

# A joint Bayesian space–time model to integrate spatially misaligned air pollution data in R-INLA

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## Abstract

In air pollution studies, dispersion models provide estimates of concentration at grid level covering the entire spatial domain and are then calibrated against measurements from monitoring stations. However, these different data sources are misaligned in space and time. If misalignment is not considered, it can bias the predictions. We aim at demonstrating how the combination of multiple data sources, such as dispersion model outputs, ground observations, and covariates, leads to more accurate predictions of air pollution at grid level. We consider nitrogen dioxide (NO<sub>2</sub>) concentration in Greater London and surroundings for the years 2007–2011 and combine two different dispersion models. Different sets of spatial and temporal effects are included in order to obtain the best predictive capability. Our proposed model is framed in between calibration and Bayesian melding techniques for data fusion. Unlike other examples, we jointly model the response (concentration level at monitoring stations) and the dispersion model outputs on different scales, accounting for the different sources of uncertainty. Our spatiotemporal model allows us to reconstruct the latent fields of each model component, and to predict daily pollution concentrations. We compare the predictive capability of our proposed model with other established methods to account for misalignment (e.g., bilinear interpolation), showing that in our case study the joint model is a better alternative.

## KEYWORDS

coregionalization model, data integration, geostatistical model, NO<sub>2</sub>, SPDE

## 1 | INTRODUCTION

Air pollution is a major concern for policy makers worldwide (EPA, 2016; European Commission, 2018; WHO, 2006), and there is extensive evidence of its negative effects, in particular on respiratory and cardiovascular diseases (Atkinson, Mills, Walton, & Anderson, 2015; COMEAP, 2015; Dominici, Peng, Barr, & Bell, 2010; Lipfert, 2017). Obtaining an accurate estimate of air pollution concentration is key for evaluating compliance with regulatory standards set by national and international environmental agencies and to reduce exposure misclassification in epidemiological studies (Berrocal, Gelfand, & Holland, 2012; Keller & Peng, 2019; Shaddick et al., 2018).

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Air pollution data come from different sources, each presenting some limitations: ground measurements from monitoring network stations, usually affected by sparse spatial resolution; estimates from land use regression models (LUR), which rely on the availability of accurate and dense monitor observations; satellite remote sensing data, sometimes poorly correlated with ground pollution level; simulations from deterministic models (e.g., chemical transport models or dispersion models), that can present prediction quality concerns despite the complete spatial coverage and high temporal resolution (Chang, 2016; Gelfand, Sahu, & Holland, 2012; Hoek et al., 2008; Johnson, Isakov, Touma, Mukerjee, & Özkaynak, 2010; Lee, Ferguson, & Scott, 2011; Shaddick et al., 2018; Shaddick & Wakefield, 2002; Shaddick, Zidek, & Liu, 2015).

Several “hybrid” approaches have been proposed to combine these data sources to draw from their strengths and to overcome their limitations, but not all of them address the discrepancy in the spatial resolution of the different data sources, which is known as *misalignment* or *change of support problem* (COSP).

## 1.1 | Main approaches to address spatial misalignment

In the context of COSP, we refer to upscaling methods when the target resolution is lower than the data resolution (e.g., point-to-area) and to downscaling when the target resolution is higher (e.g., area- or grid-to-point).

Model-based solutions for *data assimilation* (also referred to as *data fusion* or *data blending*) in environmental applications allow us to account for all sources of uncertainty while addressing COSP. These are usually set within a hierarchical Bayesian framework. Popular approaches include Bayesian melding and calibration techniques (Chang, 2016).

Bayesian melding assumes that both measurements and modeled data are error-prone realizations of an underlying latent true pollution field, and they both inform the posterior distribution of the latent process. Among the proposed melding strategies applied to misaligned air pollution data we find, for instance, the downscaling spatial Bayesian melding model by Raftery and Fuentes (2005), the upscaling spatial Bayesian melding model by Wikle and Berliner (2005), and the upscaling spatiotemporal fusion model by McMillan, Holland, Morara, and Feng (2010).

Calibration techniques assume that the model-based estimates (e.g., from dispersion models) are used in a regression framework as predictors against the monitoring site measurements. In this way the computational cost is reduced compared to melding, as the models only need to be fitted at the monitoring sites locations (Berrocal et al., 2012; Chang, 2016). Some examples are the block-averaging upscaling calibration fusion model by Sahu, Gelfand, and Holland (2010), and the spatiotemporal downscaling calibration models by Berrocal, Gelfand, and Holland (2010) and Berrocal et al. (2012), which can be considered a generalization of a Bayesian universal kriging model (Berrocal, 2019).

## 1.2 | Novelty of our approach

In this article, we are framed in the context of data integration to improve air pollution predictions at a fine grid. We combine monitoring measurements and numerical model outputs coming from two dispersion models: the pollution climate mapping (PCM) model from DEFRA (DEFRA, 2018; Ricardo Energy & Environment, 2017) and the Air Quality Unified Model (AQUM) from the Met Office (Met Office, 2018; Savage et al., 2013), and account for their associated errors.

These deterministic models have previously been used for similar purposes: Lee and Sarra (2015) provide an example of point-to-area upscaling from the PCM model grid to local authority areas for epidemiological applications and Mukhopadhyay and Sahu (2017) combine the AQUM and the monitoring observations to accurately predict NO<sub>2</sub> concentration in UK.

However, usually in the literature only one extra data source at a time is considered (Berrocal et al., 2010; Berrocal et al., 2012; Huang, Lee, & Scott, 2015; Huang, Lee, & Scott, 2017; Lee, Mukhopadhyay, Rushworth, & Sahu, 2017; Lee & Sarra, 2015; McMillan et al., 2010; Moraga, Cramb, Mengersen, & Pagano, 2017; Mukhopadhyay & Sahu, 2017; Panullo, Lee, Waclawski, & Leyland, 2016; Raftery & Fuentes, 2005; Sahu et al., 2010; Wikle & Berliner, 2005; Zidek, Le, & Liu, 2012). We show that, when more are available, these can all be put together to get better predictions while accounting for the bias which affects deterministic data.

Our approach is similar to the coregionalization model proposed by Schmidt and Gelfand (2003) to model CO, NO, and NO<sub>2</sub>, which allows us to calibrate the deterministic models against the monitor observations through a coefficient similarly to calibration techniques. However, here we treat the three sources of information on NO<sub>2</sub> as coming from the same true underlying spatiotemporal process (i.e., the true air pollution concentration field) as in Bayesian melding. The pure application of this kind of models is computationally prohibitive for the high resolution output data we have at hand.

This issue is solved by representing the spatially continuous fields as solutions to a stochastic partial differential equation (SPDE) to handle this in a computationally efficient way (Krainski et al., 2018; Lindgren, Rue, & Lindström, 2011).

Additionally, our model reconstructs the continuous latent spatial and temporal fields allowing us to account for all the sources of uncertainty: first, the one associated with the estimates from the numerical models, which is not provided as they are deterministic models, and second, the measurement error associated with ground observations. This is most useful in the perspective of using the predictions from the air pollution model as a measure of exposure in an epidemiological model, where the uncertainty could be fed forward (see Cameletti, Gómez-Rubio, & Blangiardo, 2019; Lee et al., 2017).

The inference is done under the Bayesian paradigm through the integrated nested Laplace approximations (INLA) coupled with the SPDE approach, which is implemented in the R-INLA package (Rue, 2018).

Other authors have implemented solutions for spatially misaligned air pollution data in R-INLA; however, their approaches differ from ours under several points of view. In particular, Moraga et al. (2017) show an example of area-to-point misalignment addressed via block averaging, in a spatial-only context, without accounting for the uncertainty associated with the raster data. Cameletti et al. (2019) implement a spatial upscaler from point to area comparing two different averaging methods. Kifle, Hens, and Faes (2017) compare additive and coupled spatiotemporal processes for multivariate data in a biological context (prevalence of vectors for arboviruses), where the data are not misaligned, and do not include any explanatory covariate.

To the best of our knowledge, this is the first time a spatiotemporal model for spatially misaligned point-referenced data is implemented through the INLA-SPDE approach considering more than one deterministic model output at different spatial and temporal resolutions.

We compare and contrast several models and through a cross-validation method we evaluate which one produces the most accurate predictions of NO<sub>2</sub> concentration in Greater London and surroundings for the period 2007 to 2011. We compare our method with two approaches in which the alignment is done through bilinear interpolation or kriging, hence not accounting for the measurement error associated with the misaligned covariates. The first is a simple hierarchical model that includes linear effects for the covariates and structured spatiotemporal residuals. The second is the recently proposed data integration model from Mukhopadhyay and Sahu (2017), which allows for nonstationarity in the residual spatial process.

The remainder of the article is organized as follows: Section 2 presents the study area and data; Section 3 describes the methods used in the analysis, starting with the model specification followed by a description of the competitor models; Section 4 reports the results of the application of such methods to our air pollution data; finally, Section 5 contains the conclusions and a short discussion, pointing toward further developments.

## 2 | STUDY AREA AND DATA

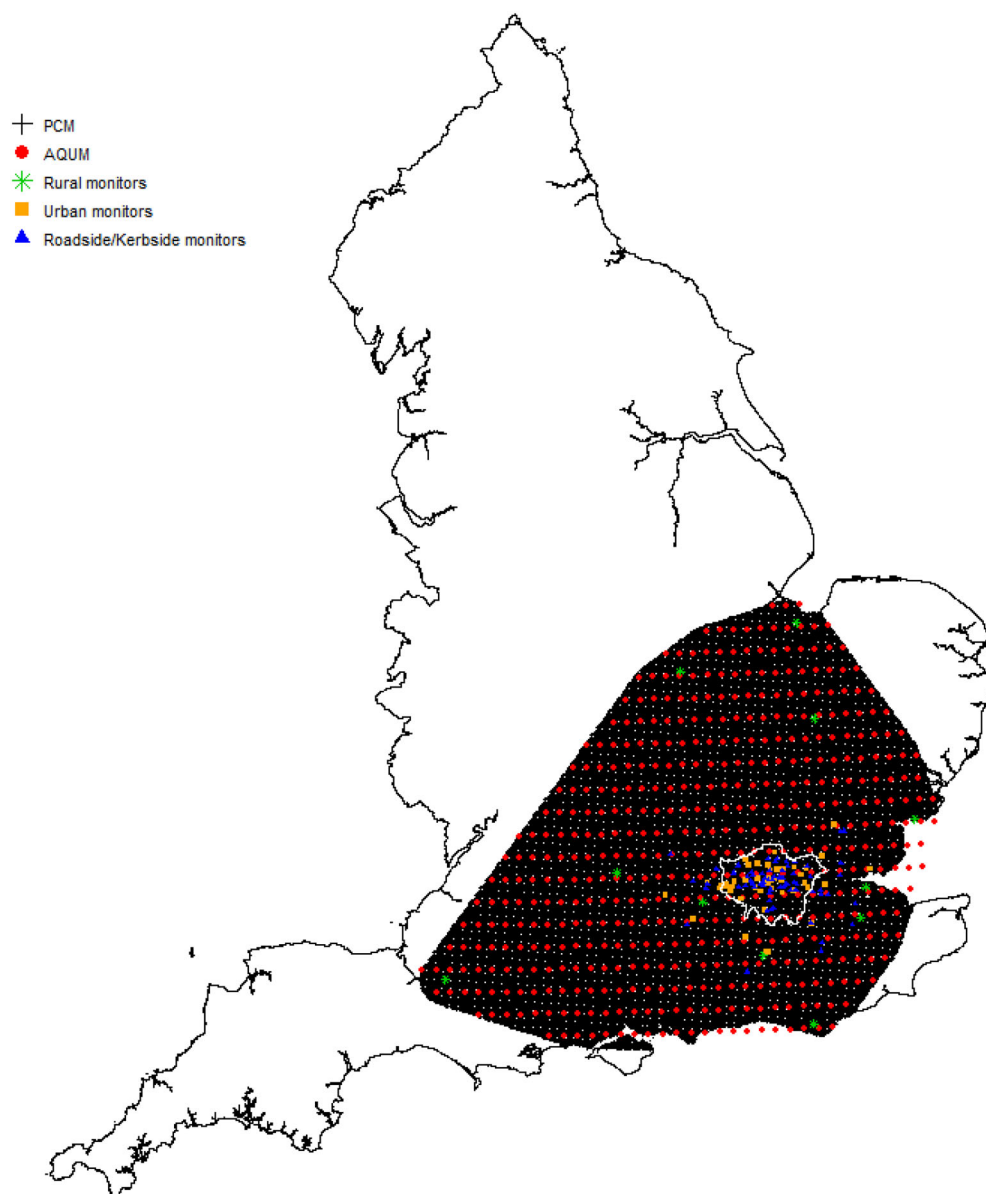
The study focuses on NO<sub>2</sub>, as it is one of the pollutants regulated by national and international directives, and it is traffic driven, hence characterized by high spatiotemporal variability.

We used daily averages of hourly observations from different monitoring networks including the AEA and the Automatic Urban and Rural Network (AURN) from the DEFRA's UK Air Quality Archive, and the London Air Quality Network (LAQN) in Greater London and surroundings, managed by the King's College London Environmental Research Group (ERG). The combined database was built as part of the Spatio/Temporal Exposure Assessment Methods (STEAM) project (King's College London ERG, 2016).

We also considered the outputs of two deterministic models: (i) annual 1 km × 1 km predictions from the PCM model provided by DEFRA (DEFRA, 2018), for 2007–2011; (ii) daily 12 km × 12 km predictions from the AQUM model, available for the years 2007–2011, provided by the Met Office (Met Office, 2018).

We consider the period 2007–2011 due to the availability of the AQUM data.

Among the 213 monitoring stations active between 01/01/2007 and 31/12/2011 for at least 1,370 consecutive days (75% of the total number of days), 126 have been included in the analysis after applying the following criteria to the NO<sub>2</sub> time series: (i) the daily average is computed only for the days where at least 18 hourly observations, that is, the 75%, are present; (ii) we eliminated nonpositive daily averages which do not allow for the logarithmic transformation required in the analysis (negative observations are due to measurement error); (iii) monitors where the resulting daily NO<sub>2</sub> is available for less than 1,370 days, not necessarily consecutive, have been excluded (this is because an active monitor does not necessarily record NO<sub>2</sub> measurements).



**FIGURE 1** NO<sub>2</sub> data locations on the study domain, on the shape of England as reference

The monitors are split into six groups maximizing similarity criteria between groups, and a six-fold cross validation is performed.

For each monitor we have information about the site-type classification that we aggregated into three categories: rural, urban, and road-kerb side.

We define our study area as that including all the selected monitors, containing 495 grid cells for AQUM and 44,117 grid cells for PCM.

The locations of the air pollution data sources described above are shown in Figure 1.

The AQUM model includes chemistry, physical and aerosol models, meteorological configuration based on the Met Office's North Atlantic and European Model (NAE), and emission data (Savage et al., 2013); the PCM model input includes emission inventory, energy projections, road traffic counts, road transport activity, and meteorological hourly data from Waddington weather station (Ricardo Energy & Environment, 2017).

Although data were available, we decided against the inclusion of meteorological variables in our models, as they are already an input for both the numerical models considered in the analysis.

Consistently with the selection criteria, all the six training and validation sets have similar distribution of daily NO<sub>2</sub> concentration by site type (see Appendix A, Figure 1). As expected, in all sets the road-kerb side monitors have higher mean and maximum levels of NO<sub>2</sub>.

**TABLE 1** Descriptive statistics of NO<sub>2</sub> concentration (µg/m<sup>3</sup>) for the three data sources

Data	Min	First qu.	Median	Mean	Third qu.	Max
PCM 2007	7.276	9.948	11.289	13.039	14.055	66.036
PCM 2008	5.615	9.107	10.439	12.064	13.198	56.123
PCM 2009	7.097	10.105	11.333	12.844	13.915	53.290
PCM 2010	5.613	10.396	11.843	13.404	14.705	62.190
PCM 2011	5.437	9.905	11.317	12.545	13.575	55.400
AQUM January	0.215	11.354	19.926	21.943	30.150	73.654
AQUM February	0.154	13.912	22.491	25.052	33.535	97.435
AQUM March	0.291	10.165	16.760	19.180	25.969	84.589
AQUM April	0.059	9.982	15.339	17.248	22.457	81.498
AQUM May	0.008	6.847	10.340	12.187	15.622	77.623
AQUM June	0.000	6.493	9.568	11.088	13.974	63.689
AQUM July	0.409	5.855	8.388	9.842	12.244	67.893
AQUM August	0.000	6.392	9.210	10.591	13.176	58.456
AQUM September	0.054	7.545	11.795	13.899	18.095	68.396
AQUM October	0.067	10.521	16.622	18.402	24.576	70.455
AQUM November	0.531	11.714	18.694	20.942	28.109	97.137
AQUM December	0.000	12.890	23.150	25.040	34.480	121.320
Monitors RUR	0.484	5.357	8.995	11.405	14.734	114.375
Monitors URB	0.679	11.938	19.091	22.286	29.049	166.792
Monitors RKS	0.245	20.208	30.524	34.903	44.422	231.292

In particular, 17 road-kerb side sites overcome the limits set by the WHO and the European Commission for the annual average of 40µg/m<sup>3</sup>, for at least 4 of the 5 years under study (see Appendix A, Figure 2). Of these, the monitor in Lambeth-Brixton Road (LB4) is also well above the threshold of 18µg/m<sup>3</sup> not to be exceeded more than 18 times annually, for every year, even though a decreasing trend can be observed (from 865 hourly exceedances in 2007, to 62 in 2011), and other six monitors exceeded this threshold between 2007 and 2008.

Table 1 reports summary statistics for PCM data by year, AQUM data by month and monitor observations by site type.

### 3 | METHODS

In this section we first present some analysis on the AQUM and PCM data, then we introduce the joint model, and finally the models that we use for comparison. Note that we will represent vector/matrices in bold typeface.

#### 3.1 | Separate models for AQUM and PCM data

In order to quantify the relevance of the temporal component for PCM ( $i = 1$ ) and the spatial component for AQUM ( $i = 2$ ), we ran three models for each data source separately: (i) one with spatial-only or temporal-only effect respectively, (ii) one with additive spatial and temporal effects, and (iii) one with a spatiotemporal interaction.

Let us define  $\mathbf{y}_i$  as the vector of air pollution concentration on the logarithmic scale across space and time for the  $i$ th numerical model. This is assumed to be normally distributed with mean  $\boldsymbol{\eta}_i$  and variance  $\sigma_{\epsilon_i}^2$ :  $\mathbf{y}_i \sim MVN(\boldsymbol{\eta}_i, \sigma_{\epsilon_i}^2 I)$

Each element of the linear predictor  $\boldsymbol{\eta}_i$  (for a time point  $t$  and location  $\mathbf{s}$  identified by UTM coordinates) for models (i), (ii), and (iii) is specified as follows:

$$\begin{aligned}\eta_1(\mathbf{s}) &= \alpha_1 + z_{11}(\mathbf{s}) \\ \eta_2(t) &= \alpha_2 + z_{22}(t),\end{aligned}\tag{i}$$

$$\begin{aligned}\eta_1(\mathbf{s}, t) &= \alpha_1 + z_{11}(\mathbf{s}) + z_{21}(t) \\ \eta_2(\mathbf{s}, t) &= \alpha_2 + z_{12}(\mathbf{s}) + z_{22}(t),\end{aligned}\tag{ii}$$

$$\begin{aligned}\eta_1(\mathbf{s}, t) &= \alpha_1 + z_{31}(\mathbf{s}, t) \\ \eta_2(\mathbf{s}, t) &= \alpha_2 + z_{32}(\mathbf{s}, t),\end{aligned}\tag{iii}$$

where  $z_{1i}(\mathbf{s})$  is the realization at location  $\mathbf{s}$  of the spatial process  $\mathbf{z}_{1i}$  with Matérn covariance function  $\mathbf{z}_{1i} \sim MVN(\mathbf{0}, \sigma_{z_{1i}}^2 \boldsymbol{\Sigma})$ ,  $z_{2i}(t) \sim N(z_{2i}(t-1), \sigma_{z_{2i}}^2)$  is a temporal process modeled as a random walk and  $\mathbf{z}_{3i} \sim MVN(\mathbf{0}, \sigma_{z_{3i}}^2 \boldsymbol{\Sigma}_t \otimes \boldsymbol{\Sigma}_s)$  is a separable space–time interaction with Matérn covariance function and temporal dependence modeled as a random walk.

Based on the deviance information criterion (DIC), the results show that AQUM spatial variation is relevant but there is no need for a space–time interaction so model (ii) is selected for AQUM, while the PCM temporal variation is negligible so model (i) is selected for PCM (see Appendix B for details). Hence, we will use this specification in the joint model presented in the next section.

### 3.2 | Bayesian joint spatiotemporal model for misaligned covariates

Following Kifle et al. (2017) we implement an additive space–time model for data observed at different points in space, which share a spatial and a temporal component.

Previous similar applications consider measurements of more than one variable at the same locations, but this is not a requirement in the INLA-SPDE approach.

Our model is joint in the sense that we specify one likelihood for the response and one for each of the misaligned covariates, and they contain common components which are estimated using all the data. Even though in R-INLA the problem is computationally treated similarly to a multivariate situation, this is not our case as we ultimately consider solely the monitor observations as response variable.

We make the assumption that the same temporal dynamics govern AQUM and monitor observations, and likewise the same spatial dynamics govern PCM, AQUM, and monitor observations.

Our hierarchical model has three levels: in the first we define the likelihoods, in the second the random effect components, while the third level includes the prior distributions for the model parameters and hyperparameters.

The joint model presented below is implemented via INLA, a computationally efficient alternative to Markov chain Monte Carlo (MCMC) methods, that works specifically on hierarchical Gaussian Markov random fields (GMRF). Details on how this is done in R-INLA can be found in Appendix E.

#### 3.2.1 | Level 1: Likelihoods and linear predictors

Let  $y_i(\mathbf{s}, t)$  denote the PCM ( $i=1$ ) and AQUM ( $i=2$ ) data and the observed  $\text{NO}_2$  concentration ( $i=3$ ) at the generic time point  $t$  and site  $\mathbf{s}$ , on the logarithmic scale. These are assumed to be normally distributed, with mean  $\eta_i(\mathbf{s}, t)$  and measurement error variance  $\sigma_{\epsilon_i}^2$ :

$$\begin{aligned}y_1(\mathbf{s}, t) &\sim N(\eta_1(\mathbf{s}), \sigma_{\epsilon_1}^2) \quad (\text{PCM}) \\ y_2(\mathbf{s}, t) &\sim N(\eta_2(\mathbf{s}, t), \sigma_{\epsilon_2}^2) \quad (\text{AQUM}) \\ y_3(\mathbf{s}, t) &\sim N(\eta_3(\mathbf{s}, t), \sigma_{\epsilon_3}^2) \quad (\text{Ground observations}).\end{aligned}$$

Based on the results from Section 3.1 we model the PCM data with an intercept and a spatial component and the AQUM data with an intercept and additive spatial and temporal components. These are shared between the three linear predictors, which are the following:

$$\eta_1(\mathbf{s}) = \alpha_1 + z_1(\mathbf{s}),\tag{1}$$



$$\eta_2(\mathbf{s}, t) = \alpha_2 + \lambda_{1,2}\mathbf{z}_1(\mathbf{s}) + z_2(t), \quad (2)$$

$$\eta_3(\mathbf{s}, t) = \alpha_3 + \beta_{k_s} + \lambda_{1,3}\mathbf{z}_1(\mathbf{s}) + \lambda_{2,3}z_2(t) + z_3(t, k_s), \quad (3)$$

where  $\alpha_i$  are the intercepts,  $\lambda_{i,j}$  are the scaling parameters for the shared components from  $\eta_i$  to  $\eta_j$ ,  $\beta_{k_s}$  is the fixed effect for the site type as categorical variable ( $k_s = 0$ : rural [reference],  $k_s = 1$ : urban and  $k_s = 2$ : road-kerb side), and  $\mathbf{z}_1$  and  $\mathbf{z}_2$  are the shared random effects. The linear predictor for the ground observations  $\eta_3$  also contains an interaction term  $\mathbf{z}_3$ , which allows for a different residual temporal trend for each site type.

Note that even though PCM is assumed to be governed only by a spatial effect, its output does vary in both space and time, so the deterministic model output  $\mathbf{y}_1$  has space and time indices (here the locations are the centroids of the 44,117 PCM grid cell, and the time points are the years), while its latent field  $\mathbf{z}_1$  has only a spatial index.

For AQUM, the space and time indices of  $\mathbf{y}_2$  correspond to the centroids of the 495 AQUM grid cell and the 1,826 days, respectively.

Finally,  $\mathbf{y}_3$  is measured at the 126 monitors on 1,826 days.

### 3.2.2 | Level 2: Latent fields

In Equation (3),  $\mathbf{z}_1 \sim MVN(\mathbf{0}, \sigma_{z_1}^2 \mathbf{\Sigma})$  is the common spatial latent field, with  $\mathbf{\Sigma}$  being the correlation matrix defined by the Matérn stationary and isotropic covariance function (see Appendix D). It is important to note that  $\mathbf{z}_1$  is then rescaled for AQUM and monitor observations through  $\lambda_{1,2}$  (Equation (2)) and  $\lambda_{1,3}$  (Equation (3)).

In the same equation,  $z_2(t)$  is the  $t$ th element of the temporal latent field  $\mathbf{z}_2$ , and is modeled as a random walk:  $z_2(t) \sim N(z_2(t-1), \sigma_{z_2}^2)$ . Similarly to  $\mathbf{z}_1$ ,  $\mathbf{z}_2$  is rescaled for the monitor observations through  $\lambda_{2,3}$  (Equation (3)).

Finally,  $\mathbf{z}_3$  is the residual temporal trend assumed to be different for each site type (rural, urban, and road-kerb side), and modeled as first-order autoregressive  $z_3(t, k_s) \sim N(\rho z_3(t-1, k_s), \sigma_{z_3}^2)$ . In other words, we assume conditionally independent replications of the same latent field for each site type, with shared hyperparameters (Martins, Simpson, Lindgren, & Rue, 2013).

### 3.2.3 | Level 3: Priors

The priors on the model parameters are specified as follows.

According to Fuglstad, Simpson, Lindgren, and Rue (2019), we choose a penalized complexity prior (Simpson, Rue, Riebler, Martins, & Sørbye, 2017) for range and variance of the latent spatial field  $\mathbf{z}_1$  such that  $P(r < r_0) = 0.95$  and  $P(\sigma_{z_1} > \sigma_0) = 0.5$ , where  $r_0 = 1/5$  of the domain size and  $\sigma_0 = 100$  (see Appendix D).

For the standard deviation of the random walk we assume a penalized complexity prior such that the probability that  $\sigma_{z_2}$  is greater than the empirical standard deviation of the AQUM data is 1%, that is,  $P(\sigma_{z_2} > \text{SD}(\text{AQUM})) = 0.01$ .

For the time-site-type interaction we assume the default vague prior defined on the log-precision:  $\log(1/\sigma_{z_3}^2) \sim \log\text{Gamma}(1, 5e-05)$ ; for the autoregressive parameter we assume  $\rho \sim N(0.3, 0.5)$  using information from previous modeling exercise.

The precisions of response variable, AQUM data, and PCM data are assigned the default vague prior  $\log(1/\sigma_{e_i}^2) \sim \log\text{Gamma}(1, 5e-05)$ ,  $i = 1, 2, 3$ .

On the scaling coefficients we put a Normal prior centered on a positive values around 1 with a large variance to ensure minimal information:  $\lambda_{1,2} \sim N(1.1, 100)$ ,  $\lambda_{1,3} \sim N(1.3, 100)$ , and  $\lambda_{2,3} \sim N(0.9, 100)$ .

Finally on the coefficients of the fixed effects  $\alpha_i$  and  $\beta_{k_s}$  we assume the weak Normal prior distribution  $N(0, 1,000)$ .

## 3.3 | Competitor models

We compared our model to three different competitors: (i) a joint model that includes only one misaligned covariate (either AQUM or PCM), (ii) a simple hierarchical model that includes a covariate aligned at the monitoring sites through

bilinear interpolation (Akima, 1978) or kriging, and (iii) a complex hierarchical model that allows for nonstationarity after interpolating the misaligned covariates via bilinear interpolation (Mukhopadhyay & Sahu, 2017).

The aim of this comparison is to evaluate if the inclusion of more than one extra data source actually improves the model predictive capability and can counterbalance the need for complex random effect structures, and if there is a gain in moving from a simple interpolation to a modeling framework.

We describe the three comparators in the rest of this section.

### 3.3.1 | Joint models with one misaligned covariate only

The joint model that includes PCM only is specified as follows:

$$y_1(\mathbf{s}, t) \sim N(\eta_1(\mathbf{s}), \sigma_{\epsilon_1}^2) \quad (\text{PCM})$$

and

$$y_2(\mathbf{s}, t) \sim N(\eta_2(\mathbf{s}, t), \sigma_{\epsilon_2}^2) \quad (\text{Ground observations})$$

with

$$\eta_1(\mathbf{s}) = \alpha_1 + z_1(\mathbf{s}) \quad (\text{PCM})$$

$$\eta_2(\mathbf{s}, t) = \alpha_2 + \beta_{k_s} + \lambda_{1,2}z_1(\mathbf{s}) + z_3(t, k_s) \quad (\text{Ground observations})$$

Similarly, the joint model that includes AQUM only is defined as:

$$y_1(\mathbf{s}, t) \sim N(\eta_1(\mathbf{s}, t), \sigma_{\epsilon_1}^2) \quad (\text{AQUM})$$

and

$$y_2(\mathbf{s}, t) \sim N(\eta_2(\mathbf{s}, t), \sigma_{\epsilon_2}^2) \quad (\text{Ground observations})$$

with

$$\eta_1(\mathbf{s}, t) = \alpha_1 + z_1(\mathbf{s}) + z_2(t) \quad (\text{AQUM})$$

$$\eta_2(\mathbf{s}, t) = \alpha_2 + \beta_{k_s} + \lambda_{1,2}z_1(\mathbf{s}) + \lambda_{2,2}z_2(t) + z_3(t, k_s) \quad (\text{Ground observations})$$

For these models we considered either fixed to 1 or varying calibration coefficients  $\lambda_{i,j}$ , and different priors. The final choice of priors is the one reported in Section 3.2.3.

### 3.3.2 | Data integration model via interpolation

We implement two models that use interpolation techniques to obtain values of AQUM and PCM at the monitoring stations. The first is a naive bilinear interpolation, the second can be considered as Bayesian kriging, as we predict AQUM and PCM at the monitoring stations from the models described in Section 3.1.

In both cases, after aligning the AQUM ( $\mathbf{X}_1$ ) and PCM ( $\mathbf{X}_2$ ) values, we consider a linear effect on the covariates, a spatially structured residual  $\mathbf{z}_1$ , a temporally structured residual  $\mathbf{z}_2$  and the site-type-specific temporal effect  $\mathbf{z}_3$  specified as in Section 3.2. We also keep the fixed effects for the site type  $\beta_{k_s}$  as in the joint model.



We specify a normal likelihood  $y(\mathbf{s}, t) \sim N(\eta(\mathbf{s}, t), \sigma_\epsilon^2)$  and the linear predictor as follows:

$$\eta(\mathbf{s}, t) = \beta_0 + \beta_1 X_1(\mathbf{s}, t) + \beta_2 X_2(\mathbf{s}, t) + \beta_{k_s} + z_1(\mathbf{s}) + z_2(t) + z_3(t, k_s).$$

### 3.3.3 | Data integration model with nonstationarity

Mukhopadhyay and Sahu (2017) developed a site-type-specific regression on the AQUM data using our same classification for the site type. The key feature of their model is the specification of a nonstationary spatiotemporal process, which leads to a better predictive performance compared to the stationary Gaussian process (GP) in their application.

To obtain a like-for-like comparison, we also include a site-type-specific regression on the PCM data and implement both the stationary and the nonstationary versions of this model.

Both AQUM ( $\mathbf{X}_1$ ) and PCM ( $\mathbf{X}_2$ ) are interpolated at the monitoring site locations through bilinear interpolation.

The hierarchical model specification in this case is:

$$y(\mathbf{s}, t) \sim N(\eta(\mathbf{s}, t), \sigma_\epsilon^2),$$

$$\eta(\mathbf{s}, t) = \mu(\mathbf{s}, t) + v(\mathbf{s}, t),$$

with

$$\mu(\mathbf{s}, t) = \gamma_0 + \gamma_1 X_1(\mathbf{s}, t) + \sum_{k=1}^2 \delta_k(\mathbf{s})(\gamma_{0k} + \gamma_{1k} X_1(\mathbf{s}, t))$$

for the model with AQUM only, and

$$\mu(\mathbf{s}, t) = \gamma_0 + \gamma_1 X_1(\mathbf{s}, t) + \gamma_2 X_2(\mathbf{s}, t) + \sum_{k=1}^2 \delta_k(\mathbf{s})(\gamma_{0k} + \gamma_{1k} X_1(\mathbf{s}, t) + \gamma_{2k} X_2(\mathbf{s}, t))$$

for the model with AQUM and PCM.

Here  $k = 0$  indicates rural site type (baseline),  $k = 1$  urban and  $k = 2$  road-kerb side,  $\delta_k(\mathbf{s})$  is an indicator function equal to 1 if site  $\mathbf{s}$  is of type  $k$  and 0 otherwise,  $\gamma_0$ ,  $\gamma_1$ , and  $\gamma_2$  are the baseline intercept and slopes for  $\mathbf{X}_1$  and  $\mathbf{X}_2$ , while  $\gamma_{0k}$ ,  $\gamma_{1k}$ , and  $\gamma_{2k}$  are site-type-specific adjustments to the baseline intercept and slopes.

For the spatiotemporal process  $\mathbf{v}$  we first assume a stationary time-independent GP with zero mean and exponential correlation function (note that  $v_t(\mathbf{s}) = v(\mathbf{s}, t)$ ):

$$\mathbf{v}_t \sim N(\mathbf{0}, \sigma_v^2 \mathbf{H}_v(\phi)), \quad \text{where } \mathbf{H}_v(\phi) = \text{corr}(v_t(\mathbf{s}), v_t(\mathbf{s}')) = \exp(-\|\mathbf{s} - \mathbf{s}'\| \phi).$$

Then we specify a nonstationary covariance structure as in Sahu and Mukhopadhyay (2015): given a GP  $\mathbf{v}_t^*$  defined on a set of  $m = 25$  knot locations  $\mathbf{v}_t^* \sim \text{MVN}(\mathbf{0}, \sigma_v^2 \mathbf{H}_{v^*}(\phi))$ , the Gaussian predictive process (GPP) at a new location  $\mathbf{s}$  is defined as  $\tilde{v}_t(\mathbf{s}) = E[v_t(\mathbf{s}) | \mathbf{v}_t^*]$ . From multivariate Gaussian theory it follows that  $\tilde{\mathbf{v}}_t = \mathbf{C}^* \mathbf{H}_{v^*}^{-1}(\phi) \mathbf{v}_t^*$  with  $\mathbf{C}^*$  being the cross-correlation function between  $\mathbf{v}_t$  and  $\mathbf{v}_t^*$ .

The nonstationarity and the anisotropy are given by the fact that  $\text{corr}(\tilde{v}_t(\mathbf{s}), \tilde{v}_t(\mathbf{s}')) = \mathbf{c}^*(\mathbf{s})^T \mathbf{H}_{v^*}^{-1}(\phi) \mathbf{c}^*(\mathbf{s}')$ , which depends on both  $\mathbf{s}$  and  $\mathbf{s}'$  and not only on the separation vector or the distance between locations.

To introduce temporal dependence we specify a first-order autoregressive model for  $\mathbf{v}_t^*$ .

The choice of knot locations, model specification, and prior distributions is based on Mukhopadhyay and Sahu (2017). This is justified by the fact that we use the same data sources on a subregion of their study area.

## 3.4 | Validation and predictive capability measures

We compared the predictive capability through proper scoring rules (Gneiting & Raftery, 2007) such as the cross-validated logarithmic score (logScore), the Continuous Ranked Probability Score (CRPS), and the root mean squared error (RMSE), and also the predictive model choice criterion (PMCC) proposed by Gelfand and Ghosh (1998).

Furthermore, we reported the correlation between the observed and the predicted values for the validation sites (COR), the mean absolute percentage error (MAPE), and the 95% coverage (COV), defined as the percentage of times that the observed value falls within the 95% credibility interval of the sampled posterior marginal.

To measure the predictive capability we need to report the fitted values at the validation sites on the scale of the outcome, as cannot compare the observed values with the fitted values because they are not accounting for the measurement error, but only for the uncertainty associated with the model parameters. In order to do so, we draw 50 values from the marginal posterior of the measurement error  $p(\sigma_{\epsilon_3}^2 | \mathbf{y}_3)$  first, then draw  $\boldsymbol{\eta}_3$  from its conditional posterior  $p(\boldsymbol{\eta}_3 | \sigma_{\epsilon_3}^2, \mathbf{y}_3)$  using the simulated values of  $\sigma_{\epsilon_3}^2$  (Gelman et al., 2013). These values are used as mean and variance of a Normal distribution, from which we sampled values at each site (sample size = 100).

The following are the formulas for the different measures of predictive capability used in the analysis. For simplicity we apply a slight change of notation here:  $y_{jt}$  indicates the observed value at monitor  $j$  ( $m$  is the number of validation monitors) and day  $t$  ( $t = 1, \dots, T$ ,  $T = 1,826$ ), and  $\hat{y}_{jt}$  is the corresponding predicted value obtained as mean of the vector of  $Q = 100 \times 50$  sampled values  $\hat{\mathbf{y}}_{jt} = \hat{y}_{j1}, \dots, \hat{y}_{jQ} \sim F_{jt}$ ,  $F_{jt}$  being the empirical distribution function of  $\hat{\mathbf{y}}_{jt}$ .

$$\begin{aligned} \text{RMSE} &= \sqrt{\frac{1}{mT} \sum_{j=1}^m \sum_{t=1}^T (y_{jt} - \hat{y}_{jt})^2} \\ \text{MAPE} &= \frac{1}{mT} \sum_{j=1}^m \sum_{t=1}^T \frac{|y_{jt} - \hat{y}_{jt}|}{y_{jt}} \cdot 100 \\ \text{PMCC} &= \sum_{j=1}^m \sum_{t=1}^T (y_{jt} - \hat{y}_{jt})^2 + \sum_{j=1}^m \sum_{t=1}^T \text{VAR}(\hat{\mathbf{y}}_{jt}) \\ \text{CRPS} &= \frac{1}{mT} \sum_{j=1}^m \sum_{t=1}^T \text{CRPS}(F_{jt}, y_{jt}), \quad \text{with} \\ \text{CRPS}(F_{jt}, y_{jt}) &= \frac{1}{Q} \sum_{q=1}^Q |\hat{y}_q - y_{jt}| - \frac{1}{2Q^2} \sum_{q=1}^Q \sum_{r=1}^Q |\hat{y}_q - \hat{y}_r|. \end{aligned}$$

For each model under comparison, the predictive capability measures presented above are computed pooling together the six validation sets. It can be calculated by day, by site, by site type or across all sites to obtain specific and global measures, with lowest measures indicating the best predictive performance.

### 3.5 | Predictions on a regular grid

From the joint model, we extract daily predictions of  $\text{NO}_2$  concentration on a regular grid that covers the study area. For the grid we choose an intermediate spatial resolution between PCM and AQUM data to limit the computational burden while retaining spatial variability.

In order to provide the predictions in a reasonable time, we extract samples from the joint posterior marginals and estimate the linear predictor at each time-location for the 1,826 days on the regular grid (Thomas, Shaddick, Simpson, de Hoogh, & Zidek, 2019).

We compute the predictions from the model that includes all monitors as training set.

We extract samples from the posterior marginals of the model components in order to reconstruct the linear predictor at each time-location for the 1,826 days on the regular grid, as:

$$\eta_3(\mathbf{s}, t) = \alpha_3 + \beta_{k_s} + \lambda_{1,3} \mathbf{z}_1(\mathbf{s}) + \lambda_{2,3} \mathbf{z}_2(t) + \mathbf{z}_3(t, k_s).$$

In particular, following the tutorial by Bakka (2017), we obtain samples from the posterior of the intercept  $\alpha_3$  and  $\beta_{k_s}$  for each site type, samples from the posterior of  $\lambda_{1,3} \mathbf{z}_1$  at the mesh nodes and reproject it on the prediction grid, samples from the posterior of  $\lambda_{2,3} \mathbf{z}_2$  at each time point (days), and samples from the posterior of  $\mathbf{z}_3$  for each day and site type.

Note that in order to predict at the grid locations we need to know the value of site-type classification for each grid point. With this aim we built a function which assigns each location to road-kerb side, urban, or rural depending on the

**TABLE 2** Model comparison in terms of predictive capability

Model <sup>a</sup>	Predictive capability					
	PMCC	CRPS	RMSE	MAPE	CORR	COV
AQUM( <i>s,t</i> ) joint	18,277	0.0523	0.5725	16.71%	65.83%	78.15%
PCM( <i>s</i> ) joint	14,018	0.0372	0.4615	13.54%	76.77%	86.87%
AQUM( <i>s,t</i> ) + PCM( <i>s</i> ) joint	13,621	0.0338	0.4665	13.67%	76.08%	84.66%
AQUM+PCM bilinear interpolation	82,970	0.2560	0.6911	17.57%	67.14%	68.55%
AQUM+PCM kriging estimates	35,017	0.2220	0.4964	14.58%	73.13%	75.27%
AQUM, nonstationary (Mukhopadhyay & Sahu, 2017)	79,542 <sup>b</sup>					60.74%
AQUM+PCM, nonstationary (Mukhopadhyay & Sahu, 2017)	75,506 <sup>b</sup>					62.13%
AQUM+PCM, stationary (Mukhopadhyay & Sahu, 2017)	75,510 <sup>b</sup>					62.13%

<sup>a</sup>(*s*) indicates spatial-only random effects; (*t*) indicates temporal-only random effects; (*s,t*) indicates additive spatial and temporal random effects. When not specified, a linear effect is assumed as described in Section 3.3.

<sup>b</sup>As provided by spT.Gibbs function in R package spAir.

distance from any road as well as using the Corine land cover for the year 2012 for the UK, Jersey, and Guernsey shapefile from the Centre for Ecology and Hydrology (Cole et al., 2015). See Appendix F for more details.

For each sample we then sum up the samples from the fixed effects and random effects to reconstruct the linear predictor, then the prediction is given by average across all samples.

## 4 | RESULTS

In this section we present the results of the model comparison, with particular focus on the advantages of the proposed joint model, and the daily predictions that we obtained from the best model.

### 4.1 | Model comparison

In order to show whether the inclusion of more than one extra data source actually improves the model predictive capability, we compare our proposed joint model with the corresponding models that include only AQUM or PCM.

For AQUM we assume a spatiotemporal effect or temporal-only effect when PCM is included.

We also compare our joint model with other well-established data integration techniques, the simple interpolation models described in Section 3.3.2, and the more complex ones described in Section 3.3.3.

Besides providing information about all the sources of uncertainty, all the joint models have better performance than the models where the misaligned data are interpolated, even allowing for nonstationarity (see Table 2).

However, the AQUM data do not seem to provide much information, in fact the model that includes only AQUM has a far worse performance than the one only including PCM. In addition, allowing for a spatial effect on AQUM does not improve the prediction, for the model where PCM is also included. This can be explained by the fact that the time–site-type interaction  $\mathbf{z}_3$  replaces the role of AQUM in capturing the temporal trend when we remove AQUM from the model and the temporal information is still provided by the numerous monitoring stations, while there is no other structured spatial component that compensates for PCM when it is removed.

Furthermore, as we focus here on spatial prediction rather than temporal forecasting, removing AQUM is less of a burden on the model performance in terms of predictive capability.

Nevertheless, the model including both AQUM and PCM has the best performance in terms of PMCC and CRPS and we will report the results from this model in the next section.

Note that the predictive capability measures of the models in Section 3.3.3 cannot be compared with the others due to the different model structure. Only the PMCC and the 95% coverage are comparable and reported in Table 2.

	mean	SD	0.025q	median	0.975q
$\alpha_1$	2.0653	0.0308	2.0048	2.0653	2.1258
$\alpha_2$	2.5793	0.0259	2.5285	2.5793	2.6301
$\alpha_3$	2.4722	0.0236	2.4258	2.4722	2.5186
$\beta_{\text{URB}}$	-0.1716	0.0047	-0.1808	-0.1716	-0.1624
$\beta_{\text{RKS}}$	0.3764	0.0047	0.3673	0.3764	0.3856
$\sigma_{\epsilon_1}^2$	0.0003	0.0000	0.0003	0.0003	0.0003
$\sigma_{\epsilon_2}^2$	0.0303	0.0000	0.0303	0.0303	0.0303
$\sigma_{\epsilon_3}^2$	0.0213	0.0000	0.0213	0.0213	0.0213
$\sigma_{z_1}^2$	2.0729	0.0385	1.9815	2.0803	2.1225
$\sigma_{z_2}^2$	2626.3	7.960	2607.8	2627.7	2637.7
$\sigma_{z_3}^2$	0.0013	0.0000	0.0013	0.0013	0.0013
$r_{z_1}$ (km)	177.8	0.227	177.2	177.77	256.0
$\rho_{z_3}$	0.5702	0.0005	0.5689	0.5700	0.6869
$\lambda_{1,2}$	1.1000	0.0001	1.0996	1.0999	1.1345
$\lambda_{1,3}$	1.2999	0.0003	1.2989	1.2998	1.3990
$\lambda_{2,3}$	0.8995	0.0004	0.8977	0.8995	0.9003

**TABLE 3** Summary of model parameters and hyperparameters

With regard to these models, allowing for nonstationarity and anisotropy leads to very little gain compared with the introduction of an additional source of data at high spatial resolution. In general, their performance is almost as poor as having a linear effect on interpolated covariates.

## 4.2 | Results from the complete joint model

We report the results for the joint model that includes spatial and temporal effects on AQUM and spatial effect on PCM, ran using all monitors as training data.

Looking at the summary reported in Table 3 we see that, as expected, there is an increase in the NO<sub>2</sub> concentration going from rural to road-kerb side locations, but not for urban. For the spatial latent field  $\mathbf{z}_1$ , the estimated empirical range, that is, the distance after which the spatial correlation function drops to 0.13 (Lindgren & Rue, 2015) is 177 km, corresponding to approximately 50% of the maximum extension of the spatial domain.

The scaling parameters  $\lambda_{i,j}$  are all different from 1, meaning the spatial field for PCM needs to be rescaled for AQUM ( $\lambda_{1,2} = 1.1$ ) and for the monitor observations ( $\lambda_{1,3} = 1.3$ ), and the temporal latent field for AQUM is also calibrated against the monitor observations with  $\lambda_{2,3} = 0.9$ .

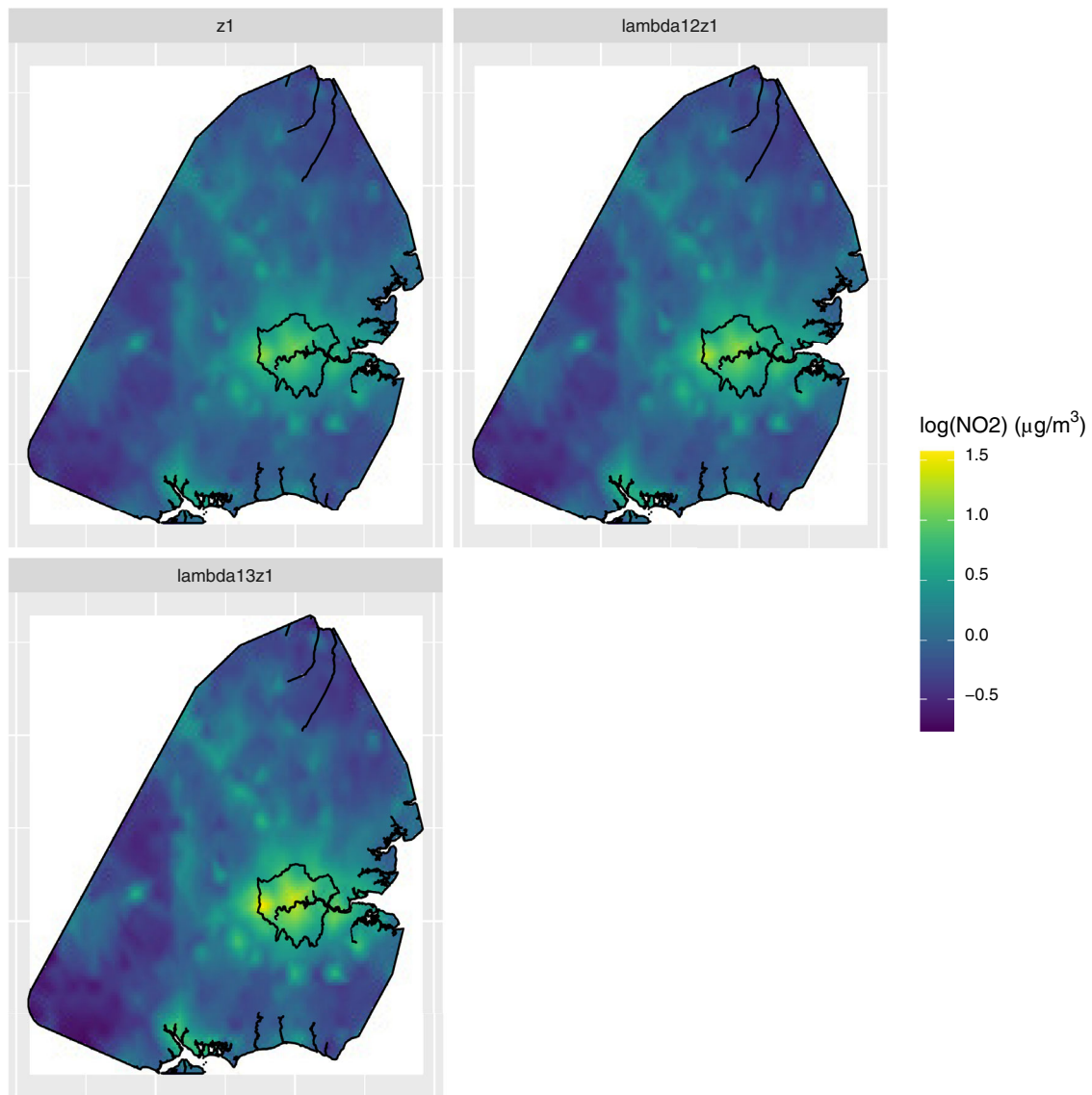
The intercepts  $\alpha_i$  represent the overall mean of PCM, AQUM, and ground observations, respectively.

The spatial latent field  $\mathbf{z}_1$  (Figure 2) shared between the PCM data, the AQUM data, and the monitor observations shows the traffic-driven characteristics of NO<sub>2</sub> as we can recognize higher values in correspondence of motorways and major city centers. The rescaled fields are reported as well and for  $\lambda_{1,3}\mathbf{z}_1$  the magnifying effect of the scaling parameter  $\lambda_{1,3} = 1.3$  is particularly visible.

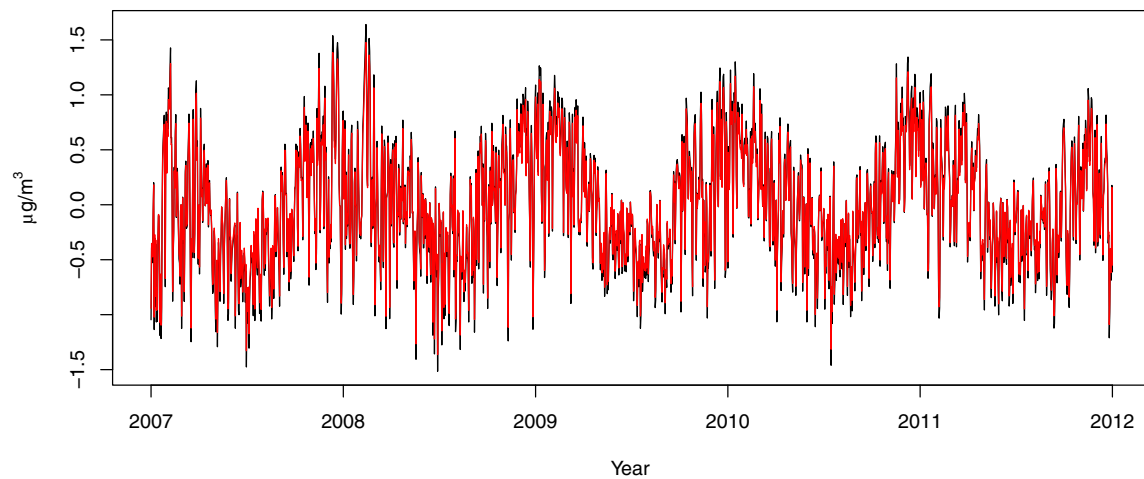
Figure 3 shows the temporal latent field  $\mathbf{z}_2$  shared between the AQUM data and the monitor observations, which captures the seasonality of NO<sub>2</sub>, and the rescaled field  $\lambda_{2,3}\mathbf{z}_2$ , which is shrunk by the scaling parameter  $\lambda_{2,3} = 0.9$ .

The latent fields  $\mathbf{z}_1$  and  $\mathbf{z}_2$  are both centered in zero as the large scale component of PCM and AQUM is captured by their intercepts  $\alpha_1$  and  $\alpha_2$ .

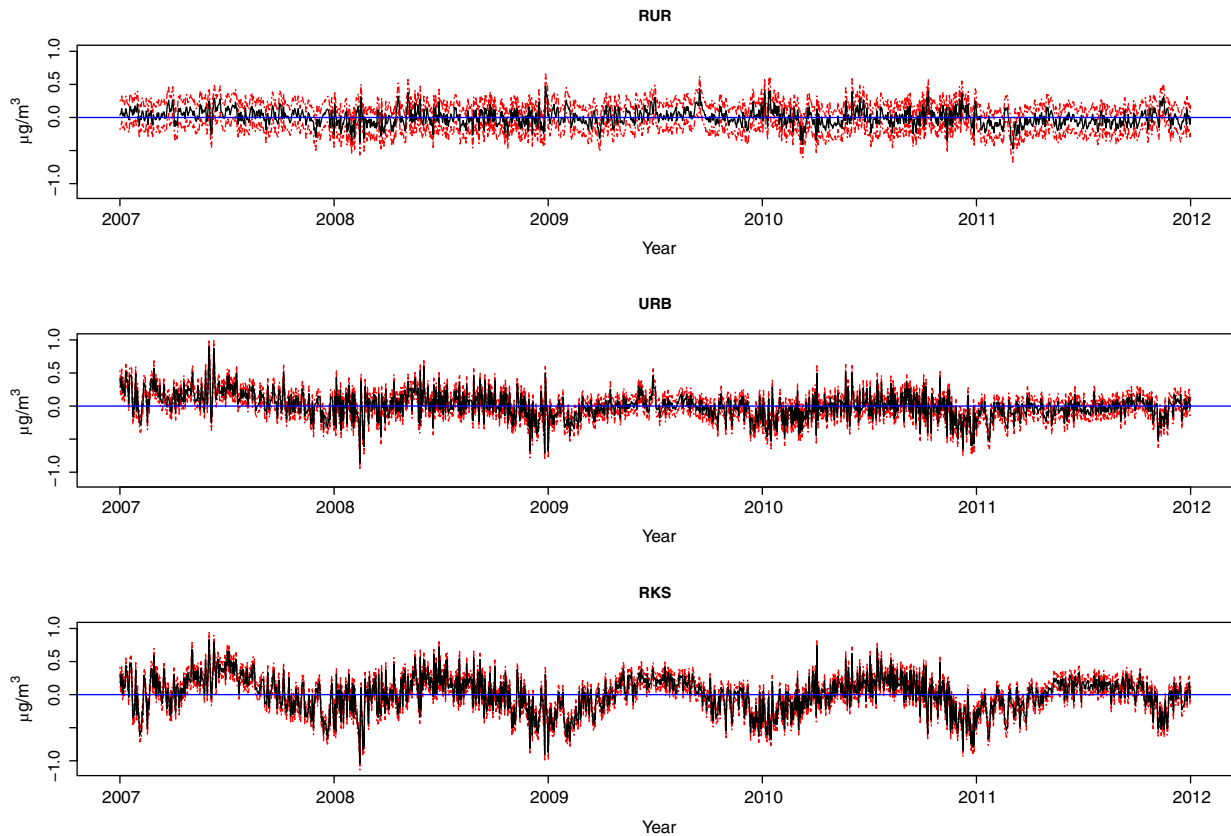
Finally, the time-site-type interaction  $\mathbf{z}_3$  in Figure 4 shows that there is some residual site-type-specific temporal variability, especially for urban and road-kerb side monitors, which is not captured by the main temporal component  $\mathbf{z}_2$ .



**FIGURE 2** Posterior mean of the latent spatial field  $z_1$  and of the rescaled spatial fields  $\lambda_{1,2}z_1$  and  $\lambda_{1,3}z_1$   
 $z_2$  (black) and  $\lambda_{2,3}z_2$  (red) – posterior mean



**FIGURE 3** Posterior mean of the latent temporal field  $z_2$  (black line) and of the rescaled temporal field  $\lambda_{2,3}z_2$  (red line)



**FIGURE 4** Time-site-type interaction  $z_3$ . Posterior mean in red, 95% CI in black dashed lines

#### 4.2.1 | Daily predictions

We selected four  $\text{NO}_2$  pollution episodes reported by the LondonAir website (King's College London, 2018) and compared the predictions for these 4 days with four randomly selected summer Sundays across the study period, where we expect to see low levels of  $\text{NO}_2$ . The predictions show the expected behavior, with high predicted concentrations during the pollution episodes and low concentrations during the selected Sundays (Figure 5).

A layer with the roads classified as motorways is plotted on top of each map, showing correspondence between the highest predicted levels of  $\text{NO}_2$  and the major roads. This is expected because  $\text{NO}_2$  is a highly traffic-driven pollutant. A peak of  $\text{NO}_2$  concentration can also be observed in the area of Heathrow airport, on the left of Greater London, which is characterized by the highest levels also on low concentration days.

## 5 | CONCLUSION AND DISCUSSION

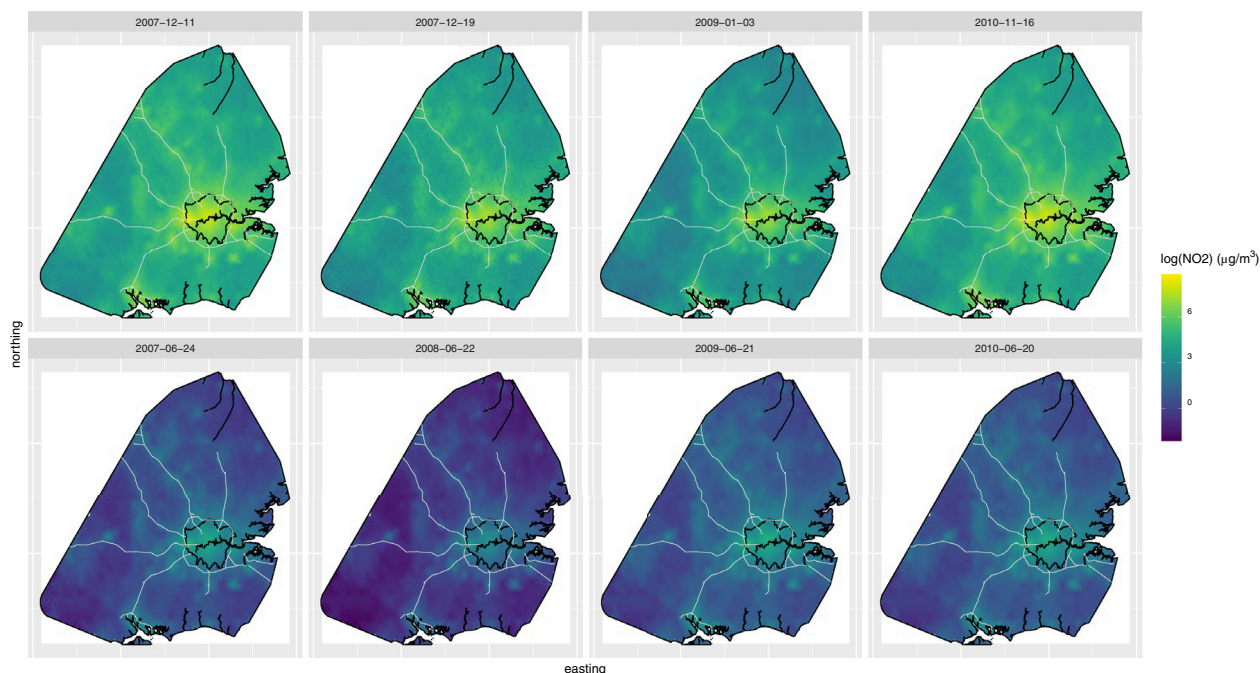
We implemented a hierarchical Bayesian model to estimate air pollution concentration, combining misaligned data sources with a joint approach. This approach can be considered in between Bayesian melding and calibration, and it is the first attempt at implementing such methods on spatiotemporal air pollution data in R-INLA.

The proposed model includes information on the site type as well as output from two different numerical models characterized by spatial and temporal variability and accounting for traffic, chemistry, land use, and meteorological covariates. Our method is transferable to any available data sources; however, the interpretation of the results may change according to their intrinsic characteristics, in particular referring to the information included in the deterministic or LUR models.

We show that including more than one covariate at different spatial and temporal resolution increases model predictive capability. However, removing AQUM has proven not to be detrimental, but this could be justified with the fact that we are not doing temporal forecasting.

Overall, we prove that using as much spatial and temporal information as possible is more beneficial than increasing the complexity of the random effect structure.





**FIGURE 5** Daily predictions for 4 days in which an air pollution event was registered (top row) and 4 days with reported low air pollution concentration (bottom row)

A time–site–type interaction was added to the model to account for residual temporal variability observed when looking at the site–type–specific residuals.

The advantages of our method are manyfolds: first, reconstructing the entire latent field in a Bayesian approach provides us with the marginal posterior distribution for all the uncertainty parameters, allowing us to correctly quantify the uncertainty associated with our predictions and the deterministic models, that is not possible to obtain with other downscalers and non-model-based solutions; second, unlike the spatiotemporal downscaler proposed by Berrocal et al. (2012), our model reconstructs the latent fields of the misaligned covariates as a whole, rather than locally. For the same reason, in order to obtain daily predictions at new locations there is no need to calculate the value of the misaligned covariates at the prediction locations, as the model already estimates the whole latent field.

Our analysis presents some limitations related on one side to the computational requirements of INLA due to the high number of parameters, and on the other side to the generalizability of the results, as the models are quite data-sensitive. In particular, we have very few rural sites even though we extended the study domain outside Greater London, suggesting the presence of preferential sampling that we did not account for. Furthermore, we made assumptions of stationarity and isotropy, which may not hold when extending the spatial domain to bigger areas.

As a next step we will extend the joint model to a multivariate version including other pollutants, such as  $\text{PM}_{10}$  or  $\text{O}_3$ .

In the future, the predicted air pollution concentration with associated measure of uncertainty could be used as exposure in an epidemiological model, allowing for uncertainty propagation.

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## SUPPORTING INFORMATION

Additional supporting information may be found online in the Supporting Information section at the end of this article.

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