1 **Air Quality Estimation and Forecasting via Data Fusion with Uncertainty**
2 **Quantification: Theoretical Framework and Preliminary Results**

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12 **Key Points:**

13 • The proposed data fusion method produces a-priori uncertainty assessments and
14   confidence intervals for estimates and forecasts

15 • Confidence intervals were found to be mostly reasonable in a test case study for nitrogen
16   dioxide across four months and two cities

17 • The method provided overconfident estimates for sites within 100 meters of highways

18 **Abstract**

19 Integrating air quality information from models, satellites, and in-situ monitors allows for both
20 better estimation of air quality and better quantification of uncertainties in this estimation.
21 Uncertainty quantification is important to appropriately convey confidence in these estimates and
22 forecasts to users who will base decisions on these. Uncertainty quantification also allows tracing
23 the value of information provided by different data sources. This can identify gaps in the
24 monitoring network where additional data could further reduce uncertainties. This paper presents
25 a framework for data fusion with uncertainty quantification, applicable to multiple air-quality-
26 relevant pollutants. Testing of this framework in the context of nitrogen dioxide forecasting at sub-
27 city scales shows promising results, with confidence intervals typically encompassing the expected
28 number of actual measurements during cross-validation. The framework is now being
29 implemented into an online tool to support local air quality management decision-making. Future
30 work will also include the incorporation of low-cost air sensor data and the quantification of
31 uncertainty at hyper-local scales.

32 **Plain Language Summary**

33 Poor air quality has adverse impacts on human and environmental health. Estimating and
34 forecasting air quality accurately can improve early warnings and mitigation for poor air quality.
35 Furthermore, understanding the uncertainties and degree of confidence in these forecasts and
36 estimates can help air quality managers know when and where they can be relied upon, and where
37 more data might still be needed. This paper outlines a method to combine air quality information
38 from models, satellites, and ground-based monitors, and to assess the confidence in the combined
39 output. Combining all these data sources can give us a better overall understanding of air quality,
40 and making comparisons between them allows us to better understand uncertainties. Testing out
41 the method proposed in this paper, we find that the method can produce reasonable assessments of
42 the confidence it has in its estimates, with the expected numbers of actual measurements usually
43 falling within the confidence intervals produced by the method. An exception is when this method
44 is applied very close to a major pollution source (e.g., a highway, in our study). In such cases, since
45 the method does not know that there is such a source nearby, it tends to be overconfident in its
46 prediction.

47 **1 Introduction**

48   Poor air quality is a major global public health concern. The 2019 Global Burden of Disease
49 study identified air pollution as the leading environmental risk factor for human premature
50 mortality (Murray et al., 2020). To mitigate this public health problem on a global scale, air quality
51 managers and practitioners first need access to accurate and comprehensive information on the
52 state of air quality in their areas. Such information might come from a variety of disparate sources.
53 In-situ measurements of air quality, typically obtained from instruments operated by regulatory
54 bodies, e.g., the Environmental Protection Agency in the United States, are considered the trusted
55 standard for assessing air quality. At a global scale, however, the relatively low density of such
56 measurements means that regulatory instruments alone often cannot provide necessary air quality
57 information to answer basic questions relevant to public health (Martin et al., 2019). Low-cost air
58 quality sensors (LCS) are increasing in prominence to address this in-situ data gap (e.g., Tanzer et
59 al., 2019; Rose Eilenberg et al., 2020). As the name implies, these provide a less expensive
60 alternative to traditional regulatory-grade air quality monitors (RGM). As a tradeoff to achieve this

61 lower cost, LCS suffer from greater measurement uncertainties, and thus, require extensive
62 calibration and validation efforts to generate useable data (Giordano et al., 2021). LCS can also be
63 deployed to new areas which do not have the infrastructure to support RGM. LCS provide the only
64 currently feasible means of routine air quality assessment in many low-and-middle-income
65 countries (Hodoli et al., 2023; McFarlane, Isevulambire, et al., 2021; Raheja et al., 2022).

66   Even so, the availability of local air quality data from in-situ RGM or LCS may not provide
67 sufficient situational awareness to air quality managers. Other, more globally available data
68 sources may be required. One important source of such global data is satellite remote sensing
69 retrievals of atmospheric composition. These data are provided by a fleet of instruments operated
70 by national aerospace agencies and the private sector. By providing in many cases globe-spanning
71 monitoring of the chemical and physical properties of the atmosphere at increasingly fine spatial
72 resolution, satellite data can fill many gaps in our understanding of the composition of the
73 atmosphere. However, satellite remote sensing has some key limitations with respect to air quality
74 applications. Typically, remote sensing estimates take account of the entire atmospheric column,
75 rather than the surface-level concentrations which are most relevant to air quality and the
76 associated health exposure risk. The relationship between surface and column quantities is
77 dependent on many factors. Thus, while promising, certain expertise and domain knowledge is
78 required to correctly interpret satellite data for air quality purposes, which may be a barrier to its
79 routine use in many areas (Anenberg et al., 2020; Duncan et al., 2021; Holloway et al., 2021).

80   Other sources of global air quality information are atmospheric chemistry and transport
81 models (CTM). These models seek to estimate the state of the atmosphere, including parameters
82 relevant for air quality, based on mathematical representations of chemical and physical processes
83 combined with input data related to boundary conditions, e.g., the estimated emissions of various
84 pollutants into the atmosphere. These models produce spatially comprehensive datasets and have
85 the potential to forecast future air quality. However, their estimates may be biased due to
86 incomplete and/or outdated input information or by inadequate representation of some chemical
87 or physical processes. For example, inadequate temporal resolution for emissions data, differing
88 vertical representations between the model and observations, as well as boundary layer mixing
89 were found to impact the ability of the GEOS-Chem model to represent diel variations in fine
90 particulate matter ($PM_{2.5}$) over the United States (Y. Li et al., 2023). Constraining CTM with
91 observations from satellites, RGM, LCS, or a combination thereof via data assimilation is a widely
92 used approach to addressing these model shortcomings. Assimilation of satellite data is more
93 typical for global-scale CTM (Bocquet et al., 2015; Kelp et al., 2023), while in-situ data
94 assimilation is more typical for sub-city to national scale CTM (Lopez-Restrepo et al., 2021;
95 Schneider et al., 2023; Hassani et al., 2023).

96   Data fusion is an approach for bringing together various data sources. In contrast to data
97 assimilation, where observations are used to update the state of a model, data fusion combines
98 multiple data sources to produce a new data product, distinct from the inputs. A typical niche filled
99 by data fusion is "downscaling" of coarser-resolution regional or global CTM output to produce
100 more locally applicable outputs (Diao et al., 2019). A myriad of approaches using different inputs
101 and methodologies has been proposed. On a local scale, data fusion of a dispersion model and LCS
102 data has supported hourly PM_{10} mapping in Nantes, France (Gressent et al., 2020). Regionally,
103 satellite information is commonly used to support data fusion approaches; fusion of satellite
104 aerosol optical depth (AOD), land use information, and meteorological data with surface
105 observations from RGM and LCS allowed for daily 1-km resolution estimation of $PM_{2.5}$ over

106 California, USA (Bi et al., 2020). Satellite AOD, RGM, and LCS data were similarly combined
107 for $PM_{2.5}$ mapping over Taiwan (J. Li et al., 2020). Globally, data fusion approaches are used to
108 create yearly, monthly, or daily average surface $PM_{2.5}$ and constituent estimates (van Donkelaar et
109 al., 2015, 2021; Wei et al., 2023). These estimates support analysis of the global impacts of air
110 quality (Murray et al., 2020). For forecasting applications, i.e., prediction of surface concentrations
111 in advance, bias correction for an ensemble of CTM was performed using surface RGM
112 observations in both urban and rural areas to improve hourly $PM_{2.5}$ forecasting over the USA
113 (Zhang et al., 2020, 2022). CTM, satellite and RGM data are combined to improve hourly NO_2
114 forecasts at sub-city scale (Malings et al., 2021). Machine learning methods have also been used
115 for bias-correction of global CTM to produce daily $PM_{2.5}$ forecasts at 1-km resolution for
116 applications at sub-city scale (Keller et al., 2020; Duncan et al., 2021; Bi et al., 2022). These studies
117 demonstrate the wide applicability and flexibility of data fusion to incorporate models with various
118 observational datasets.

119 In contrast to deterministic methods, probabilistic estimates and forecasts for air quality
120 may be better suited to the needs of air quality managers and policy makers. For example, in a
121 decision-focused analysis of ozone forecasting based on public health protection, it was found that
122 single deterministic forecasts may produce less robust results compared to the use of multiple
123 forecasts or an ensemble of forecasts for guiding air quality decision-making (Balashov et al.,
124 2017; Garner & Thompson, 2012). This was because the ensemble forecasts more readily allowed
125 for choosing actions which would be robust under a range of outcomes, i.e., robust under
126 uncertainty. For global data fusion estimates of monthly $PM_{2.5}$, uncertainty quantification also
127 supports analyzing the impact of this uncertainty on global health and epidemiological assessments
128 (van Donkelaar et al., 2021). Several recent efforts have aimed at the quantification of uncertainty
129 in air quality estimation and forecasting. Most of these approaches make use of ensembles of
130 deterministic models (Garaud & Mallet, 2011; Gilliam et al., 2015; Riccio & Chianese, 2024) or
131 machine learning methods, e.g., using generative models to produce a simulated ensemble
132 (Fanfarillo et al., 2019). Data fusion approaches making use of geostatistical methods, especially
133 Gaussian process or kriging approaches, have inherent capabilities to constrain estimates and
134 quantify uncertainties for air quality estimation and forecasting (Wang et al., 2021). Kriging is
135 referred to as "objective analysis" or "optimum interpolation" in the early numerical weather
136 prediction literature (Diggle, 2010, p. 8). A major barrier to the wider use of probabilistic forecasts
137 in air quality applications has been the difficulty associated with the interpretation of probabilistic
138 forecasts by decision-makers and effectively communicating these to the public. Recent work has
139 aimed at addressing these issues by explicitly analyzing different interpretation strategies
140 corresponding with different desired outcomes (Balashov et al., 2023).

141 This paper presents a framework for combining CTM output, satellite remote sensing data,
142 and in-situ measurements from a combination of RGM and LCS via a data fusion approach to
143 support air quality estimation and/or forecasting. This framework includes explicit quantification
144 of uncertainties associated with outputs from each stage, i.e., as each additional dataset is added.
145 This paper aims at presenting a simple, generalizable method for data fusion with uncertainty
146 quantification which can be implemented for near-real-time applications, with more limited
147 computational requirements than a full data assimilation approach. We demonstrate this framework
148 with a case study, focusing on estimation and forecasting of nitrogen dioxide in two US cities (San
149 Francisco and New York City) in 2019. Nitrogen dioxide (NO_2), a regulated pollutant in the US
150 (US EPA, 2017), represents a useful test case since it is known to vary on fine spatial scales in
151 urban areas, which may not be captured even in high-resolution satellite datasets (e.g., Judd et al.,

152   2019). The ability to characterize this variability is an informative illustration of the capabilities
153   of the proposed framework. The development of analysis tools and data products which combine
154   multiple sources of air quality information, alongside methods to express confidence in or
155   quantification of uncertainties in these products, has been suggested as a key need of air quality
156   managers worldwide (Duncan et al., 2021). The methods presented in this paper are being
157   implemented as part of a NASA-funded project to develop such tools for air quality data managers.

2 Methods

158   **2 Methods**

159   2.1 Input datasets

160   The proposed data fusion approach makes use of three categories of input information:
161   CTM-based estimates and forecasts, satellite remote sensing data, and ground monitor data.

162   The NASA Global Earth Observing System Composition Forecast (GEOS-CF) system
163   generates CTM outputs used in this paper. GEOS-CF couples the GEOS atmospheric general
164   circulation model with the GEOS-Chem chemistry module (Keller et al., 2021). GEOS-CF
165   produces 5-day forecasts initialized every day, following a 24-hour historical simulation for the
166   previous day with the meteorology constrained by assimilated fields, to provide the best estimates
167   for the past atmospheric composition. Both forecast and historical model output are used here.
168   Hourly-average "surface-level" (average for the GEOS model's lowest level, nominally 130 m
169   thick) nitrogen dioxide concentrations along with tropospheric column concentrations are used for
170   the year 2019. GEOS-CF outputs are on a 0.25° or roughly 25 km latitude-longitude grid.

171   The TROPOMI instrument on the Sentinel 5P satellite provides retrievals related to
172   tropospheric column concentrations of NO_2 (Veefkind et al., 2012). Through an agreement with
173   the European Space Agency, TROPOMI data are also hosted at the [NASA Goddard Earth Sciences](#)
174   [Data and Information Services Center (GES DISC)](#), searchable via the [Common Metadata](#)
175   [Repository](#) system; these systems were used to identify and access relevant TROPOMI datasets.
176   Tropospheric NO_2 concentration data products are used here, with recommended data quality
177   filters for "good quality" retrievals. The latest high-resolution data product with a nominal pixel
178   size of 5.5 by 3.5 km is used.

179   This paper presents a case study focused on San Francisco, California, USA (defined as
180   between 37° N and 39° N and between 121° W and 123° W). Data for the month of September
181   2019 were used for the primary analysis; additional data from calendar year 2019 were also
182   included as potential inputs for calibration purposes and for additional analysis presented in
183   Section 3.3. An additional case study focused on New York City, New York, USA is also presented
184   in the supplemental materials, described in supplemental text S1. These locations were selected
185   due to their relatively high density of RGM for NO_2, as well as for comparability with previous
186   related work (Malings et al., 2021). Ground monitoring data for hourly NO_2 were obtained from
187   the US EPA's RGM network. Relevant data were queried using the [Air Quality System API](#).

188   2.2 Data fusion approach and uncertainty quantification

189   The method for air quality data fusion outlined here is adapted from prior work (Malings
190   et al., 2021). The major improvements presented here include (1) a generalization of the
191   methodology and notation, where relevant changes to corresponding elements of the prior work
192   will be noted, and (2) development of a framework for quantifying the uncertainty in fused
193   estimates of surface air quality, which was not present in the prior work. The method is separated

194   into four phases: phase 1 involves model-based historical estimates and forecasts only; phase 2
195   fuses satellite with model data; phase 3 integrates in-situ measurements in an "offline" manner,
196   useful mainly for bias correction; phase 4 integrates in-situ measurements in an "online" manner,
197   useful for near-term estimate and forecast updating.

198   *2.2.1 Phase 1: model-based estimation and uncertainty*

199   This data fusion approach starts with air quality estimate and forecast model outputs. Let
200     $M(x, t, \tau)$ denote the estimated surface concentration of a given pollutant applicable at location x
201   and time t produced by an air quality model (the GEOS-CF model in the current work). The
202   forecasting lead-time is denoted by τ. If target time t is in the future, lead-time τ will be the
203   difference between t and when the model forecast was initialized. If t is in the past, then $\tau = 0$,
204   and the latest available model output covering time t is used. Lead-time τ may not always be
205   explicitly noted for notational convenience; when it is omitted, assume $\tau = 0$. The phase 1 estimate
206   is simply the relevant model output:

207     $$E_1(x, t, \tau) = M(x, t, \tau). \tag{1}$$

208   Practically, it is important to note that while x represents a location on the Earth's surface
209   to arbitrary precision, the spatial resolution on which E_1 will be defined is limited to the spatial
210   resolution of the model. In future work, it is considered that an ensemble of air quality models,
211   either from different modeling systems or multiple initializations of the same model system, may
212   be used to inform the data fusion. In that case, $E_1(x, t, \tau)$ could be the mean of multiple available
213   models. Furthermore, the ensemble spread could be used for uncertainty quantification.

214   To better inform end-users on the uncertainty in data fusion estimates, we also aim to
215   quantify the uncertainty of $E_1(x, t, \tau)$ in terms of the expected mean square error of the estimate
216   with respect to the true concentration. We denote this uncertainty as $V_1(x, t, \tau)$. We estimate this
217   uncertainty as the sum of four components, where independence between the components is
218   assumed. These components are the uncertainty in the forecast due solely to its lead-time,
219     $V_{F1}(x, t, \tau)$, the uncertainty due to local variability in the air quality model output, $V_M(x, t)$, the
220   uncertainty due to potential bias in the air quality model, $V_{B1}(x, t)$, and the uncertainty due to the
221   representational error of the model, $V_{R1}(x, t)$, due to its relatively coarse spatial resolution. Thus:

222     $$V_1(x, t, \tau) = V_{F1}(x, t, \tau) + V_M(x, t) + V_{B1}(x, t) + V_{R1}(x, t). \tag{2}$$

223   Model-based uncertainties $V_{F1}(x, t, \tau)$ and $V_M(x, t)$ are estimated empirically using model
224   outputs. $V_{F1}(x, t, \tau)$ is estimated using the mean square difference of past model forecasts at lead-
225   time τ and estimates at lead-time 0 for location x. This is evaluated over a set of times denoted
226     $T_{c.t.o.d.}(t)$, representing times during a calibration period in the recent past, e.g., the prior week, at
227   the same time-of-day (t.o.d.) as the time of interest t. This is meant to account for potential
228   systematic differences in forecasting capabilities at different times of the day due to diel cycles or
229   initialization times.

230     $$V_{F1}(x, t, \tau) \cong \mathbb{E}_{t' \in T_{c.t.o.d.}(t)} \left[\left(M(x, t', \tau) - M(x, t', 0) \right)^2 \right], \tag{3}$$

231   where $\mathbb{E}_i[\cdot]$ denotes the expected value, i.e., the mean, of the expression in brackets with respect
232   to indexing parameter i. Note that $V_{F1}(x, t, 0) = 0$ by design, and so this term can be ignored for
233     $\tau = 0$.

234        $V_M(x,t)$ is estimated as the expected square difference of model outputs in the immediate
235   vicinity of location x and time t, i.e., the mean square difference of the model outputs in the grid
236   cells immediately surrounding it in space and time:

237        $$V_M(x,t) \cong \mathbb{E}_{x' \in X_n(x), t' \in T_n(t)} \left[\left(M(x',t') - M(x,t) \right)^2 \right],\tag{4}$$

238   where $X_n(x)$ represents the neighborhood of location x, i.e., its adjoining model grid cells
239   depending on the model spatial resolution, and $T_n(t)$ represents the neighborhood of time t, i.e.,
240   the preceding and subsequent time steps according to the model temporal resolution. The logic
241   behind this estimate is that, where model outputs are "smooth" in space and time, there is less
242   uncertainty in the model outputs, while when the model outputs are more variable in space and
243   time, there is greater uncertainty. This estimate depends on the model resolution, with lower
244   uncertainties estimated for finer resolutions, all else being equal. We consider this to be reasonable,
245   as finer resolution models will tend to explicitly represent processes at the relevant scale. However,
246   simply interpolating model outputs to a finer resolution would artificially reduce the uncertainty
247   estimate. This analysis should therefore be conducted at the native resolution of the model. A
248   schematic for this phase is provided in Supplemental Figure S1.

249   The remaining terms $V_{B1}(x,t)$ and $V_{R1}(x,t)$ are impossible to assess using the model alone
250   and must be estimated using external information, as will be discussed later (see Section 2.2.5).
251   Note that, if an ensemble of models is used, it may be possible to estimate $V_{B1}(x,t)$ using the mean
252   square differences between models in the ensemble (Riccio & Chianese, 2024). However, it may
253   still be the case that all models within an ensemble are systematically biased due to some common
254   underlying factor, e.g., all models using the same emissions dataset.

255   *2.2.2 Phase 2: model downscaling with satellite data*

256   In phase 2, relationships between column concentrations from model and satellite data are
257   used to inform the sub-model-grid variability of the pollutant of interest. The phase 2 estimate of
258   the concentration of this pollutant at time t and location x, $E_2(x,t,\tau)$, is the phase 1 estimate
259   modified by the satellite-informed sub-grid difference pattern $D(x,t)$:

260        $$E_2(x,t,\tau) = E_1(x,t,\tau) + D(x,t),\tag{5}$$

261   where:

262        $$D(x,t) = \mathbb{E}_{t' \in T_{c,overpass}(t)} \left[\left(S_{col}(x,t') - E_{1,col}(x,t') \right) \phi(x,t') \, \psi(x,t,t') \right].\tag{6}$$

263   This difference pattern is the mean of the difference between the satellite-retrieved column
264   concentration of the pollutant of interest, S_{col}, and the estimate of the same column quantity by the
265   model used in phase 1, $E_{1,col}$, multiplied by two scaling factors ϕ and ψ. This mean is calculated
266   during the calibration period associated with time of interest t considering only times when the
267   satellite was overhead, denoted $T_{c,overpass}(t)$. Practically, both ϕ and ψ are informed by the
268   model, which provides simulated data for all relevant surface and column quantities. Scaling
269   factor $\phi(x,t)$ accounts for the change in surface concentration corresponding with a unit change
270   in column concentration at location x and time t. We approximate this sensitivity using a ratio of
271   model values at this location and time:

272        $$\phi(x,t) \cong \frac{M(x,t,0)}{M_{col}(x,t,0)}.\tag{7}$$

273   Scaling factor $\psi(x, t, t')$ accounts for the ratio of changes in surface concentrations at
274   location x and time t to changes at location x and time t'. Again, we approximate this with a ratio
275   of model values:

276        $$\psi(x, t, t') \cong \frac{M(x, t, 0)}{M(x, t\prime, 0)}. \tag{8}$$

277   The definition of $D(x, t)$ presented in equation 6 is a generalization of "typical pattern"
278   extraction described in equations 1 and 2 of Malings et al. (2021). This generalization now
279   explicitly captures the relationship between surface concentrations and column quantities, which
280   was only implicit before. Equation 5 here then replaces equation 3 of Malings et al. (2021). A
281   schematic for this phase is provided in Supplemental Figure S2.

282   In general, it may be necessary to consider the observational operator and air mass factor
283   used in the satellite retrieval algorithm, as these affect the comparability between satellite retrieved
284   S_{col} and modeled $E_{1,col}$ (e.g., Cooper et al., 2020). No explicit consideration of this is made here;
285   instead, this will contribute to variability as discussed below. Future work may explicitly consider
286   these impacts, likely leading to a reduced uncertainty. Note that in the case of PM$_{2.5}$, AOD would
287   be the column quantity considered.

288   Similar to phase 1, the uncertainty of the phase 2 estimate, $V_2(x, t, \tau)$, is estimated as the
289   sum of the uncertainty due to forecast lead-time, $V_{F2}(x, t, \tau)$, the local variability of the model,
290   $V_M(x, t)$, the variance in the satellite-informed sub-grid difference pattern, $V_D(x, t)$, twice the co-
291   variance of the model and sub-grid difference pattern, $V_{MD}(x, t)$, the uncertainty due to the
292   potential bias in the model-and-satellite-derived surface concentration estimates, $V_{B2}(x, t)$, and the
293   uncertainty due to the representational error of the model-and-satellite-derived surface
294   concentration estimates, $V_{R2}(x, t)$:

295        $$V_2(x, t, \tau) = V_{F2}(x, t, \tau) + V_M(x, t) + V_D(x, t) + 2V_{MD}(x, t) + V_{B2}(x, t) + V_{R2}(x, t). \tag{9}$$

296   Model local variability $V_M(x, t)$ is carried from phase 1, and as in phase 1, $V_{F2}(x, t, \tau)$ can
297   be empirically estimated by examining the mean squared difference of forecasts with lead time τ
298   over the calibration interval at the same time of day:

299        $$V_{F2}(x, t, \tau) \cong \mathbb{E}_{t' \in T_{c,t.o.d.}(t)}\left[\left(E_2(x, t', \tau) - E_2(x, t', 0)\right)^2\right]. \tag{10}$$

300        $V_D(x, t)$ and $V_{MD}(x, t)$ can be estimated with the empirical variance and co-variance of
301   relevant terms involved in computation of the satellite-informed sub-grid difference pattern:

302        $$V_D(x, t) \cong \mathbb{V}_{t' \in T_{c,overpass}(t)}\left[\left(S_{col}(x, t') - E_{1,col}(x, t')\right) \phi(x, t') \, \psi(x, t, t')\right], \tag{11}$$

303   where $\mathbb{V}$ denotes a variance computation, and:

304        $$V_{MD}(x, t) \cong \mathbb{E}_{x' \in X_n(x), t' \in T_n(t)}\left[\left(E_1(x', t') - E_1(x, t)\right)\left(D(x', t') - D(x, t)\right)\right]. \tag{12}$$

305   Note that in this formulation, $X_n(x)$ now denotes the neighboring locations of x at the
306   (finer) spatial resolution of the satellite data, i.e., the adjoining pixel centroids. The final terms
307   related to bias $V_{B2}(x, t)$ and representational errors $V_{R2}(x, t)$ again cannot be estimated using the
308   model and satellite information alone and require surface-level information, as will be discussed
309   later (see Section 2.2.5).

310   Comparing $V_1(x, t, \tau)$ with $V_2(x, t, \tau)$, and assuming a zero lead-time such that forecast-
311   related uncertainty can be ignored, we can establish some constraints on the bias and
312   representational error from phase 1 using phase 2 results. Due to the inclusion of satellite data in
313   phase 2 compared to phase 1, we might assume that $V_2(x, t, \tau)$ will be less than or equal to
314    $V_1(x, t, \tau)$ generally. Thus:

315    $$V_{B1}(x, t) + V_{R1}(x, t) \geq V_D(x, t) + 2V_{MD}(x, t) + V_{B2}(x, t) + V_{R2}(x, t). \tag{13}$$

316   That is, uncertainty due to bias and representativity errors in phase 1 should be larger than
317   the analogous terms from phase 2 plus the variance and co-variance related to the satellite-
318   informed sub-model-grid difference patterns. Note that the inclusion of satellite information is
319   informing both sub-model-grid variability, which would tend to reduce (though not eliminate)
320   representational errors captured in $V_{R1}(x, t)$, as well as bringing in real-world measurement data,
321   which would tend to reduce (though not eliminate) model bias as represented in $V_{B1}(x, t)$. Using
322   this relationship, estimates of the phase 1 uncertainty terms can be made based on the relevant
323   phase 2 uncertainty terms, e.g., using the average of these terms within each model grid cell.

2.2.3 Phase 3: linear correction with reliable surface measurements

325   Phase 3 uses in-situ measurement data to correct for possible regional systematic errors in
326   the model-and-satellite-derived estimates of surface air quality from phase 2. As a simple case, a
327   linear correction is assumed with slope α and intercept β:

328    $$E_3(x, t, \tau) = \alpha E_2(x, t, \tau) + \beta. \tag{14}$$

329   This corresponds directly with equation 10 of Malings et al. (2021).

330   Coefficients α and β, as well as estimates of their variance V_α and V_β, co-variance $V_{\alpha\beta}$, and
331   residual regression variance V_{R3}, are derived from a linear regression analysis between phase 2
332   estimates $E_2(x, t)$ as the independent variable and ground-based air quality measurements $G(x, t)$
333   as the dependent variable over the calibration time interval T_c and the set of discrete surface
334   monitoring sites in the region available during the calibration time interval X_c:

335    $$\alpha, \beta, V_\alpha, V_\beta, V_{\alpha\beta}, V_{R3} = \mathbb{LR}_{t' \in T_c(t), x' \in X_c(x)}[G(x', t') \sim E_2(x', t', 0)], \tag{15}$$

336   where $\mathbb{LR}_{domain}[v_d \sim v_i]$ denotes a linear regression with independent variable v_i and
337   dependent variable v_d, conducted over a domain specified in the subscript of $\mathbb{LR}$. Since this
338   regression is being applied for historical data collected during the calibration time interval, the
339   phase 2 estimate with $\tau = 0$ is used, and so τ has been dropped here for notational convenience.
340   Note that a weighted linear regression can be applied, e.g., using a weight factor related to the
341   time-of-day as suggested in previous work (Malings et al., 2021, Section 3.5). In principle, other
342   approaches to regression can also be applied, including for example machine learning techniques
343   to account for non-linear relationships (e.g., as in Wei et al., 2023). In such a case, appropriate
344   characterization of the variance of the regression estimates and their covariance with explanatory
345   inputs would have to be performed. In this work, a linear regression approach is adopted as there
346   are well known closed-form solutions for computing the variance and covariance of the
347   parameters. A schematic for this phase is provided in Supplemental Figure S3.

348   In cases where both RGM and LCS provide in-situ data, a modified approach is
349   recommended. First, available RGM are used in phase 3 as outlined above. Then, LCS are

350 regionally calibrated before incorporating their data in phase 4. Details are provided in
351 supplemental text S2.

352   Uncertainty in the phase 3 estimate is based on the phase 2 estimated uncertainty, re-scaled
353 with regression terms, and with the uncertainties in these regression terms and residual variance
354 included:

355 $$V_3(x,t,\tau) = V_{F3}(x,t,\tau) + \alpha^2[V_M(x,t) + V_D(x,t) + 2V_{MD}(x,t)] + V_\alpha E_2(x,t)^2 +$$
356 $$2V_{\alpha\beta}E_2(x,t) + V_\beta + V_{R3}. \tag{16}$$

357   Now that in-situ data have been included, systematic bias due to the misrepresentation of
358 the surface air quality due to model and satellite information only, as well as representational issues
359 due to the limited spatial resolutions of the model and satellite data with respect to specific points
360 represented in the surface data, are considered to be captured in terms related to regression
361 coefficient variance and residual variance. However, practical limitations on the availability of
362 surface air quality measurement sites, as well as the tendencies of such sites to be clustered in
363 high-population-density areas, might mean that there are some residual biases which are not fully
364 captured in this formulation. In other words, by necessity, the data fusion process will be tailored
365 towards better representing locations where surface monitors already exist, and the above
366 formulation for phase 3 uncertainty will tend to be more appropriate in those types of areas, rather
367 than, e.g., more rural areas which are not covered by surface-based monitors. Furthermore, biases
368 in the in-situ data will not be accounted for, e.g., the known sensitivity of NO_2 monitors to other
369 species (e.g., Steinbacher et al., 2007).

370   Comparing the phase 2 and 3 variance estimates, assuming zero lead-time, and assuming
371 that inclusion of surface information will tend to decrease phase 3 uncertainty with respect to phase
372 2, we can establish that:

373 $$V_{B2}(x,t) + V_{R2}(x,t) \geq (\alpha^2 - 1)[V_M(x,t) + V_D(x,t) + 2V_{MD}(x,t)] + V_\alpha E_2(x,t)^2 +$$
374 $$2V_{\alpha\beta}E_2(x,t) + V_\beta + V_{R3}. \tag{17}$$

375   Note that we have now established a "chain" of relationships connecting various bias and
376 representational error terms, which could not be directly quantified, to terms which can be
377 empirically estimated based on the data fusion process. This gives us a basis for quantifying these
378 uncertainties in earlier phases as well; this will be discussed further in Section 2.2.5.

379   *2.2.4 Phase 4: updating with recent, nearby in-situ data*

380   Phase 4 enables the use of recent and nearby surface measurement data to provide updates
381 to estimates and forecasts from phase 3 via a spatio-temporal kriging approach. This process is
382 expressed as:

383 $$E_4(x,t,\tau) = E_3(x,t,\tau) + \sum_{x'\in X_{near}(x), t'\in T_{recent}(t)} K(x,x',t,t') [G(x',t') - E_3(x',t')],$$
384 $$\tag{18}$$

385 where $X_{near}(x)$ denotes surface measurement locations arbitrarily "nearby" to x, $T_{recent}(t)$
386 denotes times arbitrarily "recent" with respect to t, and $K(x,x',t,t')$ is the kriging update factor,
387 encompassing the relationship between concentrations at spatio-temporal coordinates x,t and
388 x',t'. This relationship is a combination of variance and co-variance relationships between the
389 locations as well as the measurement noise. $K(x,x',t,t')$ is evaluated with the assistance of a
390 kernel function, used in Gaussian process regression to parameterize these co-variances based on,

391   e.g., the difference in space and time between the two sets of coordinates (Rasmussen & Williams,
392   2006). Recent work has proposed the use of Gaussian process regression for interpolating air
393   quality data in space and/or time based on sparse measurements, and have proposed using square
394   exponential, Matérn, and periodic kernel functions for this purpose for different pollutants of
395   interest (Jang et al., 2020; Malings et al., 2021; Wang et al., 2021). The approach used here to
396   determine appropriate kernel functions and parameters is described in (Malings et al., 2021, section
397   3.7). Equation 18 combines equations 11 and 14 of Malings et al. (2021), using a more generic
398   notation of the kernel. A schematic for this phase is provided in Supplemental Figure S4.

399   Spatio-temporal kriging also quantifies the resulting uncertainty reduction:

400   $$V_4(x,t,\tau) = V_3(x,t,\tau) - \sum_{x' \in X_{near}(x), t' \in T_{recent}(t)} K(x,x',t,t') \, \text{cov}[E_3(x',t'), E_3(x,t)],$$
401   $$(19)$$

402   where $\text{cov}[E_3(x',t'), E_3(x,t)]$ denotes the covariance between surface concentrations of the
403   pollutant of interest between spatio-temporal coordinates x,t and x',t', which is again evaluated
404   using the kernel function.

405   For practical purposes, appropriate definitions for $X_{near}(x)$ and $T_{recent}(t)$ will have to be
406   chosen to balance accuracy with the computational intensiveness of considering many
407   measurements in this updating, which is a typical limitation of Gaussian process regression. In this
408   paper, we use all surface measurement locations in our application region but use only the most
409   recent measurement from each location.

410   *2.2.5 Quantifying uncertainties in phases 1 and 2*

411   Following phases 1 and 2 of the data fusion approach outlined above, there remain several
412   terms related to potential bias and representativity errors which are not quantifiable given the
413   inputs available at these phases. However, following phase 3, the inclusion of ground-based
414   monitor data allowed the full quantification of uncertainty as expressed in equation (16). Using
415   this fact, alongside the inequality relationships presented in equations (13) and (17), we conducted
416   an empirical analysis comparing the quantified uncertainties at different phases. Based on this
417   analysis, we propose the following parametric estimates for the unquantified portions of the
418   uncertainties in phases 1 and 2:

419   $$V_{B1}(x,t) + V_{R1}(x,t) \cong \eta_1^2(t \bmod 24\text{h}) \, \mathbb{E}_{t' \in T_c(t)} \, V_M(x,t'),$$ $$(20)$$

420   $$V_{B2}(x,t) + V_{R2}(x,t) \cong \eta_2^2(t \bmod 24\text{h}) \, \mathbb{E}_{t' \in T_c(t)}[V_M(x,t') + V_D(x,t') + 2V_{MD}(x,t')].$$
421   $$(21)$$

422   In these estimates, the unquantified portions of the uncertainty are related to the quantified
423   performance via empirically determined factors η_1 for phase 1 and η_2 for phase 2. These factors
424   are assumed to vary as a function of time-of-day, based on observations for how relationships
425   between different portions of the quantified uncertainty varied over the calibration period
426   investigated here. Empirically determined values of η_1 and η_2 for San Francisco are presented
427   Supplemental Figure S5; values for New York City are presented in Supplemental Figure S6.

428   This proposed approach has important limitations. Most notably, it relies on proceeding to
429   phase 3 of the data fusion approach. In regions without ground-based monitoring, or where only a
430   small number of ground-based monitors are available, the results from phase 3 of the data fusion
431   approach will be unavailable or highly unreliable. Empirically determined values of η_1 and η_2

432 from another region might be used, but there is no reason to expect these to generalize well. Thus,
433 in the absence of surface data, full uncertainty quantification in phase 1 or 2 of the data fusion
434 approach becomes unreliable.

435 2.3 Confidence interval determination

436 Following the approaches for data fusion with uncertainty quantification presented in the
437 previous section, for a location of interest x and time of interest t, with forecast lead time τ, and
438 for data fusion phase p, a data fusion "best estimate" for the quantity of interest $E_p(x, t, \tau)$ will be
439 available, along with an uncertainty estimate for this quantity, $V_p(x, t, \tau)$. To make practical use of
440 these outputs, in this work, we use them to define confidence intervals (CI) for our estimates or
441 forecasts. To do this, a probabilistic distribution must be assumed for the quantity of interest. In
442 this work, we assume a lognormal distribution, which is a typical assumption for many non-
443 negative quantities relevant to air quality. This distribution is parameterized by the mean μ and
444 standard deviation σ of the associated normal distribution. These are calculated from the outputs
445 of the data fusion process as follows:

446
$$\mu_p(x, t, \tau) = \log \left[\frac{E_p(x, t, \tau)}{\sqrt{1 + \frac{V_p(x, t, \tau)}{E_p(x, t, \tau)^2}}} \right], \tag{22}$$

447
$$\sigma_p(x, t, \tau) = \sqrt{\log \left[1 + \frac{V_p(x, t, \tau)}{E_p(x, t, \tau)^2} \right]}. \tag{23}$$

448 The quantity of interest $F_p(x, t, \tau)$ is then a lognormally distributed random variable:

449
$$F_p(x, t, \tau) \sim \text{LN} \left(\mu_p(x, t, \tau), \sigma_p(x, t, \tau) \right). \tag{24}$$

450 where $\text{LN}(\mu, \sigma)$ denotes a lognormal distribution with mean μ and standard deviation σ for the
451 associated normal distribution. This distribution can be used to determine a CI for the quantity of
452 interest. For example, the 75 % confidence range is defined with a lower bound, representing the
453 12.5[th] percentile of the lognormal distribution, and an upper bound, representing the 87.5[th]
454 percentile of the lognormal distribution.

455 The lognormal distribution assumption is of course an approximation of the true
456 distribution of the quantity of interest. Therefore, the CI determined as described above would not
457 necessarily correspond to the actual CI for the quantity of interest, even if the mean and variance
458 were known exactly. However, some assumption about the distribution of the quantity of interest
459 is necessary, as its true distribution will not be known a priori.

460 **3 Results**

461 In this section, we investigate the performance of the proposed data fusion framework
462 described above through testing with actual data. In all cases, a leave-one-site-out cross-validation
463 approach is used. For the given domain of interest, data from all but one of the active ground
464 monitoring sites are considered as inputs to the data fusion algorithm. Concentrations are estimated
465 or forecast via the data fusion approach for the location of the single held-out site. All sites are
466 cycled through in this manner, resulting in estimates and forecasts of concentrations at each
467 monitoring site using data from all other sites. This allows for comparisons to be made between

468 actual concentration measurements at each site and the estimates or forecasts from the data fusion
469 using all information except for any measurements at the site in question. This allows for
470 evaluating how the method would perform at an arbitrary location without in-situ data. A 14-day
471 moving calibration time window is used across all phases, i.e., for a given time of interest t and
472 forecast lead time τ, the calibration interval T_c ranges from $t - \tau - 14$ days to $t - \tau$. This ensures
473 that only input data available at or before a given time are used, with lead time measured from the
474 time of the most recently available data. However, data latency effects are not considered, e.g.,
475 satellite data are assumed to be available as soon as the satellite passes overhead. Data latency
476 effects can be estimated by inflating the lead time, e.g., performance of a 1-day forecast using
477 inputs with a 1-day data latency is assumed to be similar to a 2-day forecast.

478   For illustrative purposes, an example of time series output from the data fusion approach
479 is presented in Figure 1. Outputs from phase 4 of the data fusion process, the colored line, including
480 a 50 % CI, the colored area, are compared to actual measurements from the RGM at this location,
481 the black line. In the figure, local midnight of September 17th is considered to be "the present"
482 (marked by grey dotted vertical line). Before this time, estimates are shown considering zero lead
483 time, i.e., GEOS-CF historical outputs are used together with satellite and RGM data available up
484 to and including the indicated time. After midnight of September 17th, forecasts are shown with
485 increasing lead time, i.e., the latest GEOS-CF forecast initialized 12 UTC the previous day is used,
486 together with satellite and RGM data collected prior to September 17th. For the historical estimates,
487 availability of in-situ measurements at other RGM sites has allowed short-term spikes to be better
488 represented, with the CI likewise being wider to capture the variability. For the forecasts, such
489 spikes are not specifically captured, but the CI tends to be wider throughout the timeseries,
490 accounting for the potential for such spikes to occur. In this example, the estimated CI tend to be
491 underconfident: 75 % of actual measurements fell within the 50 % CI depicted. An analysis of the
492 accuracy and precision of the forecasts (not considering their confidence estimates) is presented in
493 Supplemental Figure S7.

494
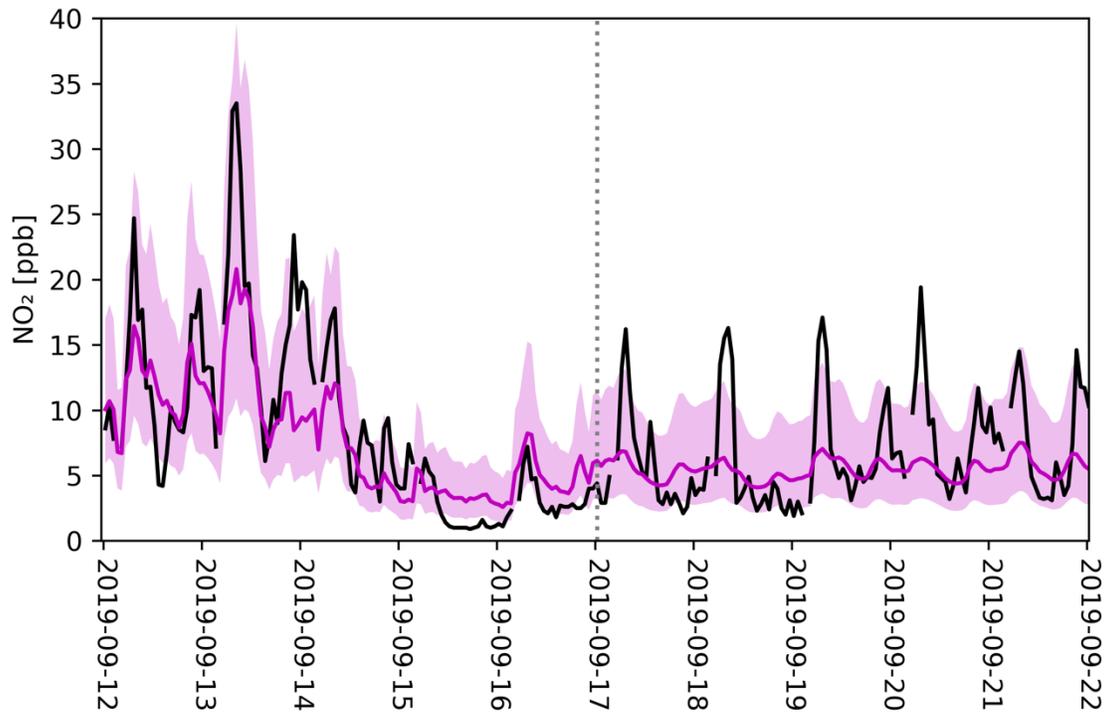
Figure 1. Representative example of probabilistic estimates and forecasts for hourly surface-level NO$_2$ concentrations at the Redwood City monitor site (AQS ID 06-081-1001) in San Francisco, between September 12 and 22, 2019 local time. The black line indicates the reported concentrations from the regulatory monitor, i.e., the true concentration. The colored line indicates the mean estimated concentration from phase 4 of the data fusion process, $E_4(x, t)$. The colored shaded areas denote the 50 % CI for the estimates. Estimates are presented with zero lead time up to midnight on September 17th, denoted with a vertical dotted line. Beyond this, forecasts with an increasing lead time are presented.

503   3.1 Assessment of confidence interval coverage for different phases of data fusion

504   To investigate the accuracy of the assessed uncertainties in the data fusion, the fraction of
505   actual measurements falling within the estimated 75 % CI across different phases of the data fusion
506   approach is presented in Figure 2. This analysis considers all NO$_2$ monitor sites operating during
507   September 2019 in the San Francisco study region, a total of 25 sites. The fraction of measurements
508   falling within the 75 % CI is calculated for each site and considering the estimates for each phase
509   of the data fusion process. Total uncertainties for phases 1 and 2 are estimated as outlined in section
510   2.2.5. Horizontal colored solid and dotted lines indicate the median, 25th percentile, and 75th
511   percentile values of these fractions across all sites for each phase. Furthermore, sites are divided
512   into types based on their assumed scale of spatial representativity, which is assessed for each
513   monitoring site by US EPA. The five site types are microscale (0-0.1 km; 5 sites), middle (0.1-0.5
514   km; 3 sites), neighborhood (0.5-4 km; 13 sites), urban (4-50 km; 3 sites) and regional (50+ km; 1
515   site), as defined in 40 CFR Part 58. By investigating the capacity of the data fusion system to
516   capture uncertainties at different spatial scales in this way, its benefits and limitations can be better
517   understood.

14
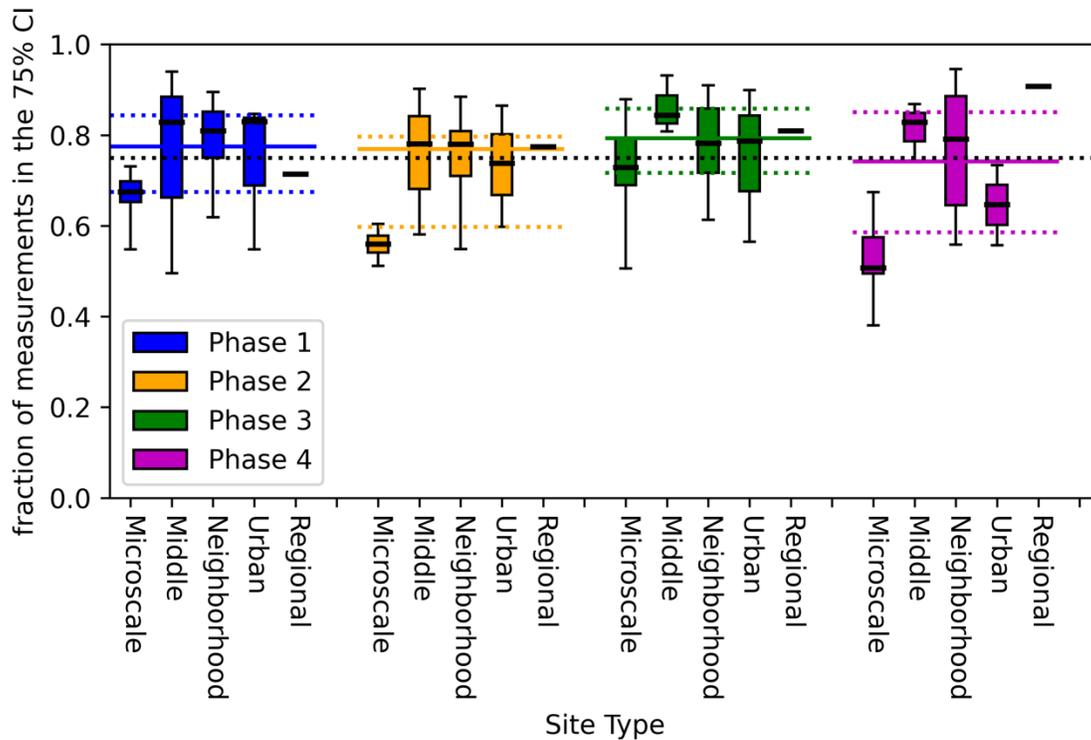
Figure 2. Assessment of the fraction of actual measurements falling within the estimated 75 % CI for different phases of the data fusion process, with phases represented by different colors. The analysis represents data from 25 active NO$_2$ ground monitoring sites in the San Francisco study region for September 2019. A horizontal dotted line across the figure indicates the goal, i.e., 75 % of measurements falling within the 75 % CI. For each ground monitor site, the fraction of measurements at that site falling within the 75 % CI is calculated. For each phase, a solid horizonal line in the corresponding color indicates the median of these fractions across sites, and two horizontal dotted colored lines indicate the 25th percentile and 75th percentile of these fractions across sites. Furthermore, monitoring sites are divided into different site types. The spread in fraction of measurements falling within the 75 % CI for each site type is indicated with a box-and-whisker plot. In each box-and-whisker plot, the horizontal line inside the box denotes the median, the box denotes the 25th-to-75th-percentile range, and the whiskers denote the full range.

Overall, for all phases of the data fusion process, the estimated 75 % CI captures roughly 75 % of measured data. Performance is most consistent for phases 1 and 3, which have the smallest inter-quartile spreads in fraction of measurements falling within the 75 % CI. Focusing on phase 1, where only model outputs are considered, performance is consistent across most site types. There is a slight bias towards underconfidence, i.e., more measurements falling within the 75 % CI than expected. For microscale sites, however, estimates are systematically overconfident, with fewer measurements falling within the 75 % CI than expected. Considering the native spatial resolution of the model, better representation of uncertainties at urban and regional scales is to be expected. There is a lack of information at this stage to make informed assessments of confidence at finer spatial scales. This manifests in the results with a slightly larger spread in performance for middle scale sites and the overconfidence noted for microscale sites.

15

543   In phase 2, this is exacerbated, with increased overconfidence for estimates of microscale
544   sites. Again, this can be explained by considering that, at phase 2, satellite data from TROPOMI
545   with a nominal spatial resolution on the order of 5 km has been incorporated. This would be
546   expected to improve assessments at neighborhood sites. This is reflected in the results with a slight
547   decrease in the underconfidence of estimates for sites at this scale. However, there continues to be
548   a lack of relevant information at finer spatial scales, and so while uncertainty estimates seem to
549   have been improved for most scales, they have substantially degraded for microscale sites.

550   In phase 3, with the incorporation of ground-based data, uncertainties at microscale sites
551   are now better represented overall, although one microscale site (denoted with the lower whisker)
552   continues to be quite overconfidently estimated. However, middle scale sites are now being
553   represented with systematic underconfidence. This might be a consequence of the relative numbers
554   of sites in each type. There are 5 microscale and 3 middle scale sites in the study domain.
555   Furthermore, because of the cross-validation approach, data from the site being evaluated are not
556   included, underrepresenting that type. Thus, the approach of phase 3 would tend to better represent
557   the more numerous site type. This could be accounted for by assigning lesser weights to certain
558   types of sites when conducting the linear regression in phase 3. However, because one would not
559   know a-priori the characteristics of the site at which concentrations are to be estimated, weighting
560   different types of sites differently might not be an appropriate approach. Uncertainty estimates for
561   neighborhood, urban, and regional sites appear reasonable, if slightly underconfident overall.

562   In phase 4, while uncertainty estimates seem to be most accurate in the median, the spread
563   in performance has increased. Microscale sites are again exhibiting systematic overconfidence,
564   along with urban scale sites, while middle scale and regional sites are underconfident. With only a
565   single regional site, however, that latter result is not necessarily robust. This varied performance
566   might be understood by considering that, due to the heterogeneity of urban areas, monitoring sites
567   of different types will tend to be interspersed with one another. For a given site, the closest site
568   which will have the greatest influence in the kriging approach of phase 4 is likely to be of a
569   different type than the site being estimated for in the cross-validation. Neighborhood sites are least
570   susceptible to this effect since, as the most numerous site type in the study area, the closest RGM
571   to a neighborhood site is often another neighborhood scale site. The microscale sites, on the other
572   hand, are closest to either neighborhood or urban scale sites, and the neighborhood or urban scale
573   sites likewise are often closest to microscale sites. A kernel function for the kriging approach not
574   based solely on distance might alleviate this difficulty, e.g., by defining similarities based on
575   similar land use and land cover factors (e.g., Gilpin et al., 2023). Such an approach would require
576   additional input information and is left as a subject for future improvements.

577   Across all phases, the best and most consistent results were observed for neighborhood
578   scale sites. This is probably due in part to their relative abundance, but also to the fact that their
579   representative scale (0.5-4 km) is of the same order as the satellite input data, which provides the
580   most relevant information about spatial heterogeneity of pollutant concentrations. Overall, this is
581   consistent with what might be expected, given the way in which the data fusion and associated
582   uncertainty quantification are being conducted. Results were also similar for different CI (see
583   Supplemental Figure S8).

584   3.2 Assessment of confidence interval coverage for different forecast lead times

585   Figure 3 presents an analysis of the fraction of measurements falling within the 75 % CI of
586   the uncertainty estimate as a function of the forecasting lead time. Several discrete lead times are

587 considered, and results for zero lead time are also presented for comparison; these were previously
588 presented in Figure 2.
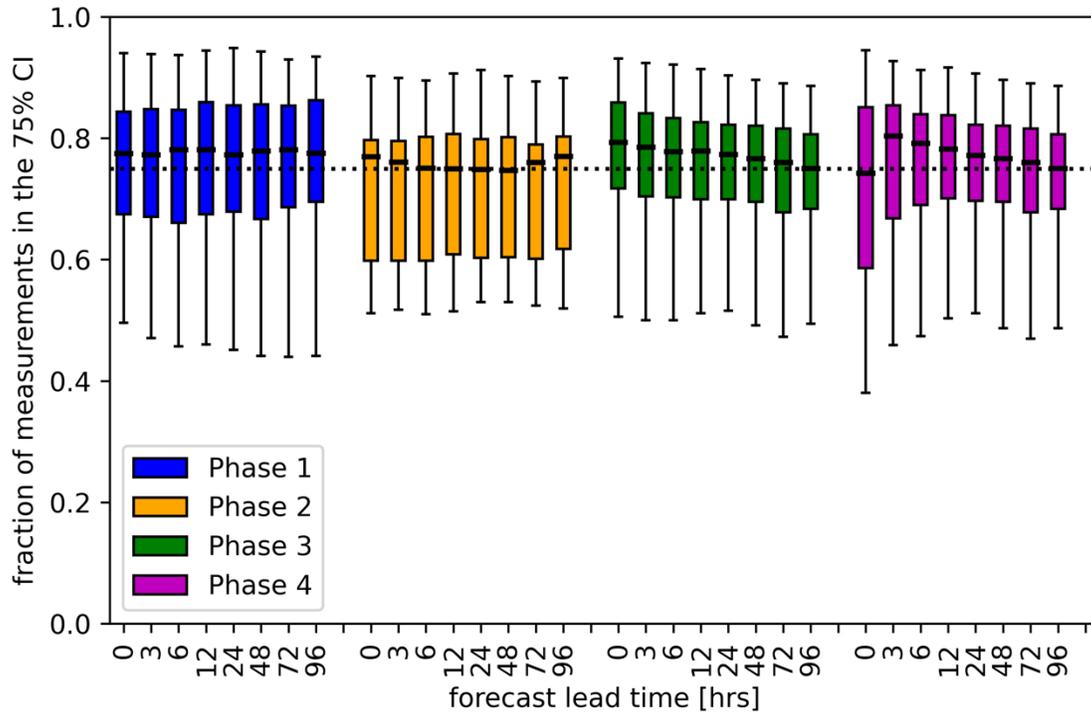
589

590 **Figure 3. Assessment of the fraction of actual measurements falling within the estimated 75**
591 **% CI for different phases of the data fusion process, with phases represented by different**
592 **colors, as a function of forecasting lead time, in hours. The analysis represents data from 25**
593 **active NO$_2$ ground monitoring sites in the San Francisco study region for September 2019. A**
594 **horizontal dotted line across the figure indicates the goal, i.e., 75 % of measurements falling**
595 **within the 75 % CI. For each ground monitor site, the fraction of measurements at that site**
596 **falling within the 75 % CI is calculated. The box-and-whisker plots denote the ranges of these**
597 **fractions across sites, with the horizontal line in the box denoting the median, the box**
598 **denoting the 25th-to-75th-percentile range, and the whiskers denoting the full range.**

599 Overall, there is little variation in the CI coverage as lead time increases, indicating that
600 the uncertainty quantification approach is applicable for forecasts as well as historical estimates.
601 For phase 3, there appears to be a tendency towards underconfidence at shorter lead times. For
602 phase 4, the spread in coverage decreases as the forecasting lead time increases. As noted
603 previously, the kriging approach of phase 4 with a distance-based kernel tends to induce under- or
604 overconfidence at nearby sites. As the forecasting lead time increases, the influence of the most
605 recent measurement data decreases, and the uncertainty quantification resembles that of phase 3.
606 While the incorporation of near-real-time data in phase 4 has notable benefits in terms of near-
607 term forecast accuracy, as noted in previous work (Malings et al., 2021), these results indicate that
608 there is also a trade-off in terms of slightly less realistic uncertainty estimates in the phase 4 near-
609 term forecasts compared to the other phases and to longer lead times.

610   3.3 Assessment of confidence interval coverage across different times of year

611   As an additional assessment, the methodology was applied across different months. Results
612   for CI coverage at zero forecast lead time in March 2019, June 2019, September 2019 (as presented
613   previously), and December 2019 are shown in Figure 4. There is some variability in performance
614   for different phases in different months. For example, in December 2019, phases 1, 3, and 4 show
615   a tendency for underconfidence in their estimates, although this is not apparent in phase 2.
616   Conversely, phase 2 exhibits overconfidence in June 2019, while this is not apparent for other
617   phases. This might indicate monthly or seasonally varying biases in the input data sources which
618   are not accounted for in the current method.

619
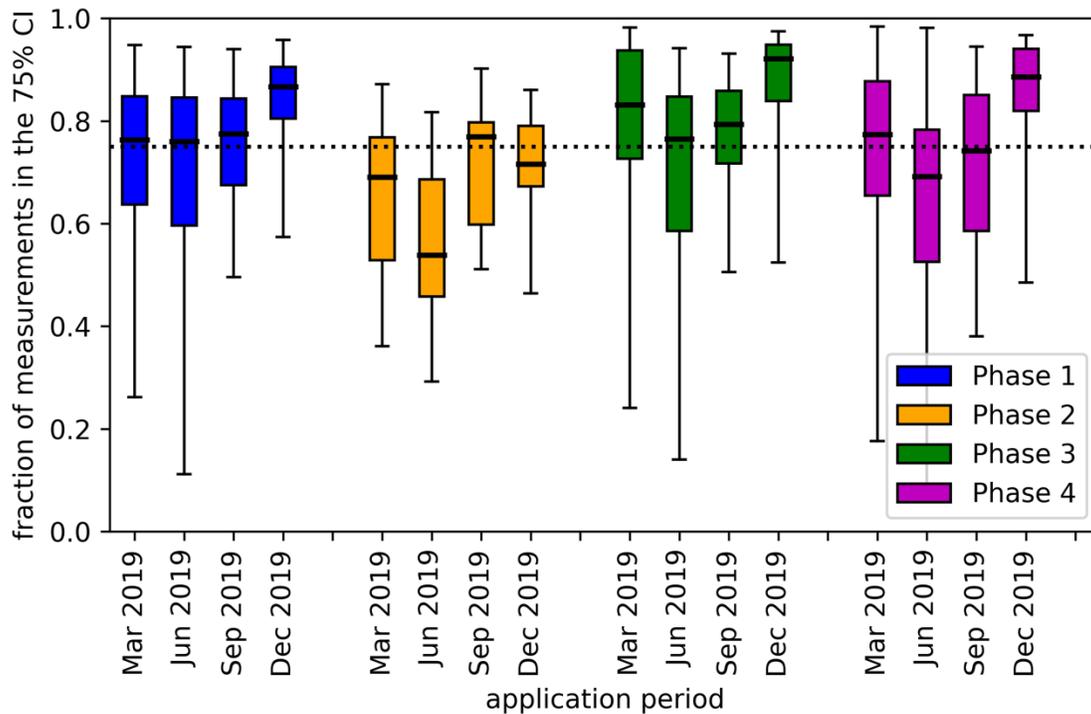
Figure 4. Fractions of measurements falling within the estimated 75 % CI for different
phases of the data fusion process, with phases represented by different colors, presented for
different application months. Box-and-whisker plots denote ranges of these fractions across
active NO$_2$ monitor sites in San Francisco during that month, with the horizontal line in the
box denoting the median, the box denoting the 25th-to-75th-percentile range, and the whiskers
denoting the full range. The horizontal dotted line across the figure indicates the goal, i.e., 75
% of measurements falling within the 75 % CI.

627   A similar assessment was conducted for the region of New York City, as discussed in the
628   supplemental materials. Results for CI coverage at zero forecast lead time in March 2019, June
629   2019, September 2019, and December 2019 are shown in Supplemental Figure S9. Similar
630   variability in performance for different phases in different months is observed as was noted above.
631   Underconfidence in December 2019 seems to be more extreme, especially in phase 1, than in the
632   case of San Francisco. Overconfidence in phase 2 also appears to be more severe. Again, monthly
633   or seasonal differences in relevant parameters, especially the factors η_1 and η_2 calculated for the
634   domain and kriging spatial and temporal scales associated with phase 4, might be influencing this.

635 The fact that month-to-month differences appear to be greater in New York City, where seasonal
636 differences in prevailing meteorological conditions are relatively greater than in San Francisco,
637 where such changes are relatively smaller, seems to corroborate this hypothesis. Thus, future
638 development should focus on better capturing such seasonal changes through dynamically
639 recalculating relevant parameters as part of the calibration process.

640 **4 Conclusions**

641 Overall, the proposed framework to estimate uncertainties and CI for concentration
642 estimates from data fusion produced reasonable results in most cases, with most CI coverage being
643 within about 10 percentage points of the theoretical value. There were also few instances of
644 extreme overconfidence (few measurements falling within the prescribed CI) or extreme
645 underconfidence (almost all measurements falling within the prescribed CI) observed in the results
646 presented here. These findings are encouraging given the various assumptions made in defining
647 the uncertainty quantification framework, including the assumption of lognormally distributed
648 concentrations.

649 The uncertainty quantification was found to be least accurate overall for microscale sites,
650 which are most impacted by hyperlocal sources. In the San Francisco case study, these sites were
651 adjacent to highways, which are most heavily impacted by NO_2 pollution. This finding is useful to
652 convey to any user of this system, i.e., that results may not be reliable within about 100 meters of
653 a major source like a highway or other intense combustion activity. Similar limitations are likely,
654 should the method be applied to other constituents measured near their respective sources.

655 It is also important to note that CI assessments are not being provided for independent data,
656 but rather there is significant autocorrelation in the data. For example, while a measurement might
657 have a 50 % chance of falling within a 50 % CI a-priori, if it is known that a recent measurement
658 fell outside this CI, it becomes much less likely that a new measurement will fall within the CI.
659 This effect can be noted on September 15th in Figure 1, when multiple measurements in sequence
660 were observed outside the 50 % CI.

661 Several areas of theoretical and practical improvement are noted for future work. As
662 suggested in Section 2.2.1, use of an ensemble of models rather than a single model in phase 1
663 would allow for estimating uncertainties at that phase based on variability across the ensemble.
664 For incorporating satellite data in phase 2, multiple sources of satellite data might be considered,
665 offering coverage at different times of day. Geostationary instruments like the recently launched
666 TEMPO might be particularly useful in establishing different values of $D(x,t)$ corresponding to
667 different times of day. Better definitions for the calibration dataset might also be explored, in
668 contrast to a simple moving time window as presented in Section 2.2.2. For example, forecasted
669 conditions might be matched to similar past conditions for which satellite data were available, in
670 an attempt to identify past situations which approximately match forecasted future conditions in
671 order to define a more suitable calibration dataset. There is also the possibility to include ancillary
672 datasets, such as land use information, as additional co-variates to explain local variability. These
673 might be incorporated using more sophisticated regression techniques, such as machine learning
674 approaches, in contrast to the linear techniques presented for phase 3 in Section 2.2.3. While it
675 would be necessary to develop customized uncertainty quantification schemes for these
676 techniques, they might be better suited to capturing non-linear relationships in the data. Finally,
677 the limitation of ground data availability and the resulting tendency of the approach to be biased
678 towards such areas, as mentioned in Section 2.2.3, might be addressed in a more systematic way,

679   e.g., via resampling or application of different weightings to data from different types of
680   monitoring sites in order to create a more unbiased calibration dataset.

681   Nevertheless, the framework established here presents a reasonable prior CI for the
682   estimates and forecasts of the proposed data fusion system, and this fact supports effective and
683   appropriate interpretation of its output by users. For example, these uncertainty estimates might be
684   applied with respect to a given regulatory pollutant threshold to estimate the probability of
685   exceeding that threshold. Such information could support air quality management decision-
686   making. In an ongoing project supported by the NASA Health and Air Quality Applied Sciences
687   Program, the authors are implementing the data fusion and uncertainty quantification scheme
688   presented here in an online application via the Google Earth Engine platform. It is hoped that this
689   application will present a useful tool for local air quality managers to visualize sub-city-scale
690   atmospheric composition and variability using a combination of model, satellite, and in-situ data.
691   This project is being conducted in collaboration with local environmental managers in the USA,
692   Brazil, and Senegal. An example prototype for this tool is presented in Figure 5. As part of this
693   project, the framework will also be extended to other relevant pollutants, primarily $PM_{2.5}$ and O_3.
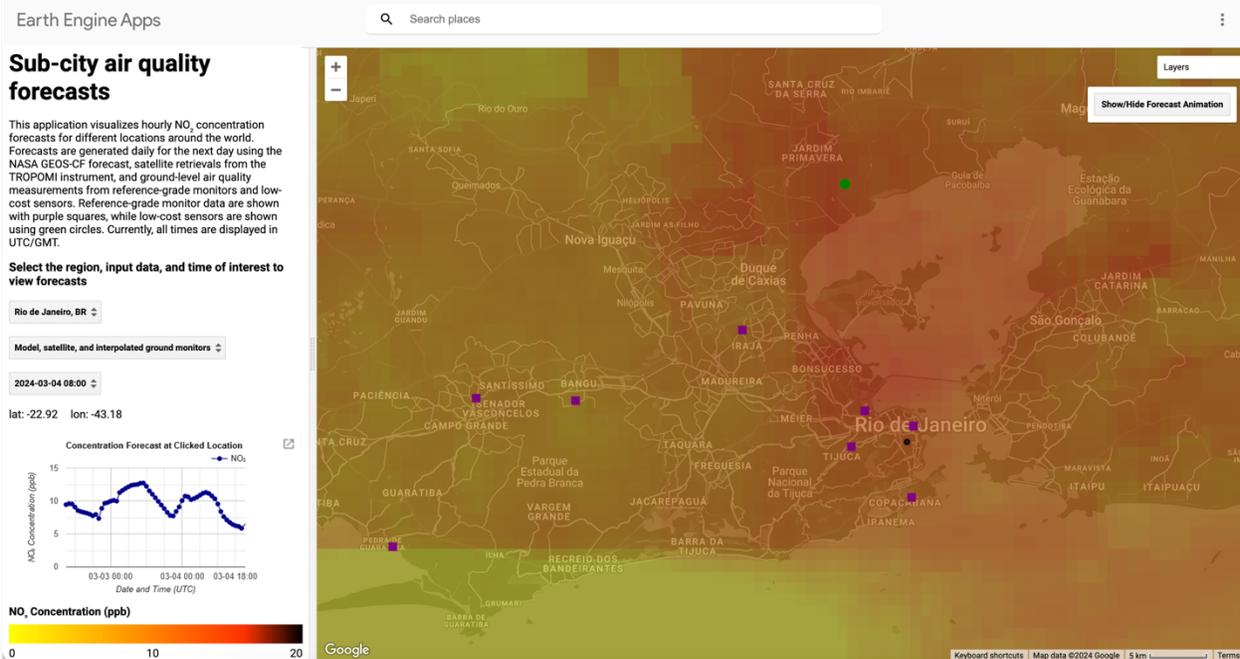
694

695 **Figure 5. Screenshot of an application currently under development which will implement**
696 **the data fusion framework presented here, including uncertainty quantification, via the**
697 **Google Earth Engine platform. This application will enable air quality managers to access**
698 **and visualize estimates and forecasts of relevant air quality parameters such as NO_2, O_3,**
699 **$PM_{2.5}$, along with associated expressions of confidence. Example outputs are presented for**
700 **the city of Rio de Janeiro, Brazil, one of the partners for this project.**

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Open Research

714 GEOS-CF outputs are available via the GMAO website; "AQC" and "XQC" collection files have
715 been used here. Other input data are available via NASA GES DISC and the US EPA Air Quality
716 System. Data and code used to generate the figures presented in this paper are available in an
717 online Zenodo archive (Malings, 2024), governed under a CC BY-NC License.

Author Contributions

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