAir API.

228 (<https://community.purpleair.com/t/api-use-guidelines/1589>; last access on February 18 2026)

229 3.2.1 PurpleAir PM_{2.5} quality control and correction

230 Quality control and correction of PurpleAir data followed the methodology described in Barkjohn et al. (2021).

231 Readers are referred to that paper for further details. A correction is required because the PurpleAir raw data usually
232 overestimate PM_{2.5} concentrations under typical ambient and smoke-impacted conditions. The following quality
233 control (QC) filters were applied to the raw PurpleAir PM_{2.5} measurements:

- 234 • Reported PM_{2.5} values from two Plantower sensors within the PurpleAir sensor (channels A and B) must
235 be nonnegative.
- 236 • The PurpleAir sensor channel A and B consistency:
 - 237 ○ Absolute difference < 5 µg/m³, *or*
 - 238 ○ Relative difference within 61%.
- 239 • PM_{2.5} values must not exceed PM10 values.
- 240 • PM_{2.5} values must be less than 3000 µg/m³ (upper threshold).
- 241 • Gross check of relative humidity with range 0-100%.

242 Only PurpleAir PM_{2.5} measurements that passed all the above QC criteria were retained for subsequent correction.

243 3.2.2 PurpleAir PM_{2.5} correction

244 Correction of PurpleAir PM_{2.5} measurements was performed using a multiple linear regression model based on
245 sensor-reported PM_{2.5} (PA) and relative humidity (RH), following the correction formula proposed by Barkjohn et
246 al. (2021):

$$247 \text{PM}_{2.5} = 0.524 \times \text{PA} - 0.0862 \times \text{RH} + 5.75 \quad (6)$$

248 We adopt the above equation because it was United States-wide valid by fitting data from September 2017 until
249 January 2020. In addition, although the correction was originally derived for 24-hour averaged PM_{2.5}, it is
250 consistent with a regression equation obtained from the September 2020 dataset based on 1-hour averaged PM_{2.5}.

251 3.2.3 Observation error assignment

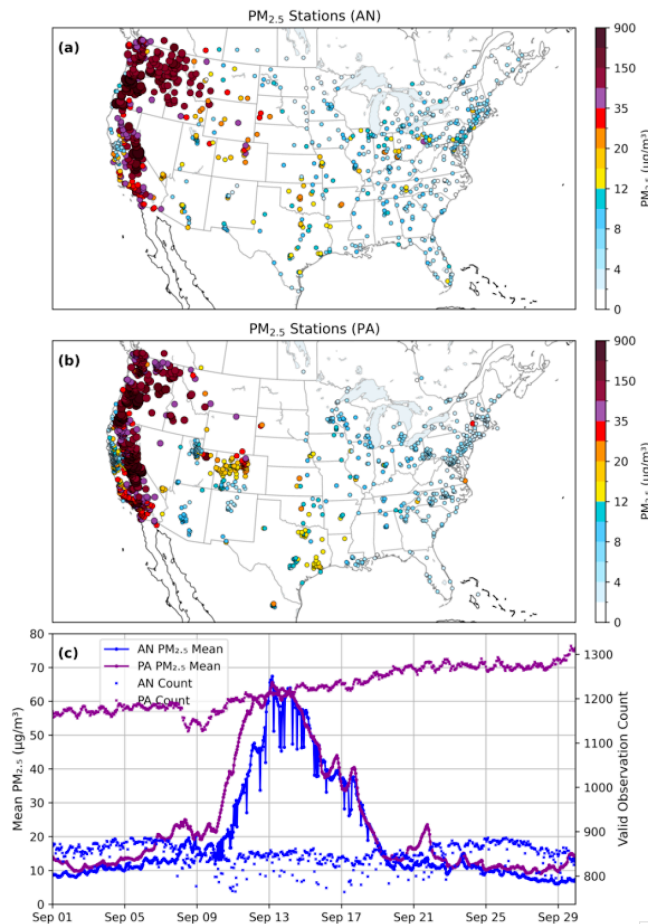
252 Observation error standard deviations were assigned to each network:

- 253 • AirNow PM_{2.5}: 5% of observed value

254 • PurpleAir PM_{2.5}: 10% of observed value

255 The values above are based on the EPA's definition of acceptable measurement uncertainty, which specifies a 10%
256 coefficient of variation for total precision. The AirNow PM_{2.5} observation errors were set to 5% of the observed
257 values. For PurpleAir PM_{2.5} data, the observation errors were set to 10%, reflecting the higher likelihood of greater
258 uncertainties associated with lower-cost sensors.

259 Figure 1a–b shows the spatial distribution of AirNow and PurpleAir PM_{2.5} monitoring stations at 1200 UTC on
260 September 16, 2020. PurpleAir sensors are especially concentrated in densely populated areas, leading to notable
261 spatial variability in observation coverage during the September 2020 wildfire events. Coverage is particularly dense
262 in urban regions of the western United States (e.g. California, Oregon, Washington, Utah, Arizona and Colorado),
263 while rural and remote areas have significantly fewer sensors, for example, Nevada and North Dakota. Figure 1c
264 displays the time series of domain averaged PM_{2.5} values and station counts from the AirNow and PurpleAir
265 networks, including matched stations between the two. The number of AirNow stations ranges from approximately
266 800 to 900, while PurpleAir stations number between 1,160 and 1,300. Dropouts in the AirNow network lead to
267 sudden decreases in station count and corresponding drops in the PM_{2.5} time series. In contrast, the PurpleAir
268 network shows a general upward trend in station count, with no major data dropouts observed.



269

270 **Figure 1.** (a-b). Spatial distribution of AirNow(AN) and PurpleAir(PA) PM_{2.5} monitoring stations on 1200 UTC 16
 271 September 2020. (c). Time series of domain averaged PM_{2.5} values and numbers from AirNow and PurpleAir
 272 observing networks.

273 3.3 Background error covariance

274 In this study, the background error standard deviation (Σ) for each control variable is constructed based on the
 275 background forecast; specifically, the error standard deviations of an aerosol variable are prescribed as proportional
 276 to its background values.

277 The proportional scaling factor s is approximately estimated by building a linear relationship between the PM_{2.5}
 278 standard error (Σ) and the background forecast $PM_{2.5}^{bkg}$ PM_{2.5} concentrations:

$$279 \Sigma = s \cdot PM_{2.5}^{bkg} \quad (7)$$

280 The scaling factor s is subsequently applied to all PM_{2.5} components, i.e., the 70 prognostic aerosol variables, to
 281 construct their error standard deviations.

282 This proportionality-based approach has also been adopted in the MOCAGE operational system (Colette et al.,
 283 2024), where background error standard deviations are similarly prescribed relative to background concentrations as
 284 a first-order approximation.

285 Tang et al. (2023) tested a similar method, in which the background PM_{2.5} error variance is first estimated using the
 286 Hollingsworth–Lönnberg method (Hollingsworth and Lönnberg, 1986). A linear relationship is then established
 287 between the estimated PM_{2.5} standard error and the background forecast $PM_{2.5}^{bkg}$.

288 Here we take the same idea but using an alternative approach to roughly estimate the background PM_{2.5} forecast
 289 error variance. The background PM_{2.5} error variance (Σ^2) is estimated using PM_{2.5} innovation information d
 290 defined in the subsection 2.2, and observation error information R specified in the subsection 3.2.3, specifically,

$$291 \Sigma^2 = E(d d^T) - R \quad (8)$$

292 In Eq. 8, $E(\cdot)$ denotes the mathematical expectation operator. The superscript T denotes the transpose of a vector.
 293 Equation 9 is valid under the assumption that observation and background errors are uncorrelated. This assumption
 294 is reasonable when the innovation vector d is calculated using forecasts from a free-running model without any
 295 aerosol data assimilation.

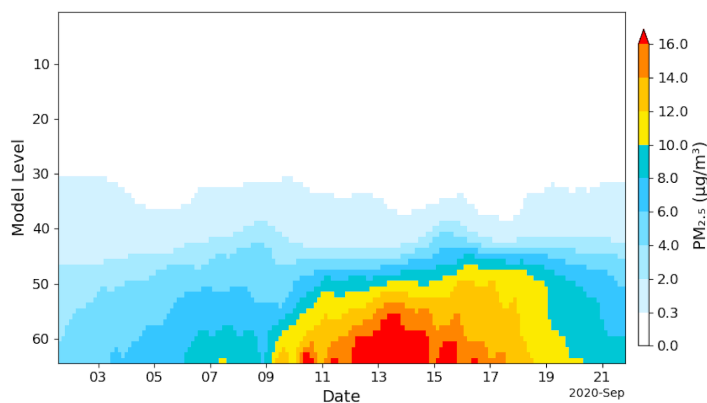
296 In this study, short-term (e.g., 3-hour) PM_{2.5} forecasts from a free run conducted during 1–21 September 2020 were
 297 used to compute the innovation vector d . This free run, referred to as the *control run*, is described in detail in the

298 following section. Using the innovations and observation errors from subsection 2.2 and 3.2.3 as inputs to Eq. 8, the
299 background error variance of $PM_{2.5}$ was first estimated. This error, along with the background values, was then used
300 in Equation 7 to estimate the scaling factor, s . This scaling factor was subsequently applied in all assimilation
301 experiments presented in this study.

302 This proportionality-based approach implicitly assumes that displacement errors in background don't dominate,
303 focusing the assimilation process on correcting amplitude. It offers several benefits:

- 304 • It helps constrain analysis increments to physically meaningful regions. For example, it prevents the
305 generation of sea salt aerosol increments over inland areas where no sea salt is present in the background.
306 This is a problem that can occur when using GSI's height-dependent or latitude–height-dependent
307 background error variance formulations, particularly when individual aerosol species are used as control
308 variables.
- 309 • It introduces location- and time-dependent background error variance information, improving the realism of
310 background error specification. Moreover, the aerosol variables that dominate background errors vary by
311 location and assimilation cycle, rather than being consistently dominated by the same species when using
312 constant static background error statistics. For example, organic and black carbon typically exhibit the
313 largest errors in wildfire regions and downwind areas affected by smoke, whereas other regions may be
314 dominated by non-organic aerosols.

315 An example of domain averaged background $PM_{2.5}$ error standard deviation from a data assimilation run that
316 assimilated both AirNow and PurpleAir $PM_{2.5}$ is shown in Figure 2. This figure is intended to illustrate the main
317 difference to static constant background errors, though the actual errors used in the data assimilation experiments are
318 the errors of the individual aerosol control variables. It is obvious that this approach produces dynamically location-
319 and time-dependent varying error estimates that yields particularly large error variances during the peak fire events
320 from 10 to 20 September 2020.



321

322 **Figure 2.** Domain averaged $PM_{2.5}$ error standard deviations for the data assimilation run that assimilated both
323 AirNow and PurpleAir $PM_{2.5}$.

324 The background error correlation matrix C is modeled using a generic diffusion correlation operator designed for
325 short length scales, as implemented in the System-Agnostic Background Error Representation (SABER) repository
326 (Sluka, 2024). A horizontal cutoff scale of 100 km is applied, consistent with estimates derived from NMC statistics
327 in previous GSI applications (Wang et al., 2021). For vertical correlations, this study uses a cutoff scale of 12 model
328 levels, which helps confine the influence of surface $PM_{2.5}$ observations within the average daytime planetary
329 boundary layer (PBL) height (~ 1450 m) and has demonstrated improved surface $PM_{2.5}$ prediction as will be
330 discussed in Section 4.

331 3.4 Update of total particle number and surface area concentrations

332 After the aerosol mass concentration has been analyzed, total particle number concentration, total surface area
333 concentration can be updated accordingly. For simplicity, it is assumed that the ratio of the particle number
334 concentration to total particulate volume within each mode (I, J, K) remains the same as in the background. Total
335 particulate volume is used instead of mass mixing ratio because it is proportional to the particle number
336 concentration (see Eq. 3 in Binkowski and Roselle, 2003). A similar assumption was adopted by Li (2013) to update
337 number concentrations for the WRF-Chem model.

338 The number of particles is updated using the following relation:

$$339 N_a = N_b / V_b \times V_a \quad (9)$$

340 Where:

- 341 • N_a and N_b are the number of particles in the analysis and background, respectively, within each mode.
- 342 • V_a and V_b are the total particulate volumes in the analysis and background, respectively, within the same
343 mode.

344 The total particulate volume (V_a or V_b) within each mode is calculated by dividing the mass concentration of each
345 aerosol variable by its corresponding density in that mode, and then summing the results. This updating approach
346 implicitly assumes that changes in volume across the three modes are driven solely by variations in particle number,
347 rather than shifts in the aerosol size distribution. The total particulate surface area within each mode is then updated
348 using the same volume ratio, i.e., V_a / V_b (Eq. 9) multiplied by the background surface area.

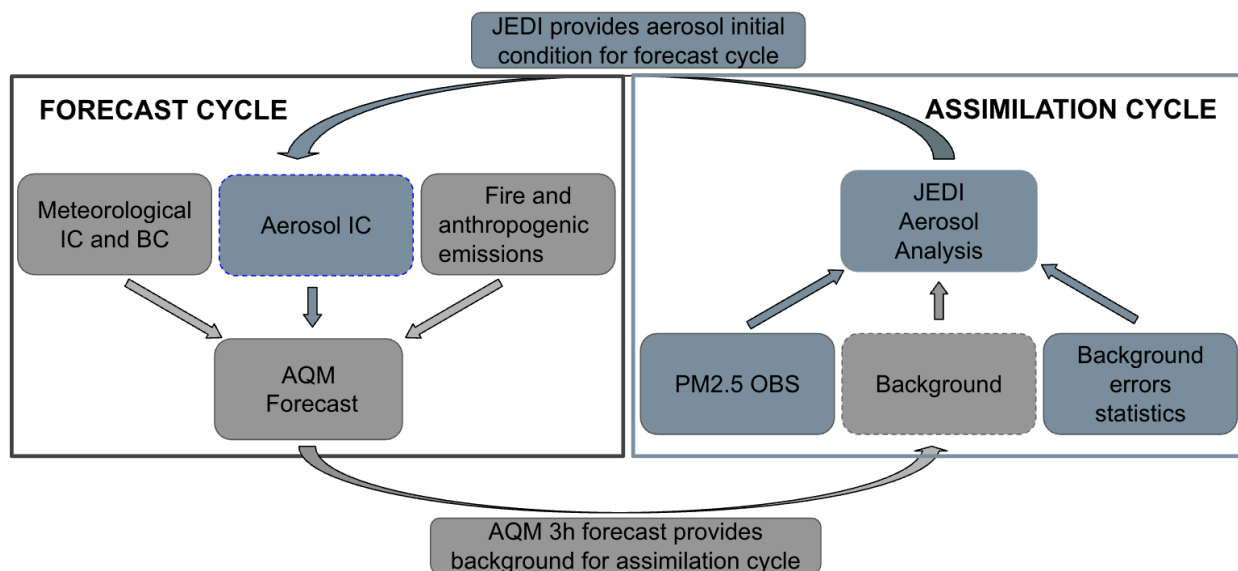
349 In preparatory work for this study, six-hourly cycling experiments (Wang et al., 2025) have shown that updating
350 these variables is crucial for improving AQMv7 performance. In contrast, previous work using GSI with earlier
351 developmental versions of AQM did not update these variables, primarily because those model versions were less
352 advanced than the current operational AQMv7. As a result, there was still significant room for improving prediction

353 skills.

354 3.5 Experiments

355 In the operational AQMv7 configuration, aerosol initial conditions (IC) are warm-started from a previous forecast
 356 cycle. In contrast, in cycling data assimilation and forecasting experiments, the data assimilation system provides
 357 aerosol initial conditions for the subsequent forecast, while the short-term (3-hour) forecast serves as the background
 358 for the next data assimilation cycle. A schematic of the data assimilation and forecasting cycles is shown in Fig. 3.

359 In the assimilation cycle, JEDI updates the aerosol analysis by combining $PM_{2.5}$ observations with the background
 360 information. The updated aerosol analysis, together with meteorological initial conditions, emissions, and other
 361 inputs, is then used to initialize the subsequent forecasts in the forecast cycle. Note that the meteorological initial
 362 conditions are not updated by JEDI but are generated from GFS forecast outputs of the previous GFS cycle.



363

364 **Figure 3.** A schematic of the data assimilation and forecasting cycles.

365 Four experiments were conducted to evaluate the performance of JEDI/AQM $PM_{2.5}$ DA. Table 1 provides a
 366 description of the experiments. The first experiment is a control run (CTR), in which meteorological initial and
 367 boundary conditions are updated every 3 hours, while chemical and aerosol fields are carried over from the 3-hour
 368 forecast of the previous cycle. The other three experiments incorporate data assimilation: DA_AN, DA_PA, and
 369 DA_ANPA, which assimilate AirNow $PM_{2.5}$ only, PurpleAir $PM_{2.5}$ only, and both AirNow and PurpleAir $PM_{2.5}$
 370 observations, respectively.

371 **Table 1. Descriptions of the experiments.**

Experiment	Data Assimilation	$PM_{2.5}$ Observations Assimilated	Aerosol Fields
------------	-------------------	-------------------------------------	----------------

CTR	No	None	Carried over from previous cycle's 3-hour forecast
DA_AN	Yes	AirNow PM _{2.5} only	Updated by Assimilation
DA_PA	Yes	PurpleAir PM _{2.5} only	Updated by Assimilation
DA_ANPA	Yes	AirNow + PurpleAir PM _{2.5}	Updated by Assimilation

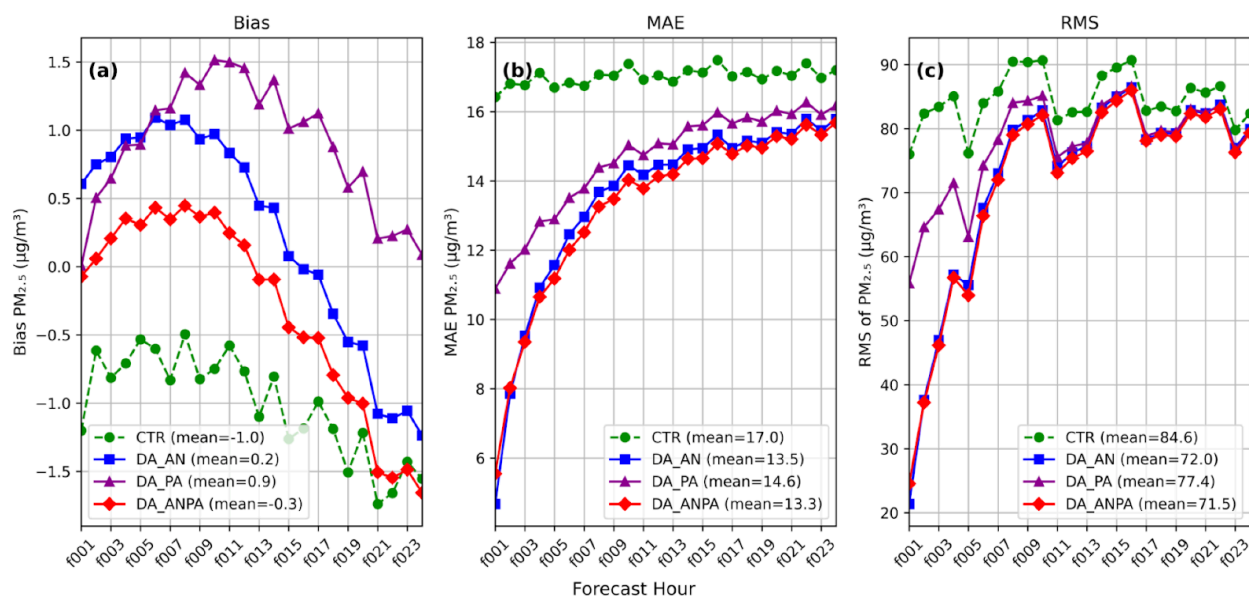
372 Like the CTR experiment, all DA experiments are conducted as 3-hourly cycling runs. Data assimilation is
373 performed every 3 hours, and a 3-hour forecast is launched at each cycle. This 3-hour forecast serves as the
374 background for the subsequent data assimilation and forecasting cycle. In addition, forecasts initialized at 0000,
375 0600, 1200, and 1800 UTC are extended to 24 hours for evaluation purposes. The experimental period spans from
376 1200 UTC on September 1 to 1800 UTC on September 21, 2020. It is noted that to reduce random sensor noise and
377 improve comparability with the model resolution (~13 km), the corrected PurpleAir PM_{2.5} data were spatially
378 averaged onto a 0.1° × 0.1° latitude–longitude grid.

379 4 Results

380 This section provides an overview of the impact of DA on PM_{2.5} forecasts. A total of 80 forecasts—initialized four
381 times daily from 0000 UTC on September 2 to 1800 UTC on September 21, 2020—are used to evaluate model
382 performance. AirNow PM_{2.5} observations are used to verify the forecast. Forecast errors are assessed using bias,
383 mean absolute error (MAE), and root mean square error (RMSE). Forecast performance is evaluated using box plots,
384 which illustrate the distribution, spread, and central tendency of forecast errors. Time series of PM_{2.5} at various
385 forecast hours are presented to examine the temporal evolution of forecast performance. Additionally, spatial
386 distributions of PM_{2.5} including observations, forecasts, forecast errors, and forecast differences are analyzed to
387 evaluate the spatial impact of data assimilation on PM_{2.5} predictions.

388 Figure 4 presents the bias, mean absolute error (MAE), and root mean square error (RMSE) for the 1–24 h forecast
389 of domain-averaged PM_{2.5}. Domain averages are computed over all states in the mainland United States. From the
390 bias statistics (Fig. 4a), it is seen that the bias in the control run follows an upward trend initially, then reverses into a
391 downward trend. The data assimilation runs show a similar trend, as data assimilation primarily corrects the model
392 state and does not fully resolve inherent model bias. The control run underpredicted surface PM_{2.5} throughout the
393 24-hour forecast period by about 1 μg m⁻³. This underprediction was improved in the data assimilation experiments.
394 The two assimilated experiments, DA_AN and DA_ANPA, reduced the 1-24h mean bias to -0.2 and -0.3 μg m⁻³,

395 respectively. The PurpleAir PM_{2.5} assimilation experiment (DA_PA) also slightly improved the 1-24h mean bias.
 396 It is seen that DA_PA produces a near zero bias at 1h forecast, however this is due to large positive and negative
 397 biases canceling out. Therefore, it should be used together with norms like Mean Absolute Error (MAE) and Root
 398 Mean Square Error (RMSE), which quantify the actual magnitude of forecast errors.
 399 In terms of MAE and RMSE, all the three data assimilation experiments reduced the surface PM_{2.5} forecast error
 400 throughout the 24-hour forecast period. The added value of assimilating PurpleAir PM_{2.5} data alongside AirNow
 401 observations is evident in the consistent MAE reduction (Fig. 4b). Its impact on RMSE (Fig. 4c) is also positive,
 402 though relatively small. Overall, all the data assimilation experiments show improved forecast skill compared to the
 403 control run.

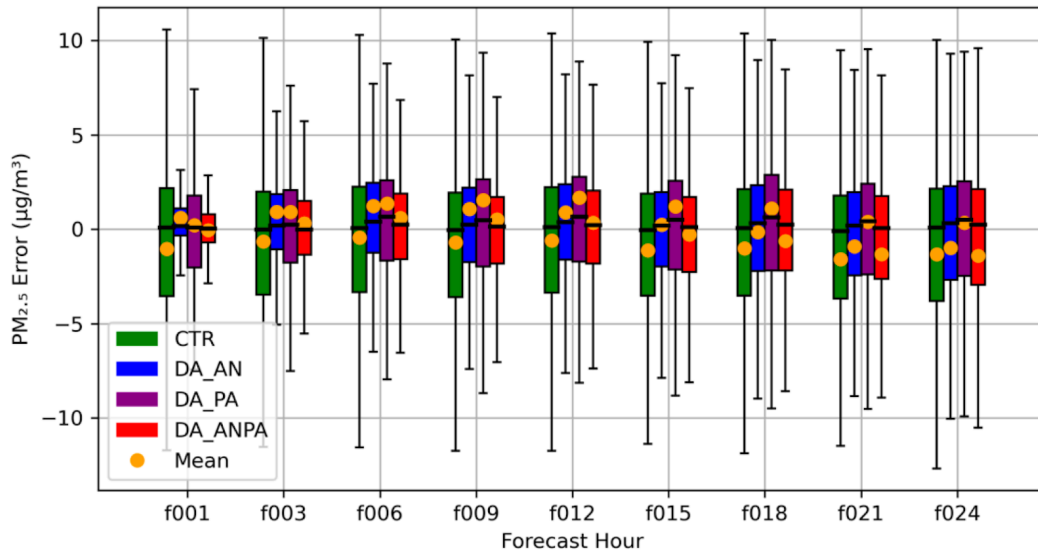


404
 405 **Figure 4.** PM_{2.5} forecast errors for 1–24 h lead times based on 80 forecasts initialized four times daily during
 406 September 2–21, 2020. Domain-averaged over CONUS. The x-axis represents forecast lead times from 1 to 24
 407 hours.

408 (a) Bias, (b) Mean Absolute Error (MAE), (c) Root Mean Square Error (RMSE).

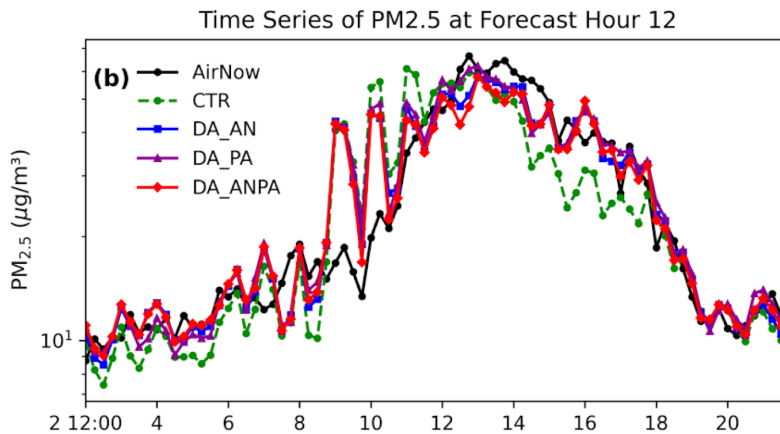
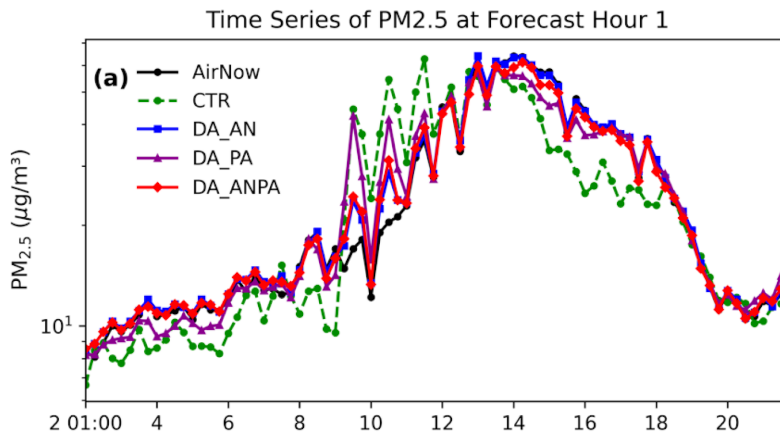
409

410 Figure 5 shows box-and-whisker plots of PM_{2.5} forecast bias. Across all forecast hours, the interquartile range
 411 (IQR)—represented by the height of the boxes—is consistently smaller for the DA experiments compared to the
 412 control run. This indicates reduced forecast error spread between the 25th and 75th percentiles and suggests more
 413 consistent forecasts in the DA experiments. Although the median forecast bias in the control run is sometimes closer
 414 to zero, the DA_ANPA experiment performs comparably in terms of central tendency while showing clear
 415 improvements in reducing the mean forecast bias, as also reflected in Fig. 4a. Among the DA experiments, DA_AN
 416 and DA_ANPA show the most consistent improvement at 24-hour lead times, with DA_ANPA slightly
 417 outperforming others during the early forecast hours (e.g., hour 1 to 12). This suggests that assimilating PurpleAir
 418 observations in addition to AirNow helps reduce bias and brings the forecasts closer to observed PM_{2.5} values in the
 419 short term.

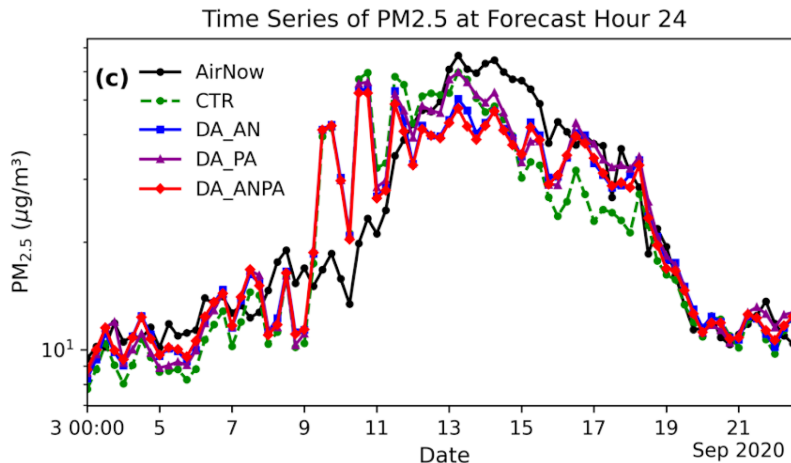


420

421 **Figure 5.** Box-and-whisker plot of $PM_{2.5}$ forecast bias. Orange dot: domain averaged mean; Bottom edge = Q1
 422 (25th percentile); Top edge = Q3 (75th percentile); Height = Interquartile Range ($IQR = Q3 - Q1$); Horizontal line
 423 inside box: The median (50th percentile); Whiskers: Extend to the min and max values within $1.5 \times IQR$ from Q1
 424 and Q3.



425



426

427 **Figure 6.** Time series of $PM_{2.5}$ averaged over CONUS for (a) forecast hour 1, (b) forecast hour 12, and (c) forecast
 428 hour 24. The y-axis is shown on a logarithmic scale.

429 Figure 6 shows time series of $PM_{2.5}$ averaged over CONUS at forecast hours 1, 12, and 24, respectively. Consistent
 430 with the evaluations in Figures 4 and 5, all DA experiments generally improve $PM_{2.5}$ forecasts. Notably, all DA
 431 experiments help correct underpredictions during September 2–9 and 14–17. In addition, the substantial
 432 overprediction during September 9–13 observed in the control run is partially mitigated by the DA experiments.
 433 Among the DA experiments, DA_AN and DA_ANPA show comparable performance and both outperform DA_PA.

434 While we have investigated the impact of DA on $PM_{2.5}$ forecasts in terms of temporal evolution, it is also important
 435 to examine the spatial distribution of forecast fields, associated errors, and the impact of $PM_{2.5}$ data assimilation.

436 Figure 7 presents the spatial distribution of temporally averaged $PM_{2.5}$ forecasts at forecast hour 1, based on 80
 437 forecasts initialized four times daily (0000 UTC, 0600 UTC, 1200 UTC, and 1800 UTC) from September 2 to 21.
 438 The effects of wildfire events are clearly seen in Fig 7a, c and e across California, Oregon, and Washington—where
 439 the fires occurred—as well as in downstream regions such as Montana, Wyoming, Utah, and Colorado impacted by
 440 smoke advection and transport.

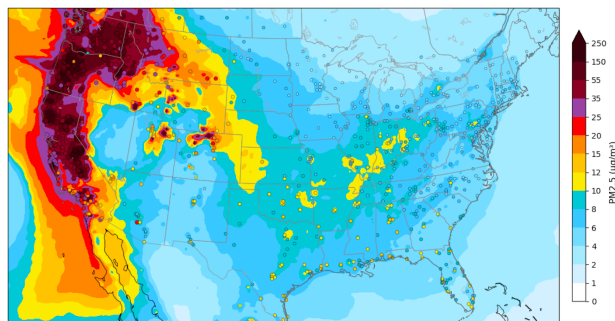
441 1-h $PM_{2.5}$ forecast errors in the control run are evident in Fig. 6a but are more clearly highlighted in Fig. 7b, which
 442 shows the difference between the control run and AirNow observations. Significant overpredictions appear along the
 443 California coast, as well as in parts of the Midwest and Northeast U.S., including Tennessee, Kentucky, West
 444 Virginia, and Virginia. Conversely, notable underpredictions are found over Colorado, New Mexico, much of Texas
 445 and Oklahoma, and several Gulf Coast states.

446 Both DA_AN (Fig. 7c-d) and DA_PA (Fig. 7e-f) show similar spatial correction patterns across California, Oregon,
 447 and Washington, particularly in reducing overpredictions along the California coast. They also produce comparable
 448 large-scale adjustments across the Northeast, Midwest, and Southern U.S., with error patterns (Fig. 7d and 7f)
 449 largely opposite in sign to those in the CTR–AirNow difference (Fig. 7b). This indicates that both DA experiments

450 effectively mitigate the control run's over- and underpredictions.

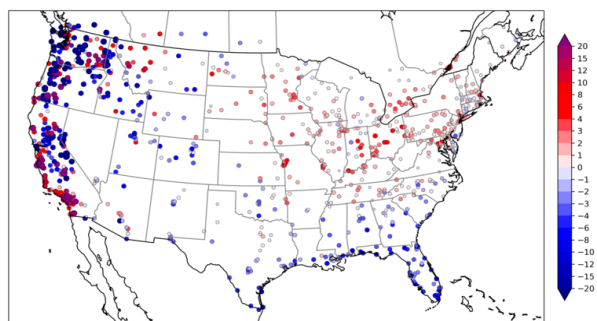
451 However, the magnitude of the corrections is generally smaller in DA_PA than in DA_AN. DA_PA shows its
452 strongest impact over Nevada, northern Utah, Colorado, and southwestern New Mexico, where it helps alleviate
453 regional underpredictions (Fig. 7e and 7f). These improvements are also observed in DA_ANPA, whose spatial
454 pattern closely resembles DA_AN except over these few states (figures not shown).

455 (a) CTR

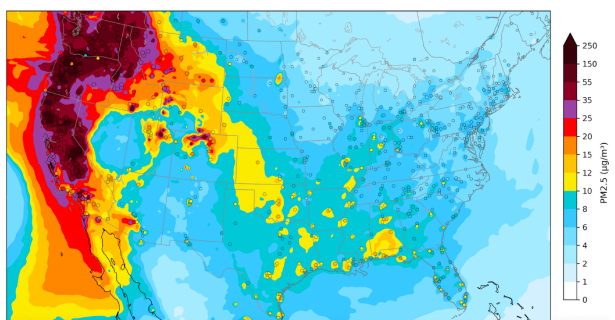


456

(b) CTR-AirNow

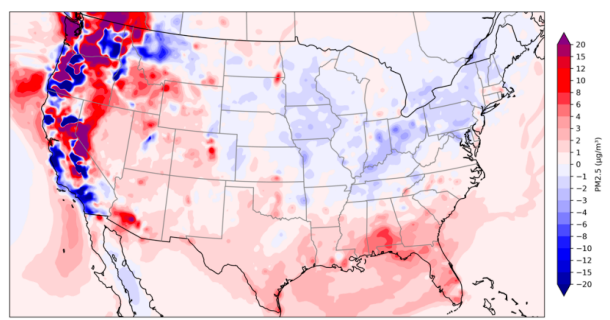


457 (c) DA_AN

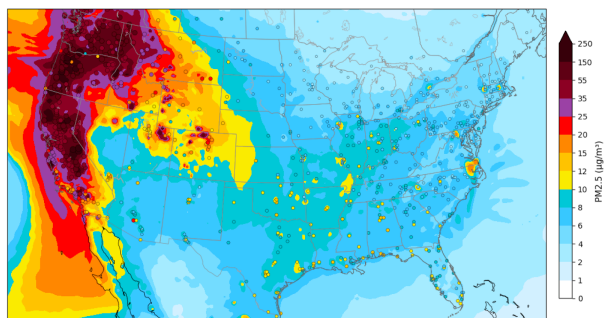


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(d) DA_AN-CTR

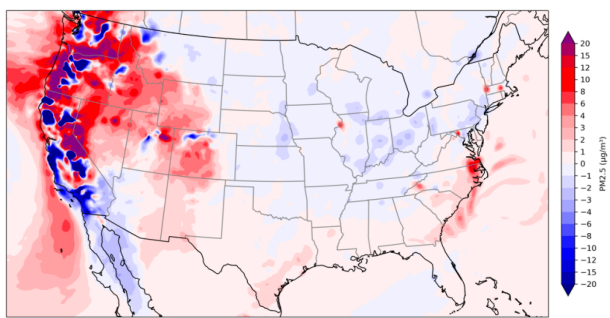


459 (e) DA_PA



460

(f) DA_PA-CTR



461 **Figure 7.** Spatial distribution of average $PM_{2.5}$ at forecast hour 1, based on 80 forecasts initialized four times daily
462 (0000 UTC, 0600 UTC, 1200 UTC, and 1800 UTC) during 2–21 September.

463 (a) $PM_{2.5}$ in experiment CTR (shaded) overlaid with AirNow $PM_{2.5}$ observations (filled dots).

464 (b) $PM_{2.5}$ bias in experiment CTR.

465 (c) $PM_{2.5}$ in experiment DA_AN (shaded) overlaid with AirNow $PM_{2.5}$ observations.

466 (d) $PM_{2.5}$ difference between experiments DA_AN and CTR.

467 (e) PM_{2.5} in experiment DA_PA (shaded) overlaid with AirNow PM_{2.5} observations.

468 (f) PM_{2.5} difference between experiments DA_PA and CTR.

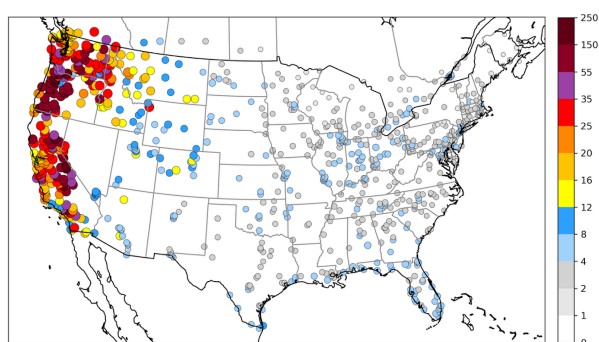
469 The above analysis shows that data assimilation effectively corrects the 1-h forecast errors in the control run,
470 particularly in the DA_AN and DA_ANPA experiments. It is therefore of interest to examine how data assimilation
471 affects longer forecast lead times. Figure 8 presents the MAE from the CTR experiment and the percentage change
472 in MAE (%) between the data assimilation (DA) experiments and the CTR experiment at the 24-h forecast lead time.
473 Negative values in Figs. 8b–d indicate a reduction in MAE.

474 It is seen from Fig. 8a that the largest MAE values occur in California, Oregon, Washington, Idaho, Montana,
475 Wyoming, Utah, Colorado, and Arizona. The PM_{2.5} MAE in these states is generally greater than 10 μg m⁻³, with
476 maximum values exceeding 150 μg m⁻³ at certain stations in California, Oregon, and Washington. In contrast,
477 regions less affected by wildfire smoke exhibit MAE values below 10 μg m⁻³.

478 All DA experiments (Figs. 8b–d) show overall reductions in MAE at most stations. MAE reduction varies by
479 location, with substantial improvements observed in regions with large forecast errors, such as California, Oregon,
480 Washington, and Idaho, where MAE is reduced by approximately 20%. On average, assimilation of AirNow PM_{2.5}
481 observations alone significantly improves the 24-h forecast skill, with MAE reductions of 6.6% based on MAE
482 percentage changes averaged over all stations. In contrast, assimilation of PurpleAir data alone reduces the MAE by
483 only 1.7%. Assimilating both AirNow and PurpleAir PM_{2.5} observations reduces the MAE by 7.6%, indicating that
484 PurpleAir data provides complementary value to AirNow in improving forecast skill.

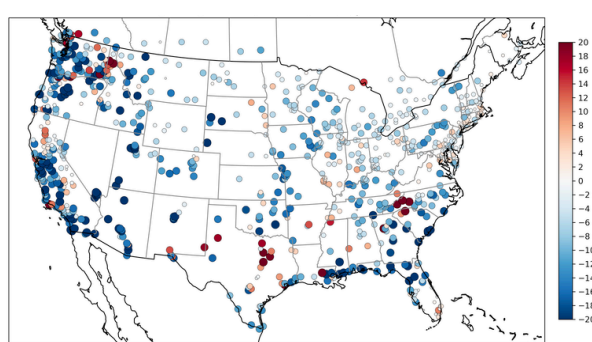
485 In the DA_PA experiment, a few eastern coastal states from Georgia to Virginia exhibit large percentage increases in
486 MAE. These increases are associated with relatively small absolute errors, as MAE values in the CTR experiment
487 over these states are typically only 2–4 μg m⁻³ (Fig. 8a). Increased MAE is also present at several stations at the 1-h
488 forecast lead time in the DA_PA experiment in these areas (figure not shown). In contrast, the MAE increase at the
489 24-h forecast lead time is much less pronounced in the experiment assimilating only AirNow PM_{2.5} observations.
490 This behavior suggests potential quality issues in the assimilated PurpleAir data in those areas that require further
491 investigation, although a contribution from model errors cannot be ruled out.

492 (a)

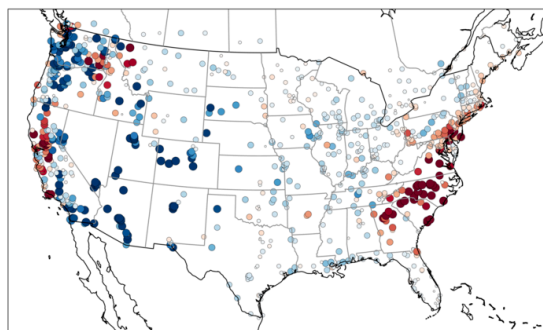


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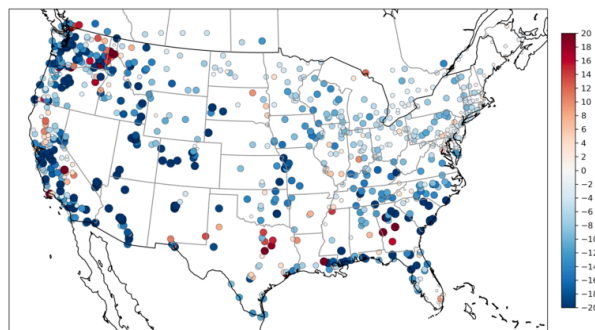
(b)



494 (c)



(d)



495

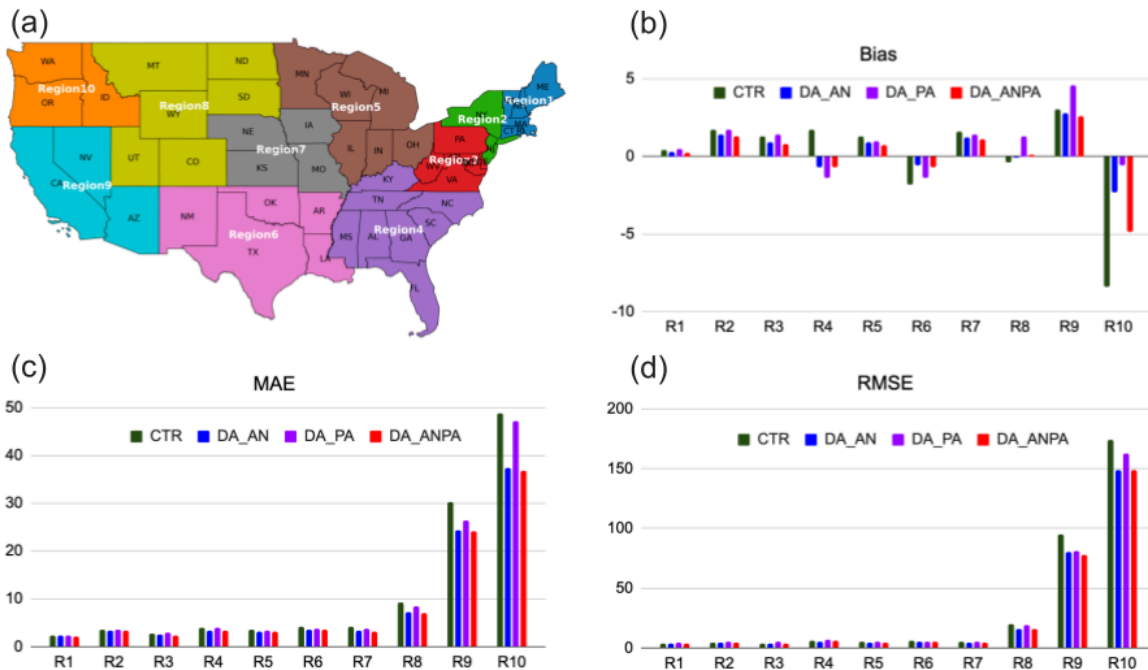
496 **Figure 8.** (a) MAE from the control (CTR) experiment.

497 Percentage change in MAE (%) relative to CTR for (b) DA_AN, (c) DA_PA, and (d) DA_ANPA. The percentage
498 change is calculated as $(MAE(DA)-MAE(CTR))/MAE(CTR) \times 100$.

499 To further examine model performance across different regions, error statistics (bias, MAE, and RMSE) for the
500 averaged 1–24 h $PM_{2.5}$ forecasts from the control and data assimilation experiments over the 10 EPA regions are
501 analyzed. Figure 9 presents the EPA Regions 1-10 and Averaged 1–24 h $PM_{2.5}$ forecasts errors statistics in each
502 EPA region.

503 In terms of bias (Fig. 9b), the DA_AN and DA_ANPA forecasts show improved performance relative to the control
504 run. The DA_PA experiment also improves bias over most EPA regions, except for increased overprediction in EPA
505 regions 8 and 9. For MAE and RMSE, the DA_AN and DA_ANPA experiments generally show improved
506 performance across all EPA regions. The DA_PA experiment also exhibits improved, or at least comparable, MAE
507 relative to the control run. However, DA_PA shows slightly increased RMSE over EPA regions 1–4, while reduced
508 RMSE is found over other EPA regions.

509 Substantial reductions in MAE and RMSE are observed over EPA regions 8–10, where fire events occurred and/or
510 where regions were most influenced by transported smoke. This is consistent with the large 1-h MAE reduction
511 shown in Fig. 8. Notably, the DA_PA experiment, which assimilates PA observations alone, reduces both MAE and
512 RMSE over EPA regions 8–10. Assimilating PurpleAir data together with AirNow data results in slightly smaller
513 MAE and RMSE over these regions, suggesting that PurpleAir observations nonetheless provide complementary
514 information to AirNow in these regions.



515

516 **Figure 9.** (a) EPA Regions 1-10. Averaged 1–24 h PM_{2.5} forecasts errors: (b) Bias, (c) MAE and (d) RMSE.

517 5 Summary and discussion

518 The latest version of NOAA's regional AQM system became operational on May 14, 2024. This system is based on
 519 the online coupling of the Finite Volume Cubed Sphere (FV3) atmospheric model with the Environmental Protection
 520 Agency (EPA)'s Community Multiscale Air Quality (CMAQ) model within the Unified Forecast System (UFS)
 521 framework.

522 To improve initial conditions for AQM and enhance predictions of wildfire impacts on air quality, the capability to
 523 assimilate PM_{2.5} observations into AQMv7 was developed within JEDI and evaluated using its 3D-Var assimilation
 524 component in this study. The developed assimilation scheme can also be used to generate analysis (reanalysis)
 525 dataset for other applications, for example, providing data for training artificial intelligent models used in air quality
 526 prediction.

527 Data assimilation experiments were conducted for the September 2020 Western U.S. wildfire episode, using
 528 3-hourly cycling with observations from the AirNow and PurpleAir networks. In the data assimilation experiments,
 529 the location- and time-dependent background error standard deviations of an aerosol variable are specified as
 530 proportional to its background values, using a diagnosed scaling factor. In addition to updating the analyzed aerosol
 531 variables in each mode, the particle number concentration and surface area of each mode are also updated. The
 532 results show that assimilating AirNow PM_{2.5} observations improves 1–24 h forecast skill. Assimilating PurpleAir
 533 data alone yields modest improvements in MAE. Combining PurpleAir with AirNow observations provides
 534 additional benefit by slightly further reducing MAE relative to AirNow-only assimilation, indicating that PurpleAir

535 observations nonetheless provide complementary information to AirNow. The AirNow data assimilation alone or
536 with PurpleAir data generally show reduced MAE and RMSE across all EPA regions, whereas the largest reductions
537 in MAE and RMSE are observed over regions affected by fire events and/or strongly influenced by transported
538 smoke. The positive impact of PurpleAir data assimilation on smoke prediction during the September 2020 wildfires
539 has also been demonstrated in an experimental Rapid Refresh Forecast System coupled with the Smoke and Dust
540 Model (Wang et al., 2023), where it significantly reduced the model’s 24-h underprediction of surface PM_{2.5}. Given
541 that PurpleAir data coverage has improved since September 2020, the results of this study further highlight its
542 potential to complement AirNow observations by filling spatial gaps and improving PM_{2.5} forecast skill.

543 In this initial development and evaluation of aerosol data assimilation in JEDI for AQMv7, the control variables are
544 defined as individual forecast aerosol variables. In previous work on aerosol data assimilation for an earlier version
545 of AQM using the GSI system (Wang et al., 2021), one option for the control variables was to define them as the
546 total aerosol mass in each of the three modes, resulting in just three control variables. A control variable transform
547 (CVT) was then applied to partition the analysis increments across these modes to individual aerosol species, based
548 on the ratio of each species’ mass to the total mass within the corresponding mode. The use of total aerosol mass in
549 the three modes as control variables—thereby reducing the number of control variables from 70 to 3—is planned for
550 a future phase of development. The use of total masses as control variables also reduces the cost of the background
551 error statistics calculation and iterative minimization (Kumar et al. 2019).

552 This study focused on surface-level PM_{2.5} and did not incorporate vertical profile constraints with satellite-based
553 aerosol optical depth (AOD) retrievals, which could further enhance forecast skill. A key challenge is the need for a
554 robust forward operator in the CRTM AOD module—specifically, the creation and validation of lookup tables
555 (LUTs) for AOD calculations with AQM. As an intermediate solution, existing LUTs in CRTM, such as the GEOS-5
556 LUTs, have been tested by grouping and mapping AQM aerosol species to those used in GEOS-5 (Wang et al.
557 2025). AOD assimilation also depends on an accurate vertical distribution of aerosols in the background field so that
558 the CRTM AOD operator can provide meaningful gradient information at the correct vertical levels to constrain the
559 analysis update. However, AQM models have shown deficiencies for the September 2020 fire events in representing
560 smoke concentrations at and above plume rise levels, largely due to how fire emissions are injected into the model.
561 This will be improved in the next update of the operational AQM.

562 Code and data availability

563 The AQMV7 model, JEDI software and PM_{2.5} and fire emission data we used in this research are publicly available
564 on on Zenodo (<https://doi.org/10.5281/zenodo.17049857>; Wang et al., 2025b).

565 Users are referred to the guidance on compiling and running the model:
566 <https://ufs-srweather-app.readthedocs.io/en/develop/UsersGuide/index.html> (Last accessed on August 26, 2025).

567 Global Forecast System analysis data were downloaded from the NCAR Research Data Archive:
568 <https://doi.org/10.5065/D65D8PWK> (last access: Aug 26 2025)

569 Author contribution

570 HW designed and developed the PM_{2.5} DA capability within JEDI for the AQM model, conducted experiments, and
571 evaluated performance; CM and JB contributed to PM_{2.5} DA methodology, advised on code implementation, and
572 assisted in performance analysis; SW contributed to PM_{2.5} DA methodology and experimental design; RL
573 conducted control experiments and contributed to workflow development; JL and KW contribute to model
574 configuration and control run setup; YT contributed to background error modeling and observational error
575 specification; HC, AT and HL contributed to workflow development; JL performed quality control and correction of
576 PurpleAir observations.

577 Competing interests

578 The authors declare that they have no conflict of interest.

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583 the PurpleAir observations.

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587 as well as any views or opinions expressed herein, are those of the authors and do not necessarily reflect those of
588 NOAA or the Department of Commerce.

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