Using Satellite Data on Remote Transportation of Air Pollutants for PM2.5 Prediction in Northern Taiwan

George William Kibirige, Ming-Chuan Yang, Chao-Lin Liu and Meng Chang Chen

Abstract—Accurate PM2.5 prediction is part of the fight against air pollution that helps governments to manage environment policy. Satellite Remote sensing aerosol optical depth (AOD) processed by The Multi-Angle Implementation of Atmospheric Correlation (MAIAC) algorithm allows us to observe the transportation of remote pollutants between regions. Here we proposed a composite neural network model, Remote Transported Pollutants (RTP) model, for such long-range pollutant transportation that predicts more accurate local PM2.5 concentrations given such satellite data. The proposed RTP model integrates several deep learning components and learns from the heterogeneous features of various domains. We also detected remote transportation pollution events (RTPEs) at two reference sites from the AOD data. Extensive experiments using real-world data show that the proposed RTP model outperforms the base model that does not account for RTPEs by 17%-30%, 23%-26% and 18%-22% and state-of-the-art models that account for RTPEs by 12%-22%, 12%-14%, and 10%-11% at +4h to +24h, +28h to +48 hours, and +52h to +72h hours respectively.

Index Terms—Remote transported pollutants(RTP), remote transportation pollution events (RTPEs), deep neural network, PM2.5 prediction, composite neural network.

I. INTRODUCTION

With the rapid urban development and industrialization in recent years have come increases in air pollution, leading to health issues such as respiratory and cardiac diseases [1]. Air pollutants consist in part of gaseous and particulate matter (PM). The impacts of PM on human health depend on its size, composition, origin, and solubility. PM2.5 has a diameter less than 2.5 micrometers (μm), and cannot be filtered by nasal passages, leading to serious respiratory diseases [2]. Many nations have constructed urban stations to monitor the presence of PM2.5 in the environment; the resultant datasets can be utilized to better understand and predict PM2.5. In addition, satellites use sensors to gauge the density of pollutants over wide areas and offer updates at regular frequencies. Prediction of future PM2.5 levels is a difficult problem [3], as the dispersion of pollutants depends heavily on meteorological features and terrain, in addition to the activities of inhabitants. Prediction is further complicated by factors such as pollutant migration from outside the observed area. Such long-range transport of air pollutants relies on wind and other meteorological effects. Specifically, in this study, we considered pollutants transported from northeastern Asia across the East China Sea to Taiwan.

In this study, due to its coverage area and strong correlation with PM2.5 [2], we used aerosol optical depth (AOD)

sensory data to better understand the air quality in remote areas. The Moderate Resolution Imaging Spectroradiometer (MODIS) sensor on satellites in the Earth Observing System measures aerosols in the atmosphere. The Multi-Angle Implementation of Atmospheric Correlation (MAIAC) algorithm is used to combine two readings per day from MODIS satellites Aqua and Terra into a single AOD dataset [4]. The MAIAC algorithm has been updated to support global calculations, improving aerosol retrieval, detection of snow and cloud, spatial resolution, and atmospheric correction of the MODIS data. The improved MAIAC product was extensively tested [5] and has been used for air quality and land sensing [6], and has demonstrated improvements in accuracy over MODIS process algorithms such as Dark Target and Deep Blues [7], [8].

The MAIAC products are provided on a 1 kilometer (km) sinusoidal grid, and the gridded data are divided into 1200x1200 square kilometers (km^2) standard MODIS tiles [4]. Each tile's location is represented by horizontal (h) and vertical (v) reading, e.g. h11v05 located at the east cost of United States of America (USA) [4]. In this study, the area in question for extracting remote pollutants consists of four satellite tiles h28v05, h29v05, h28v06 and h29v06 as shown in Fig.1.

In this study we attempted to answer two questions. The first is “Can we identified the occurrence of remote transportation of air pollutants to Taiwan?” We used Tamsui station and Wanli station as reference sites, which located on the northern shore of Taiwan in Fig.1. They are the first to be affected when such long-range air pollutants arrive. We answered this question by detecting PM2.5 hikes at either of these sites. The second question is “Can we incorporated knowledge about remote transportation of air pollutants to produce more accurate PM2.5 predictions?” To answer this question, we exploit existing neural network models by including an extra neural network model using the data on long-range pollutant transport to predict PM2.5 values for Taipei. Answering these questions entails the following challenges in terms of deep learning design and practice.

The first challenge is to prioritize the factors that influence the capture of remote pollutants, as air quality is affected by multiple factors, each with its own spatial and temporal distribution [9]. Second, we incorporated the identified factors into the design of a neural network model to capture the complex interactions between them for better PM2.5 prediction [3]. Third, we used model fusion to train the proposed neural network model on large heterogeneous datasets for improved efficiency and prediction results.

Before discussing these challenges, we reviewed useful tools for PM2.5 prediction. The influence of remote pollutants on the prediction of future local PM2.5 levels involves complex

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Fig. 1. Left side: Four tiles label 1(*h28v06*), 2(*h29v06*), 3(*h28v05*), 4(*h29v05*) with Taiwan in the middle between tiles 1 and 2. Right side: The map of Taiwan after zoom with two stations Wanli (red star) and Tamsui (green star)

factors such as the spatial-temporal correlation between remote pollutants and local pollutants. A deep learning neural network (DNN) can be trained with large meteorological and pollution history datasets to examine this complex correlation between datasets [10], [11]. However, according to [3], for complicated applications in which the problem is not well-defined and is associated with complicated natural environmental factors or social activities, such as long-term (i.e., over the subsequent 48 to 72 hours) prediction of PM_{2.5}, deep learning yields poor results. Other than the computationally expensive traditional end-to-end deep learning, one way to obtain reasonably good results is to use a composite neural network [3].

A composite neural network is a collection of pre-trained neural network models that forms a large neural network (NN) to yield greater learning capabilities without the burden of high model training expenses [12]. Yang and Chen predict PM_{2.5} levels using a composite neural network with pre-trained and non-instantiated components using data from sources such as meteorological and pollution history data. In [13], a performance bound is provided for the composition model that yields good performance on PM_{2.5} prediction using real-world data. In this study, we used the composition network model proposed in [3] as a baseline.

We addressed the first challenge by considering the AOD data and weather data of remote areas typically provided in coarse-grained grids. Generally, remote transportation pollution events (RTPEs) are caused by monsoon and frontal surfaces which are synoptic; therefore, we considered wind speed, direction, and related features. AOD data measurements are available from the earth's surface to the top of the atmosphere, including weather features at different altitudes of atmospheric pressure from 10mb (millibar) to 1000mb to allow deep learning methods to learn temporal and spatial associations.

We tackled the second challenge by extending the pre-trained DNN base model [3] to the remote transported pollutant composite neural network (RTP model), which includes a DNN component to incorporate long-range pollutants for

PM_{2.5} prediction [9], [10], [14]–[18]. This new component learns the spatial correlation between remote AOD and local PM_{2.5} and grasps spatial-temporal features from remote areas.

For the third challenge, we break the new large DNN component into two parts: one for feature extraction and one for prediction. This reduces the number of training parameters and thus the computational cost of the training process with virtually equivalent prediction performance.

Apart from the main task, we also improved daily PM_{2.5} prediction by filling a new heterogeneous AOD dataset for Taipei and by changing the topology of the base model [3] to an extended local satellite dataset (ESD) model, which extracts spatial-temporal knowledge from AOD features.

This research work offers the following contributions.

- 1) To the best of our knowledge, this is the first work to use deep learning to capture extra knowledge from RTPEs from satellite datasets for local PM_{2.5} prediction. The proposed RTP model efficiently captures RTPEs and significantly improves PM_{2.5} prediction in comparison with the base model and state-of-the-art models.
- 2) This paper addressed challenges using RTPEs as features for local PM_{2.5} prediction. These challenges are addressed in a combined fashion to learn from selected features and models.
- 3) We developed a classification algorithm to classify RTPEs of two reference sites at different PM_{2.5} levels and increase rates.
- 4) We applied a composite neural network [3] to develop neural network models incrementally to demonstrate the design rationale and contributions of each component for PM_{2.5} prediction.

In the remainder of this paper, we cover related work in Section II, preliminary knowledge in Section III, the proposed models in Section IV, the classification of RTPEs in Section V, our methodology in Section IV, datasets and preprocessing in Section VI, and the experiments, results, and discussion in Section VII. Finally, section VIII covers the conclusion.

II. RELATED WORK

This section covers research related to PM_{2.5} prediction using satellite AOD data, RTPEs, and composite neural networks.

Satellite-based AOD measurements have been used to estimate and predict PM_{2.5} levels due to their high correlation with PM_{2.5} and their large spatial coverage area [2], [19]–[22]. Lee et al. predict daily PM_{2.5} concentrations in the southern and eastern parts of the United States of America (US) at 1km x 1km resolution using AOD data processed by MAIAC, which yields better performance than other algorithms with 10km x 10km resolution [2]. Kloog et al. use MODIS satellite, land usage, and meteorological data for daily prediction of PM_{2.5} [21]. Similarly, Di et al. develop a neural network with convolutional layers to predict PM_{2.5} concentrations over the US. They use convolutional layers to aggregate information in neighboring grid cells to capture spatial and temporal auto-correlations [20]. Chudnovsky et al. study the relationship between PM_{2.5} and AOD, and find a high correlation of determination between them, concluding that AOD data can be used as a proxy for PM_{2.5} ground concentrations [22].

Some use ensemble models for improving PM_{2.5} prediction [23]–[25]. In an ensemble model, a linear combination of the outputs from different individual models is used for PM_{2.5} prediction, yielding results superior to the individual prediction results. Popular ensemble models in a broad sense include AdaBoost (AD) [23], generalized additive models (GAMs) [24], [25], random forests (RFs) [23]–[25], and extreme gradient boosting (XGB) [23]–[25]. Here we compared these ensemble and machine learning models with the proposed RTP model.

Several studies simulate and quantify RTPEs from Asia to Taiwan [26]–[30]. Most use trajectory statistics (TS) and chemical transport modeling (CTM) approaches. TS uses the frequency of backward trajectories in an area to determine whether that area's pollutants result from remote pollutants. CTM involves a brute-force-based method, which further involves two simulations: one simulation without pollutants from the local area and a normal simulation. The difference between these simulations then determines the pollutant quantities from the remote area. Lin et al. study RTPEs in Taiwan and discover that during winter and spring, 50% to 75% of PM₁₀ in northern Taiwan is due to RTPEs [27]. Chuang et al. study and simulate RTPEs in Taiwan using CTM, showing up to 35% increases in sulfate PM_{2.5} [28]. Similarly, Chen et al. discover that RTPEs are more severe in winter and autumn, increasing the pollutant concentrations by 39% and 41%, respectively [29]. However, approaches which use classical models yield low accuracy for PM_{2.5} prediction due to computational complexity [9] and uncertainty [26]. In this work we used deep neural network models to capture remote pollutants and improve local PM_{2.5} prediction.

One approach for better PM_{2.5} predictions is to use a composite neural network. Yang and Chen predict PM_{2.5} concentrations using a composite neural network base model [3] which consists of six nearest neighbors (NNs) in two groups: pre-trained networks, and non-instantiated networks. The idea behind the base model relies on Yang and Chen's

[13] proposal, which focuses on the performance constraints of the two groups w.r.t. PM_{2.5} prediction. The six NNs are connected to form a rooted directed graph, and the objective of which is to produce superior final prediction results. In computational physics, Meng and Karniadakis propose a composite neural network comprised of three NNs, each of which uses a different heterogeneous dataset [12]. We adopted the same approach by extending the base model and forming two composite neural networks.

III. PRELIMINARY KNOWLEDGE

A. Convolutional Neural Network

Convolutional neural networks (CNNs) are popular networks for image classification [20], [31]. A CNN uses a convolutional kernel to scan through the height and width of an image to extract the spatial features of grids within the kernel, as shown in Fig. 2. It also uses a pooling kernel after convolution to reduce the spatial dimensions of the input image. In this work, we used two-dimension (2-D) convolution to extract spatial features from adjacent grid cells in the satellite image followed by an average pooling layer.

Fig. 2. CNN with 2x2 convolutional kernel, stride of 2, and 2x2 max pooling kernel on 300x300x1 (height x width x channel) satellite tiles

B. Convolutional LSTM

Convolutional Long Short-Term Memory (ConvLSTM), which combines CNN and long short-term memory (LSTM), is used for spatial-temporal prediction [32]–[34]. LSTM is a recurrent neural network (RNN) structure designed to model sequence or time-dependent behavior. LSTM models long-time dependencies by preventing vanishing gradients during model training [35]. Fig.3 shows the inner structure of a LSTM cell: it consists of an input gate i_t , a forget gate f_t , and an output gate o_t . At time t the cell receives X_t as input, H_{t-1} as the previous state, and C_{t-1} as the previous cell output, and uses these to update the information inside the cell. The cell uses the forget gate to drop unimportant information from the input gate and later uses a series of sigmoid (σ) or tanh ($\tanh$) activations to update information and produce the current cell state (H_t) output through the output gate. ConvLSTM, an extension of LSTM, applies an initial convolutional operation to the input spatial data (typically an image). It uses convolutional operations for input-to-state and state-to-state transitions, producing four-dimensional data that preserves spatial and temporal information. The equations to formulate ConvLSTM are shown below with a corresponding

Fig. 3. LSTM cell structure

inner structure in Fig. 4. Input X_t and previous cell state H_{t-1} are satellite tiles of the current and previous hour. Below, $*$ represents the convolutional operator and $\circ$ denotes the Hadamard product.

$$\begin{aligned}
 i_t &= \sigma(W_{xi} * P_q + W_{hi} * H_{t-1} + W_{ci} \circ C_{t-1} + b_i) \\
 f_t &= \sigma(W_{xf} * P_q + W_{hf} * H_{t-1} + W_{cf} \circ C_{t-1} + b_f) \\
 C_t &= \tanh(W_{xc} * P_q + W_{hc} * H_{t-1} + b_c) \\
 C_t &= f_t \circ C_{t-1} + i_t \circ C_t \\
 o_t &= \sigma(W_{xo} * P_q + W_{ho} * H_{t-1} + W_{co} \circ C_t + b_o) \\
 H_T &= o_t \circ \tanh(C_t)
 \end{aligned} \quad (1)$$

where W represents the weight and b the bias. For instance, for i_t the $*$ operator captures spatial features from the input satellite tile X_t and previous cell state H_{t-1} . Input weight W_{xi} , previous state weight W_{hi} , and previous cell output weight W_{ci} with input bias b_i are used to process new input information and accumulate them in the cell before forwarding to f_t , which drops unnecessary information from the cell state. Then C_t uses $\tanh$ to create a new vector of values after being updated using σ . Lastly, o_t uses σ on C_t to decide the values of the cell state and H_t uses $\tanh$ again to filter other values to produce the final cell state H_t . Here we used ConvLSTM to extract spatial-temporal features from satellite tiles.

Fig. 4. ConvLSTM cell structure

IV. PROPOSED MODELS

In this section we describe the proposed composite neural network models ESD and RTP. We explain their components

before discussing the main composite models.

A. spatial-temporal remote information neural network Model

The spatial-temporal remote information neural network (STRI), as depicted in Fig. 5, predicts the PM2.5 concentrations of the 18 Environmental Protection Administration (EPA) stations in Taipei using meteorological and AOD features from remote areas with local meteorological features and PM2.5 value. Due to the size of the STRI model with available graphics processing unit (GPU) memory, to reduce computational costs we divide the model into the STRI_fe and STRI_p submodels (or called components). There are two phases of training that the first phase trains the whole STRI model and the second phase fine-tunes the STRI_p model by freezing the STRI_fe model trained in the first phase. In the first training phase, spatial-temporal features from the remote area are extracted by the STRI_fe model, and the STRI_p model learns to predict the PM2.5 of Taipei area from the extracted features of the STRI_fe model and its input of local meteorological and PM2.5 values. In the second training phase, the STRI_p model is further refined by fixing the STRI_fe model and using the input of local meteorological and PM2.5 values. The STRI_p model is relatively small and converges promptly during the second phase of training, providing opportunities for better prediction results.

In the first training phase, the STRI_fe model receives the current input from four satellite tiles, each of which contains 300x300 values downsampled from 1200x1200 during pre-processing, as will be explained in Section VI. The four-dimensional (4d for short) tensor, $[t, c, w, h]$ corresponding to time, channel, width, and height, represents the input shape of each tile. Considering the available memory and computational resources, the model uses average pooling with 3 dimensions (3d) $[c, w, h]$ on each tile to reduce their dimension along the time axis and output T_q . The convolutional and pooling layers receive T_q for capturing spatial correlation, and aggregate information between grid cells. The output from the pooling layer on the 4d tensor is denoted by P_q :

$$P_q = L(\varrho(c + b_i * v)) \quad (2)$$

where L represents the pooling layer, c is the convolutional feature from the convolutional layer, b is the additional bias, v is a vector with the same size as c , and ϱ is an activation function.

$$c = T_q * K \quad (3)$$

where T_q is the downsampled AOD data, $*$ represents the convolutional operation, and K is the convolutional kernel. The STRI_fe model uses a series of ConvLSTM layers with batch normalization, used to speed up the training process [36], in between to capture spatial-temporal information in the grid cells of each tile. The output of ConvLSTM for each tile ($H_{T1}, H_{T2}, H_{T3}, H_{T4}$) are concatenated and then flattened to produce a 1 dimension (1d) tensor $[e,]$. The flatten layer unstacks all tensors in 1d, therefore e is results of $(t \cdot c \cdot w \cdot h)$, where $\cdot$ represents multiplication.

On the right hand side of STRI_fe of Fig. 5, the ConvLSTM structure with batch normalization is applied to the current

Fig. 5. Structure of STRI, STRI_fe and STRI_p models, where red dashed circle denotes extraction of spatial-temporal features from remote areas.

remote weather dataset to extract spatial-temporal features, which represent historical weather patterns of wind and other features associated with time and location. Furthermore, the 4d tensor's output from ConvLSTM, denoted by H_W is flattened and output as 1d tensor $[x,]$ where x is the product of t, c, w, h . After that, the $[e,]$ and $[x,]$ tensors are fused together to form 1d tensor $[g,]$ where g is the sum of $|e|$ and $|x|$. The merged output is denoted by R_p , which is the extracted spatial-temporal features of remote pollutants with their corresponding weather features. The STRI_fe model uses RepeatVector to transform R_p to a 2d tensor $[t, g]$ to match output shape $[t, ps]$, where t is the time stamp and ps is the future PM2.5 values of 18 stations. Then, R_p which is transferred to the STRI_p model to be concatenated with local PM2.5 and meteorology data for PM2.5 prediction of the future hours.

In the second training phase, the STRI_p model is further refined with the fixed STRI_fe model to reduce the training time, model complexity, and model parameters for improved prediction results. As shown in Fig. 5, the STRI_p model consists of a series of fully connected (FC) layers after the concatenation layers. STRI_p receives a 2d tensor $[t, g]$ as the current extracted spatial-temporal features (R_p). It also receives 1d tensors $[pm,]$ and $[met,]$ for local sequences of PM2.5 (L_p) and meteorology data (L_m). Future weather forecast data is included in the current L_m to reflect weather fluctuations, because the current weather is not satisfactory for long-term prediction, i.e., beyond 24 hours [9]. Furthermore, the model uses RepeatVector layers on $[pm,]$ and $[met,]$ to transform them to 2d tensors $[t, pm]$ and $[t, met]$ to match other input features. Then the input features are merged together, denoted as HR , using a concatenation layer to form 2d tensor $[t, feature]$. Finally, FC layers is applied to HR to learn the complex interaction between features extracted from

the remote area and local features and make predictions.

$$V_i = \varrho(W_i \odot HR_i + b_i) \quad (4)$$

where ϱ is the rectified linear activation function (ReLU), $\odot$ denote multiplication and W_i and b_i are the weight and bias of the FC layer of STRI_p. The last FC layer with the linear function performs the prediction and outputs the result, denoted by y ; W_e and b_e are the weight and bias used by the layer

$$y = W_e \odot V_i + b_e \quad (5)$$

B. Base Model

The composite neural network [3] is comprised of six heterogeneous NNs designed for PM2.5 prediction for 18 EPA stations using local influential factors within the Taipei area (30x38 cells). The model uses 21 features from EPA and 26 features from the Center Weather Bureau (CWB) related to air quality and weather status. Among the 1140 cells (i.e., 30x38), there are 18 EPA stations and 33 CWB stations. Before the training phase, Yang and Chen [3] use 4-nearest neighbor (4-NN) clustering to fill grid cells without monitor stations. Fig. 6 shows the base model for the next 72hour prediction. For the next 24hour and 48hour predictions, the base model have the same architecture but different details, such as activation functions and weights (W).

The base model has ten weight matrices and two activation functions, Linear activation function with bias ($linear()$) and Scaled Sigmoid activation functions with bias ($Scaled_Sigmoid()$). The equation below demonstration how $linear()$ and $Scaled_Sigmoid()$ work when receiving input $\vec{h} = (h_1, \dots, h_n)$.

$$Linear(\vec{h}) = \sum_{i=1}^n \alpha_i h_i + b \quad (6)$$

$$Scaled_Sigmoid(\vec{h}) = \sum_{i=1}^n \alpha_i \left(\frac{2}{1 + e^{-2h_i}} - 1 \right) + b \quad (7)$$

Fig. 6. Base model[3]

where n number of input elements and α_i is the weight of h_i and b is the bias.

The base model combines six heterogeneous models as its components: one LSTM, two FC and three convolutional LSTMs (ConvLSTM). Each component has its own input data and its expected task. For example, ConvLSTMs extract spatial-temporal knowledge of EPA, CWB and weather forecasting datasets, and two FC are expected to automatically distillate the information from EPA and CWB data. The resultant PM2.5 prediction performance is the best of all comparisons [3].

C. Local Satellite Data Model

The local satellite data (LSD) model is a simpler composite neural network than STRI that LSD only considers local AOD data in the Taipei area. We fill the area with AOD data using satellite tiles h28v06 (tile 1) and h29v06 (tile 2), as discussed in the data preprocessing section. We also fill the Taipei area with PM2.5, weather forecast, and meteorological data, all of which are aligned as daily readings.

As shown in Fig. 7(a), the model starts with a series of CNNs on the AOD data with the 4d tensor $[t, c, w, h]$ to capture the spatial correlation from neighbors along the temporal axis. Then a pooling layer is applied after CNN to reduce the spatial dimensions and aggregate features between the grids and output K_o , a 4d tensor, at the same time the model uses the same series of CNN and pooling layers on the current 4d tensor, which includes meteorological, air quality, and weather forecast data, and outputs 4d tensor (K_l). Later, the model flattens K_o and K_l along the temporal axis, yielding two 3d tensors $[t, feature]$ concatenated using an Add layer, producing a 3d tensor. Thirdly the model uses an LSTM to extract temporal related features from this 3d tensor. Finally, the model uses the first FC layer to learn the interaction and correlation between all features in a nonlinear way [9] and then produces the PM2.5 prediction using the final FC layer.

Fig. 7. (a) Structure of LSD model, (b) RTP model, and (c) ESD model

D. Remote Transported Pollutant Model

RTP is a composite neural network consisting of a pre-trained base model as described in Section IV-B and an STRI_p component, which handles knowledge from Remote Transportation Pollution Events (RTPEs). Fig. 7(b) illustrates the RTP structure with both components trained separately, after which they are used as pre-trained components in the RTP model using a series of linear functions $linear()$ for improved overall local PM2.5 prediction for the 18 EPA stations.

The RTP model predicts PM2.5 concentrations by ensembling input from the two components. The base model yields PM2.5 predictions $O = \{o_1, o_2, \dots, o_n\}_{t=1}^z$ and STRI_p yields $X = \{x_1, x_2, \dots, x_n\}_{t=1}^z$ for $n = 18$ monitor stations for next z hour where $z = 4, 8, \dots, 72$. The RTP model then produces PM2.5 predictions for all n stations for the next 1 to z hours using O and X . The objective here is to improve local PM2.5 prediction by accounting for RTPEs.

E. Extended Local Satellite Model

As shown in Fig. 7(c), the ESD model with series of Linear() is composed of the base model and the LSD model, which handles heterogeneous satellite AOD data. AOD sensory data is composed of columnar pollutant measurements as opposed to ground measurements, and due to the difference of granularity, AOD is interpolated for the finer granularity in the Taipei region. The difference between the RTP and ESD models is that ESD has the LSD component with local AOD knowledge to improve daily PM2.5 prediction, while RTP utilizes STRI_p, which learns the remote AOD knowledge.

ESD produces predictions using these two components. Given the PM2.5 prediction output $P = \{p_1, p_2, \dots, p_n\}_{d=1}^f$ of next f days for cells with n monitor station from the base model, where $f = \{1, 2, 3\}$, as well as the PM2.5 prediction output $Y = \{y_1, y_2, \dots, y_n\}_{d=1}^f$ of next f days for the same n cells from the LSD model, then the ESD predicts the PM2.5 concentrations of the next f days of all n cells.

V. CLASSIFICATION OF REMOTE POLLUTANTS

In this section we answered the first question by classifying PM_{2.5} levels at the Wanli and Tamsui stations in the Taipei region that are affected by RTPEs. Again, as shown in Fig. 1, due to their locations in Taiwan, these stations are the first to show evidence of RTPEs. In addition, since both Wanli and Tamsui are by the seashore, their background PM_{2.5} values are stable and relatively low. The occurrence of RTPe will cause the rise of their PM_{2.5} value. Therefore, we start by producing PM_{2.5} predictions using the STRI_{fe} and SRTI_p models without considering the local PM_{2.5} influence factor. Then we use a classification algorithm for different PM_{2.5} concentrations in the prediction results. In our prediction experiment, we considered only from November to May because they are months when RTPEs have the greatest impacts on northern Taiwan [26]. The STRI_{fe} model is discussed in the previous section; here we cover the classification algorithm.

The classification algorithm classifies the PM_{2.5} concentrations for the next 24, 48, and 72 hours that are affected by RTPEs. Such remote pollutants are understood to flow across the eastern China Sea to Taiwan; however, due to variations in wind direction, not all pollutants reach Taiwan. Thus, we seek to ascertain the amount of pollutants reaching Taiwan. In the first condition, we assume that the arrival of such remote pollutants raises PM_{2.5} concentrations beyond a certain threshold at these stations. In the second condition, we focused on PM_{2.5} increases over two consecutive hours because we assume that remote pollutants increase rather than decrease the concentration of local pollutants. That is, our second assumption is that remote pollutants yield positive changes between two consecutive predictions. For example, if remote pollutants arrive in the current hour (t), then the difference between the current PM_{2.5} and that of the previous hour (t-1) must be positive.

A. Classifying remote transportation pollution events

For the two conditions, we created three thresholds each. That for the first condition is the EPA threshold (Epa_tshd). Chuang et al. show that RTPEs in northern Taiwan account for PM_{2.5} concentrations ranging from 31 to 39 [26]. These quantities were obtained by studying the contribution of RTPEs on PM_{2.5} in northern Taiwan during the monsoon winter seasons from 2005 to 2015. We used this range to select thresholds of 30, 33, and 36 for the first condition. Predictions exceed any of these thresholds are said to satisfy the first condition.

For the second condition, we considered the differential threshold (Diff_tshd). We convert the true and predicted PM_{2.5} concentrations to first-order difference vectors, after which we select differential thresholds 0.5, 1.0, and 1.5. For the second condition the difference between the current hour's predicted value and that of the previous hour must be greater than or equal to these Diff_tshd. Therefore, an RTPe is said to occur if the peak value simultaneously satisfies both conditions.

Fig. 8 is a figure of an example with the ground-truth (GT) and predicted results of the next one hour and next four hours for the Wanli station. The Epa_tshd and Diff_tshd used of the example are 30 and 0.5, respectively. The green

dashed line indicates Epa_tshd, and the colored dots represent the peaks from different predicted hours that exceed the two thresholds. The 26 red dots represent the total number of RTPEs predicted in 1 hour, compared to the 69 ground-truth events. The accuracy of RTPe detection is thus 37.7%.

Fig. 8. Prediction of +1h and +4h with ground truth at Wanli station. The dots and stars at the bottom show all peaks that meet both EPA and Differential conditions.

1) *Evaluation Metrics on Classification*: Note that an RTPe is defined by conditions that depend on the given Epa_tshd and Diff_tshd thresholds. By definition, a true positive (TP) RTPe is when the ground truth and the model prediction are both larger than the Epa_tshd and Diff_tshd. A True negative (TN) event occurs if neither ground truth nor prediction is larger than the given thresholds. False positive (FP) and False negative (FN) events are defined similarly. We used these to calculate the accuracy (A), precision (Pr), recall (R), and F1 score. In particular, the F1 score is defined as the following:

$$F1_score = \frac{(2 * TP)}{((2 * TP) + FN + FP)} \quad (8)$$

For the formulas for A, Pr, and R, see the deep learning textbook [37]; further classification details are provided in the Appendix

VI. DATASETS AND DATA PREPROCESSING

Of the two dataset groups, that used to evaluate the ESD model contains daily data and that for the RTP model contains hourly data

A. Dataset for ESD Model

The dataset for the ESD model includes daily satellite AOD data, air quality data, and meteorological data. The model is trained on two years (2014 and 2015) of data and tested on one year (2016) of data.

1) *Satellite MAIAC AOD dataset (daily)*: This is satellite AOD data at a 1x1-km resolution created using the MAIAC algorithm and downloaded from the National Aeronautics and Space Administration (NASA) website [38]. Taipei, the area in question, with an area of 30x38km², is located between tiles 1 and 2 (h28v06 and h29v06), each of which covers a 1200x1200km² area. Fig. 1 shows these two tiles, which we

used to fill the AOD data of Taipei area by matching their latitude and longitude coordinates. After matching these coordinates, we pre-processed and filled grid cells with missing or anomalous AOD data with the means of AOD data of its 3x3 neighbouring cells.

2) *Air quality dataset (daily)*: We obtained hourly air quality data from the Taiwan EPA website [39] consisting of PM10, PM2.5, Carbon monoxide (CO), Nitrogen Oxides (NOx), Ozone (O₃), and Sulfur dioxide (SO₂). In the study area there are a total of 1140 grid cells (30x38), eighteen of which have EPA monitor stations; thus we use the four nearest neighbours (4-NN) method to fill grid cells with empty values. We then convert all data to daily readings by taking 24-hour averages.

3) *Meteorological Data (daily)*: We obtained meteorological data from the Center Weather Bureau (CWB) website [40] which is provided at six-hour intervals. Each reading includes wind speed and direction, rainfall, pressure, temperature, and humidity. The data covers only 33 grid cells in the Taipei area. Again, we use 4-NN to fill those cells without monitor stations and then average these into daily readings.

B. RTP model dataset

1) *Satellite MAIAC AOD dataset (per day)*: As shown in Fig. 1, the remote area is covered by satellite tiles h28v05, h29v05, h28v06, and h29v06 with the MAIAC AOD sensory data and each tile covers a 1200x1200-km² area, for a total of 1200x1200 grid cells per tile. The satellite AOD were obtained from the NASA website [38].

First, we calculate the daily means of quality AOD values to fill missing and poor-quality AOD. If there is no quality AOD data for an entire day, we use the mean values of the previous day. We assume AOD values of grid cells over a day are the same for the whole day; thus we repeat the same value 24 times to match 24 hourly readings per day.

Secondly, to make best use of the available GPU memory and to reduce computational costs, we downscale each tile separately to reduce the spatial dimensions. Sønderby et al. downscale satellite images for precipitation from a spatial dimension of 1024x1024km² to 512x512km² using mean pooling [33]. Here we used the same approach; however, to maintain the distribution of values in each tile, we use maximum pooling instead of mean pooling. Maximum pooling is applied twice to each tile image to downscale it from 1200x1200km² to 300x300km².

2) *Remote Meteorological Data (hourly)*: We used the National Center for Environmental Prediction (NCEP) final (FNL) global analysis data [41]. These are collected all over the world and provided by the Global Data Assimilation System, and are provided over 28x28-km² grids every six hours. We converted these to one-hour intervals via linear interpolation to match the other data. The data include the following meteorological features: temperature, pressure, vertical velocity (VVEL), absolute vorticity (ABSV), lifted index (LFTX), wind speed, and wind direction. The wind speed (denoted as ws) and direction (denoted as θ) are represented as u and v components, i.e., $ws * \cos(\theta)$ and $ws * \sin(\theta)$. The

u component is the horizontal speed toward the east (known as Zonal Velocity) and v component is the horizontal wind speed toward the north (known as Meridional Velocity). The wind speed and direction, temperature, VVEL and ABSV were considered at pressure levels from 10mb to 1000mb.

3) *Air quality dataset (hourly)*: We obtained PM2.5 features for the 18 stations in Taipei from the EPA website [39]. The data were provided at one-hour intervals.

4) *Local Meteorological Data (hourly)*: We obtained meteorological data for the 18 stations in Taipei from the CWB website [40]. The data were provided at six-hour intervals, and we transformed them to hourly intervals via linear interpolation. The data consist of features for rainfall, pressure, temperature, humidity, wind speed, and wind direction.

VII. EXPERIMENTAL RESULTS AND DISCUSSION

A. Experimental settings and model parameters

We used data from 2014 to 2016 to evaluate the proposed neural network models. Data of two years (2014–2015) were used for training and one year (2016) for testing. The data for the ESD evaluation were prepared at a daily granularity, whereas for the RTP model the data were at hourly granularity.

The two models were trained on an NVIDIA GPU with 11 gigabytes (GB) and implemented on Keras with Tensor Flow backend environment. In the proposed models, we used the rectified linear activation function (Relu) for all layers except for the prediction layer. Learning rates of 0.0015 and 0.0001 were used for ESD and RTP model, respectively; 0.00001 was used for the STRI_{fe} and STRI_p models, and Adam optimization was used for all training. In addition, to reduce overfitting, we applied dropout layers, weights and bias kernel regularization to several layers.

All models were evaluated using root mean square error (RMSE), which shows the difference between the predicted and true values

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} \quad (9)$$

where n is the number of stations and y_i and $\hat{y}_i$ are the true and predicted values of the timestamp. In this work, we consider the mean RMSE of all monitor stations.

B. Performance of ESD model

In Table I we compare the PM2.5 prediction results of the ESD model with that of its components, base model and the LSD model, where $\Delta\%$ is the relative improvement in RMSE over the base model. We also include the performance of RTP model which performed in daily like other models in table. The RTP model that use RTP_{Es} from 2tile and 4tile are represented by RTP_{2tile} and RTP_{4tile} respectively.

We begin by comparing LSD, ESD and the base model and then we compare them with RTP model. For the base model, a large model with six components, converting the hourly data to daily data reduces the amount of training data, which impacts the base model training, especially for long-term prediction. The base model outperforms the LSD model at the next 1 day (+1day in short) because it uses more features than LSD.

For +2day and +3day, the LSD component outperforms the base model due to the application of AOD data in the models. For the proposed ESD model, which consists of the base model with the addition of the pre-trained LSD component, the corresponding heterogeneous AOD data improves RMSE prediction by 12.68%, 11.45%, and 6.65% for +1day, +2day, and +3day, respectively, in comparison to the base model. The topological changes of ESD with the addition of new local AOD knowledge decrease the prediction error between the true and predicted values.

For comparison of RTP model with base model, LSD model and ESD model. The RTP_2tile and RTP_4tile outperform all those three models for +1day, +2day and +3day. The results show that the RTP model captures RTPes from remote AOD and weather data and it helps improve the prediction performance for all days. With reference to the base model, the RTP_4tile provides the greatest improvement prediction performance in RMSE by 25.77% for +1day and 28.96% and 21.17% for +2day and +3day. In other words, the RTP_4tile outperforms RTP_2tile in all three days that the result demonstrates the enlarged remote area will help improve the local prediction of PM2.5. This matches with our idea of enlarging the remote area from 2tile to 4tiles with the objective of capturing more RTPes.

TABLE I
RESULTS FOR BASE, LSD, ESD AND RTP MODELS

Target	Model	RMSE	$\Delta(\%)$
+1day	base	7.299	
	LSD	8.170	-11.93
	ESD	6.373	12.68
	RTP_2tile	5.781	18.58
	RTP_4tile	5.418	25.77
+2day	base	9.802	
	LSD	8.801	10.21
	ESD	8.679	11.45
	RTP_2tile	8.342	14.89
	RTP_4tile	6.963	28.96
+3day	base	9.898	
	LSD	9.389	5.14
	ESD	9.240	6.65
	RTP_2tile	8.523	13.89
	RTP_4tile	7.803	21.17

C. Prediction of RTPes

To answer the first question that we raised in the Introduction, i.e., to predict RTPes, we predicted the local PM2.5 for the two stations first using only the local PM2.5 and weather as input to the STRI_p model with the extracted spatial-temporal features from remote areas. We predicted the RTPes by applying the thresholds Diff_tshd and Epa_tshd to the PM2.5 predictions. In order to observe the general performance, we used combinations of various thresholds that Diff_tshd=30, 33, 36 and Epa_tshd=0.5, 1.0, 1.5. Tables II to IV show the classification results in terms of accuracy (A), precision (Pr), recall (R), and F1 score (F1). The first column

indicates the data used, for instance, “P” represents the local PM2.5 values, “EP” represents the remote spatial-temporal features from four tiles, and “W” represents the local weather features. The results are shown in Tables II, III and IV.

We first note the increases in accuracy and others metrics for many forecasts when EP and W are added to the model, which demonstrates the contribution of RTPes to increasing PM2.5 concentrations at the stations. A similar trend is observed for the Epa_tshd threshold, although the increases in accuracy are lower. For example, for the +24h predictions for the Wanli station with a Diff_tshd of 0.5, the accuracy are 0.72, 0.62, and 0.46 for Epa_tshd thresholds of 30, 33, and 36, respectively. This shows that as the threshold of PM2.5 increases, the prediction of PM2.5 tends to be conservative and cannot follow the PM2.5 increase that results in low accuracy.

In terms of precision and recall, the highest recall of 0.44 is observed at Wanli whereas for Tamsui, the highest is 0.41, both at thresholds of 0.5 (Diff_tshd) and 30 (EPA_tshd) for +24h. For precision, the highest score is 0.24 and 0.30 at thresholds of 0.5 (36) for the Wanli and Tamsui stations, respectively. Overall, these results demonstrate the effects of the STRI model for the RTPes prediction of these two stations in northern Taiwan.

D. Performance of RTP Model

In this section we answer the second question about improving local PM2.5 predictions using knowledge about RTPes. We discuss the results of different training approaches for the RTP components, knowledge captured from RTPes, and the results of RTP models in comparison to other models.

We first evaluated the effect of training strategies on prediction performance by comparing the results from a full STRI model with those using the STRI_fe and STRI_p components, as described in Section IV.A. Fig. 9 shows the comparison results of STRI and STRI_p from Next 4hour (+4h in short) to Next 72hour (+72h in short). STRI_p yields better prediction results than the full STRI model. As training a full STRI model on a single GPU can be a challenge, we use STRI_fe for feature extraction and STRI_p for prediction. Furthermore, as STRI_p consists of a small number of layers, it converges quickly during training, leaving more room for model fine-tuning. The improved performance of STRI_p validates our idea of breaking the full STRI model into two components.

We also evaluated the effects of the extracted remote pollutants and local features on the STRI_p component to show whether the proposed STRI model is able to capture knowledge from remote areas. We conducted experiments using one feature and incrementally added features while observing the results in terms of root-mean-square error (RMSE). Fig. 10 shows the results of various features, including spatial-temporal features from two and four tiles (t12 and t1234) as well as the local PM2.5 (P) and weather (W) features from 18 stations. The weather features include the current and forecasted weather. Therefore, the model input sequence is P, t12 (tiles h28v06 and h29v06), the remaining two tiles t34 (tiles h28v05 and h29v05), and then W. Thus, P+t1234 indicates that P and t1234 are used as the model input.

TABLE II
CLASSIFICATION RESULTS WITH $Diff_tshd = 0.5$

Wanli Station												
<i>Epa_tshd</i>	30											
Hour	+24h				+48h				+72h			
	A	Pr	R	F1	A	Pr	R	F1	A	Pr	R	F1
P	0.44	0.20	0.32	0.25	0.19	0.10	0.17	0.12	0.08	0.06	0.08	0.07
P+EP	0.71	0.20	0.43	0.28	0.26	0.12	0.22	0.16	0.06	0.05	0.06	0.06
P+EP+W	0.72	0.23	0.44	0.30	0.33	0.14	0.26	0.18	0.21	0.12	0.18	0.14
<i>Epa_tshd</i>	33											
P	0.37	0.22	0.29	0.25	0.14	0.10	0.14	0.12	0.02	0.03	0.03	0.03
P+EP	0.61	0.22	0.41	0.29	0.10	0.08	0.10	0.09	0.02	0.02	0.02	0.02
P+EP+W	0.62	0.24	0.41	0.30	0.16	0.12	0.15	0.14	0.08	0.08	0.08	0.08
<i>Epa_tshd</i>	36											
P	0.30	0.20	0.25	0.22	0.11	0.10	0.11	0.10	0.02	0.03	0.02	0.02
P+EP	0.45	0.22	0.34	0.27	0.02	0.06	0.02	0.03	0.01	0.03	0.01	0.02
P+EP+W	0.46	0.24	0.34	0.28	0.06	0.08	0.06	0.07	0.03	0.04	0.03	0.04
Tamsui Station												
<i>Epa_tshd</i>	30											
P	0.50	0.25	0.35	0.29	0.32	0.18	0.26	0.21	0.19	0.16	0.17	0.16
P+EP	0.66	0.28	0.42	0.34	0.32	0.20	0.26	0.22	0.19	0.16	0.17	0.16
P+EP+W	0.63	0.29	0.41	0.34	0.41	0.22	0.31	0.25	0.24	0.17	0.20	0.19
<i>Epa_tshd</i>	33											
P	0.38	0.23	0.29	0.26	0.20	0.13	0.17	0.15	0.09	0.10	0.08	0.09
P+EP	0.54	0.27	0.36	0.31	0.15	0.15	0.14	0.14	0.11	0.14	0.10	0.12
P+EP+W	0.51	0.29	0.35	0.32	0.18	0.17	0.16	0.17	0.13	0.17	0.12	0.14
<i>Epa_tshd</i>	36											
P	0.29	0.22	0.24	0.23	0.08	0.09	0.08	0.09	0.02	0.05	0.02	0.03
P+EP	0.38	0.27	0.30	0.28	0.03	0.05	0.04	0.04	0.05	0.09	0.05	0.06
P+EP+W	0.37	0.30	0.29	0.29	0.07	0.15	0.08	0.10	0.06	0.13	0.06	0.08

TABLE III
CLASSIFICATION RESULTS WITH $Diff_tshd = 1.0$

Wanli Station												
<i>Epa_tshd</i>	30											
Hour	+24h				+48h				+72h			
	A	Pr	R	F1	A	Pr	R	F1	A	Pr	R	F1
P	0.35	0.17	0.32	0.22	0.14	0.07	0.16	0.10	0.05	0.04	0.07	0.05
P+EP	0.56	0.16	0.44	0.24	0.19	0.10	0.20	0.13	0.05	0.05	0.06	0.05
P+EP+W	0.54	0.18	0.43	0.25	0.27	0.12	0.27	0.16	0.17	0.10	0.19	0.13
<i>Epa_tshd</i>	33											
P	0.31	0.18	0.30	0.23	0.10	0.07	0.12	0.09	0.01	0.02	0.02	0.02
P+EP	0.51	0.19	0.41	0.26	0.07	0.07	0.09	0.07	0.02	0.03	0.02	0.02
P+EP+W	0.49	0.20	0.40	0.26	0.14	0.10	0.16	0.13	0.07	0.08	0.09	0.08
<i>Epa_tshd</i>	36											
P	0.24	0.15	0.25	0.19	0.09	0.08	0.11	0.09	0.01	0.01	0.01	0.01
P+EP	0.37	0.19	0.34	0.24	0.02	0.05	0.02	0.03	0.01	0.03	0.01	0.02
P+EP+W	0.37	0.20	0.34	0.25	0.05	0.08	0.07	0.07	0.03	0.04	0.04	0.04
Tamsui Station												
<i>Epa_tshd</i>	30											
P	0.40	0.20	0.35	0.25	0.26	0.15	0.26	0.19	0.15	0.12	0.16	0.14
P+EP	0.54	0.23	0.42	0.30	0.25	0.17	0.25	0.20	0.13	0.14	0.15	0.14
P+EP+W	0.52	0.25	0.41	0.31	0.33	0.18	0.30	0.22	0.19	0.14	0.20	0.17
<i>Epa_tshd</i>	33											
P	0.32	0.19	0.28	0.23	0.17	0.12	0.17	0.14	0.07	0.08	0.08	0.08
P+EP	0.44	0.22	0.35	0.27	0.11	0.12	0.12	0.13	0.08	0.12	0.09	0.10
P+EP+W	0.42	0.25	0.34	0.29	0.15	0.14	0.15	0.15	0.11	0.15	0.12	0.13
<i>Epa_tshd</i>	36											
P	0.23	0.17	0.23	0.20	0.06	0.06	0.07	0.07	0.02	0.05	0.03	0.04
P+EP	0.31	0.22	0.29	0.25	0.03	0.05	0.04	0.04	0.04	0.09	0.05	0.06
P+EP+W	0.30	0.24	0.28	0.26	0.06	0.12	0.07	0.09	0.05	0.13	0.06	0.09

In Fig. 10, we observed a significant gap between the performance when using P and that when using data on remote pollutants from tiles t12 (P+t12) and t1234 (P+t1234). This shows that the model captures RTEs and that these events improve the local prediction performance by reducing the prediction error for all hours. We also observed the impact from

the expanding the range from tiles t12 to t1234, mainly for +28h and longer. This impact is not present between +4h and +24h, possibly as events from the extra two tiles (t34) require additional time to make an impact, due to their distance from the study area. This fits with our goal of expanding the range to four tiles to improve prediction by capturing more RTEs. The

TABLE IV
CLASSIFICATION RESULTS WITH $Diff_tshd = 1.5$

Wanli Station												
Epa_tshd	30											
Hour	+24h				+48h				+72h			
	A	Pr	R	F1	A	Pr	R	F1	A	Pr	R	F1
P	0.44	0.17	0.32	0.22	0.17	0.07	0.16	0.10	0.06	0.04	0.06	0.05
P+EP	0.68	0.17	0.43	0.24	0.20	0.09	0.18	0.12	0.06	0.05	0.06	0.05
P+EP+W	0.66	0.18	0.42	0.26	0.33	0.12	0.26	0.16	0.20	0.10	0.18	0.13
Epa_tshd	33											
P	0.39	0.18	0.30	0.23	0.10	0.06	0.10	0.08	0.02	0.02	0.07	0.016
P+EP	0.63	0.20	0.41	0.26	0.08	0.07	0.08	0.07	0.02	0.03	0.02	0.03
P+EP+W	0.59	0.20	0.39	0.27	0.16	0.10	0.15	0.12	0.09	0.08	0.09	0.08
Epa_tshd	36											
P	0.29	0.15	0.25	0.19	0.09	0.07	0.09	0.08	0.01	0.01	0.01	0.01
P+EP	0.43	0.19	0.33	0.24	0.02	0.05	0.02	0.03	0.01	0.03	0.01	0.02
P+EP+W	0.44	0.21	0.33	0.26	0.06	0.08	0.07	0.07	0.03	0.04	0.04	0.04
Tamsui Station												
Epa_tshd	30											
P	0.46	0.20	0.34	0.25	0.30	0.14	0.25	0.18	0.16	0.11	0.15	0.13
P+EP	0.63	0.24	0.41	0.30	0.29	0.16	0.24	0.19	0.15	0.14	0.14	0.14
P+EP+W	0.61	0.25	0.40	0.31	0.38	0.18	0.30	0.22	0.22	0.15	0.19	0.17
Epa_tshd	33											
P	0.37	0.20	0.28	0.23	0.18	0.11	0.16	0.13	0.08	0.08	0.07	0.08
P+EP	0.49	0.22	0.34	0.27	0.10	0.11	0.10	0.10	0.09	0.13	0.09	0.10
P+EP+W	0.49	0.25	0.34	0.29	0.16	0.14	0.15	0.14	0.13	0.15	0.12	0.13
Epa_tshd	36											
P	0.27	0.18	0.23	0.20	0.05	0.06	0.06	0.06	0.03	0.05	0.03	0.04
P+EP	0.32	0.22	0.27	0.24	0.03	0.04	0.03	0.04	0.05	0.09	0.05	0.07
P+EP+W	0.32	0.24	0.27	0.25	0.07	0.12	0.07	0.09	0.06	0.13	0.07	0.09

Fig. 9. Performance of STRI and STRI_p components from +4h to +72h

addition of W yields superior performance, especially beyond +28h. We attribute this gap to long-term rather than short-term (+4h to +24h) weather fluctuations; that is, in the long term, the weather forecast is used to reflect weather fluctuations [9], which explains the significant gap in that period. Overall, the results show that the STRI_fe component captures knowledge from RTPs by learning spatial-temporal behavior from AOD data with their corresponding weather features from remote areas before transferring to the STRI_p component, which then learns the complex interaction between all input features, yielding improved local PM_{2.5} prediction for the 18 stations.

Third, we evaluated the performance of the RTP model in comparison with the base model [3] and other state-of-the-art ensemble models with the same settings: linear regression (LR) [16], AdaBoost (AB) [23], bagging regression (BG),

Fig. 10. Results given remote pollutant and local features using STRI_p component

random forest (RF), extreme gradient boosting (XGB) [23]–[25], and a generalized additive model (GAM) [24], [25]. We also show RTP performance when we use RTPs from 2tile(RTP_2tile) and 4tile(RTP_4tile) with the objective of showing the impact of remote pollutants towards local prediction of PM_{2.5}.

Fig. 11 shows the relative prediction improvements in RMSE of both RTP models and the other state-of-the-art models w.r.t. base model from +4h to +72h; the greater the improvement, the better the model does in comparison to the base model. The figure shows that RTP_4tile yields the greatest improvements: from 17%–30%, 23%–26%, and 18%–22% for +4h to +24h, +28h to +48h, and +52h to +72h, respectively. Similarly, the RTP_2tile provides greater improvement: from 13%–24%, 17%–23%, and 13%–17% for +4h to +24h, +28h to +48h,

and +52h to +72h. XGB and GAM, in turn, improve on the base model by 6%–8%, 10%–12%, and 8%–11% for +4h to +24h, +28h to +48h, and +52h to +72h, respectively, with scores that are similar to those for the LR model. AB is outperformed by the base model for most hours; RF is also, but to a lesser extent. The RTP_2tile and RTP_4tile outperforms other models due to its composite neural network design [13], which involves high flexibility with learning capability to model nonlinear association between input features. On the other hand, for XGB, GAM and LR yield good performance improvements but are outperformed by both RTP models because of their limited flexibility in their model structure as a result of insufficient learning capability from input features. The performance of RTP_4tile over RTP_2tile continues to demonstrate the importance of the enlarged remote area with the aim of capturing more RTPes from the remote area.

Fig. 11. Relative RMSE Improvement(%) of all models with reference to base model

VIII. CONCLUSION

We proposed RTP, a composite neural network model that captures knowledge from remote transportation pollution events (RTPes) to improve the local PM_{2.5} prediction. To the best of our knowledge, this is the first deep learning work to include knowledge from remote pollutants for PM_{2.5} prediction. RTP consists of two neural network components: a pre-trained base model and STRI model. The base model captures knowledge from local factors that influence PM_{2.5} concentrations and STRI captures knowledge from RTPes by learning spatial-temporal characteristics of AOD data and weather features from remote areas. In addition, given the size of the STRI model, to facilitate training and improve results we divide the full STRI model into two components: STRI_{fe}, which is used to extract spatial-temporal features from remote areas, and STRI_p, which predicts local PM_{2.5} concentrations using both remote and local features. The prediction results from STRI_p show that the prediction error is reduced when remote features are added to the model, demonstrating that the STRI model indeed captures knowledge from RTPes.

To characterize the occurrence of RTPes in northern Taiwan, we also developed an algorithm to classify PM_{2.5} concentrations attributable to RTPes. We use the STRI model for

the prediction of two EPA stations located at the northern tip of Taiwan and apply the classification algorithm to the results. This yields improvements in accuracy when remote features are added to the model, which demonstrates the impact of RTPes at the stations.

We perform local PM_{2.5} prediction using the RTP model for all stations from +4h to +72h. The RMSE results show that the RTP model outperforms the base model and other state-of-the-art ensemble models by 12%–30%, 12%–18%, and 10%–14% for +4h to +24h, +28h to +48h, and +52h to +72h, respectively, due to RTP's composite neural network [13]. The ESD model, although it just considers local AOD data, still improves PM_{2.5} prediction, as evidenced by lower RMSE scores than the those for the base model by 12.68% for +1day and 11.45% and 6.65% for +2day and +3day.

Future work will focus on expanding the remote area, using data that is updated at a higher frequency compared to the AOD data, considering other possible features and re-analyzing weather features.

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APPENDIX A DOWNSCALE SATELLITE TILES

We show how we downscale each satellite tiles in the remote area from 1200x1200 km² to 300x300 km². The max pooling of 2x2 kernel with 2x2 stride is used to downscale satellite tiles while maintaining the distribution of values like the original tile. The kernel window slides on the satellite image and summarizes each sub-region with the maximum value. Fig.1 shows how max pooling works on satellite tiles with the following shape [hours, height, width], where hours represent all hours in year. The Fig.2 illustrates the way maximum kernel reduce the pixel values inside the kernel .

APPENDIX B CLASSIFICATION DETAILS

The numerical prediction score of PM2.5 is converted into decision by checking if the score is above the defined threshold values. Base on he International Organization for Standardization (ISO) 5725, numeric accuracy is the decomposition of numerical quantities into numerical version of trueness and precision. Therefore, we calculate the score of the evaluation metrics including accuracy, precision, recall and F1_score between prediction results and true values using three defined thresholds of PM2.5. We use the confusion matrix as a tool to calculate those metrics, the confusion matrix contains all the information that can be used to analyze the errors and confusion of the end results [31]. Furthermore, the confusion matrix consists of true positive (TP) information which in this work we define as predicted PM2.5 value which satisfy both thresholds condition. The matrix also contains true negative (TN), false positive (FP) and false negative (FN) information, Table I shows the details of the remote transportation event confusion matrix that match with this task. The equations below show how to calculate all classification metrics.

Given PM2.5 ground truth(GT) values and their predicted values as remote transportation (RT) with their corresponding first order differential vector GTD and RTD. Moreover given the Epa_tshd(β_1), Diff_tshd(β_2) and the total number of hours that used in prediction(all hours in winter and autumn seasons). We obtain four events(E) after applying those thresholds

Fig. 12. Downscale of Satellite tile from spatial dimension of 1200x1200 to 300x300 using Maximum pooling with kernel size of 2x2

Fig. 13. Illustration of the max pooling with kernel of 2x2 applied to input image with shape 6x6

$$P(RT \cap RT') = \frac{\text{count}\{E_3 \cap E_4\}}{\text{total}\{t\}} == P(RT|RT')P(RT') \quad (17)$$

TABLE V
CONFUSION MATRIX OF REMOTE EVENT

		Predicted PM2.5 values	
Ground Truth PM2.5	Remote Event=Yes	TP= $(GT \cap GT') \cap (RT \cap RT')$	FN= $(GT \cap GT') \cap \neg(RT \cap RT')$
	Remote event=No	FP= $\neg(GT \cap GT') \cap (RT \cap RT')$	TN= $\neg(GT \cap GT') \cap \neg(RT \cap RT')$

to PM2.5 values.

$$E_1: GT > \beta_1, E_2: GTD > \beta_2, E_3: RT > \beta_1, E_4: RTD > \beta_2$$

Then we use probability(P) to obtain the number of remote transportation pollution events by considering their occurrence with total number of hours(t). Later, the confusion matrix in Table I shows how to calculate true positive(TP), false negative(FN), false positive(FP), and true negative(TN), which show the full picture of our model performance.

$$P(GT) = \frac{\text{count}\{E_1\}}{\text{total}\{t\}} \quad (10)$$

$$P(GT') = \frac{\text{count}\{E_2\}}{\text{total}\{t\}} \quad (11)$$

$$P(GT|GT') = \frac{\text{count}\{E_1 \cap E_2\}}{E_2} \quad (12)$$

$$P(GT \cap GT') = \frac{\text{count}\{E_1 \cap E_2\}}{\text{total}\{t\}} == P(GT|GT')P(GT') \quad (13)$$

$$P(RT) = \frac{\text{count}\{E_3\}}{\text{total}\{t\}} \quad (14)$$

$$P(RT') = \frac{\text{count}\{E_4\}}{\text{total}\{t\}} \quad (15)$$

$$P(RT|RT') = \frac{\text{count}\{E_3 \cap E_4\}}{E_4} \quad (16)$$

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