Eulerian Neural Network Informed by Chemical Transport for Air Quality Forecasting

Xukai Zhang[1], Shuliang Wang[1], Guangyin Jin[2], Ziqiang Yuan[1], Hanning Yuan[1*] , Sijie Ruan[1*]

[1]Beijing Institute of Technology, [2]Sapienza University of Rome

{xkzhang,slwang2011,ziqiangy,yhn6,sjruan}@bit.edu.cn, jinguangyin96@gmail.com

Our Laboratory

Code and Data

NEURAL INFORMATION PROCESSING SYSTEMS

Introduction

➢ Background

- Accurate air quality prediction is crucial for
  - mitigating health risks
  - guiding public health
  - shaping policies
  - enhancing environmental monitoring in smart, sustainable cities

➢ Problem Statement

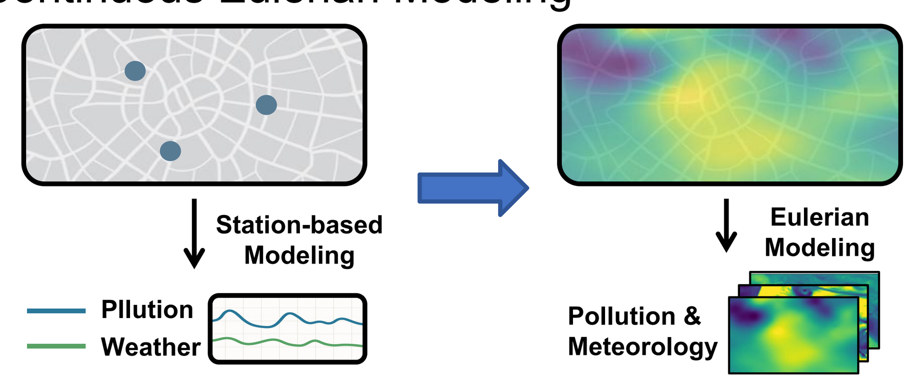
- **Input:**
  - ✓ Historical pollutant concentration data $P_{1:T} \in \mathbb{R}^{T\times C_P\times N}$ from N observation stations located at spatial coordinates $\mathcal{S} = \{(h_n, w_n)\}_{n=1}^{N}$
  - ✓ Continuous meteorological data $M_{1:T} \in \mathbb{R}^{T\times C_M\times H\times W}$, where C_M denotes the number of channels, including wind components as well as other meteorological variables
- **Output:**
  - ✓ The pollutant concentrations at all station locations over the future time period from $T+1$ to $T+\tau$, denoted by $\hat{P}_{T+1:T+\tau}$
- **Task:**
  - ✓ To learn the function $\mathcal{F}$:

$$\hat{P}_{T+1:T+\tau} = \mathcal{F}(P_{1:T}, M_{1:T}),\ \hat{P}_{T+1:T+\tau} \in \mathbb{R}^{\tau\times C_P\times N}$$

➢ Challenge and Contribution

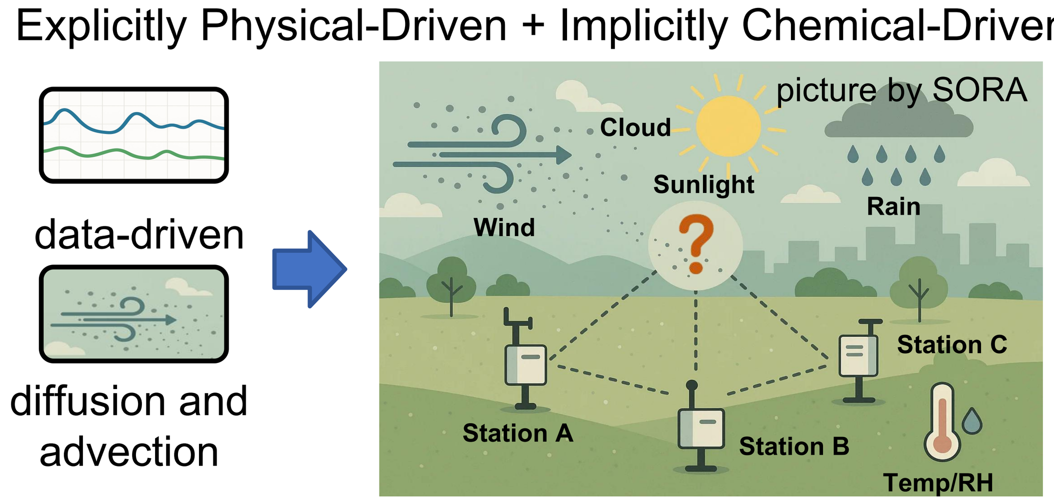
① **Data Representation**

- ✦ **Traditional Discrete Modeling**
  - Multivariate time series / Spatial-temporal graph
  - Ignoring spatial continuity
- ✦ **Our Eulerian Modeling**
  - Continuous Eulerian Modeling



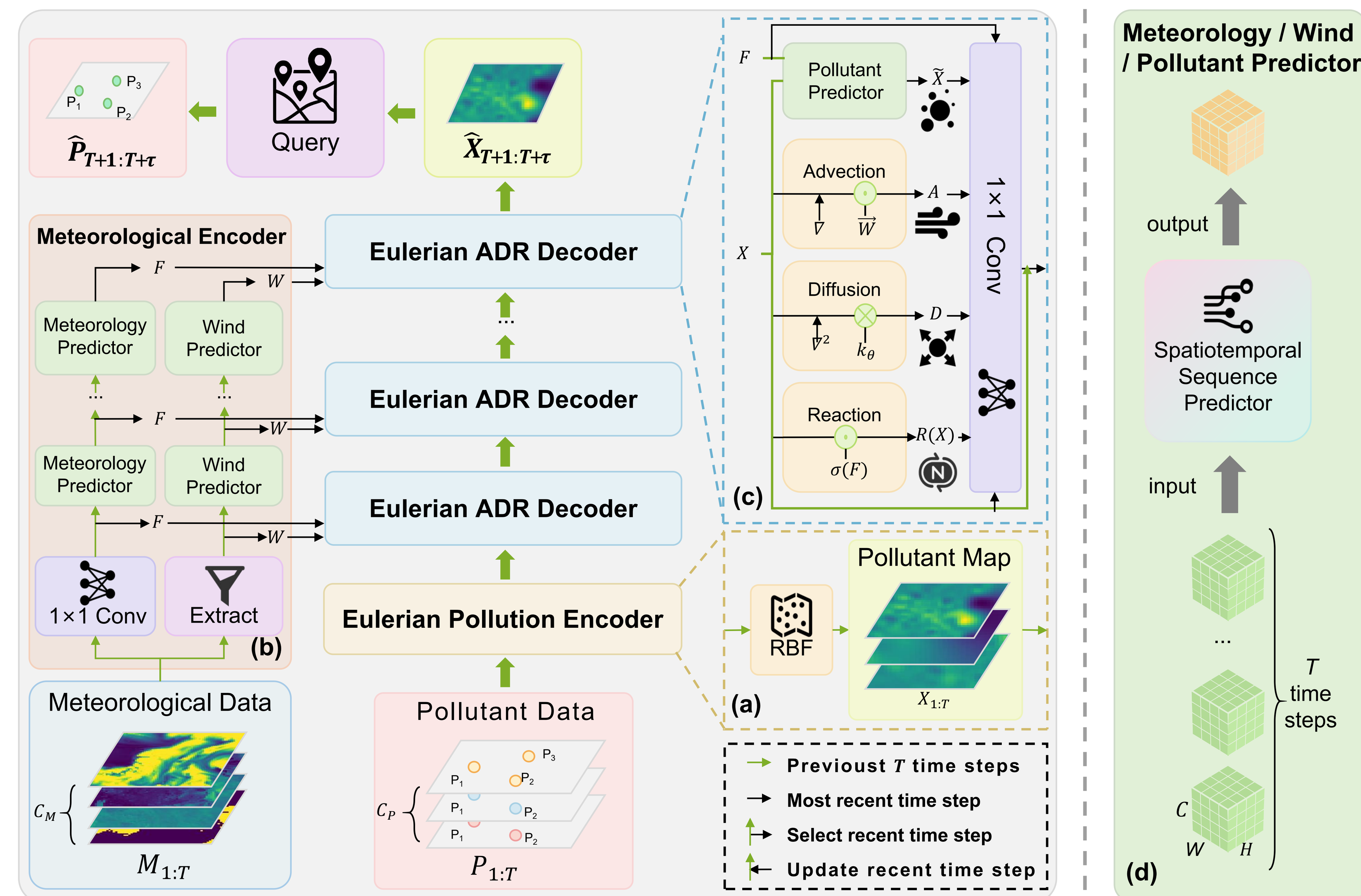
② **Evolutionary Mechanism**

- ✦ **Traditional Drivers**
  - Purely data-driven / only physical drivers
  - Ignoring secondary pollutant generation (e.g., photochemistry)
- ✦ **Our Physicochemical Driver**
  - Explicitly Physical-Driven + Implicitly Chemical-Driven



Methodology

Structure of our propossed CTENet



(a) Eulerian Pollution Encoder
employs RBF interpolation to construct smooth pollutant fields from discrete observations, preserving spatial gradients and variability.

$$rbf(x) = \sum_{i=1}^{n_t} \lambda_i^{(t)} \phi\left(\left\|\mathbf{x} - \mathbf{x}_i^{(t)}\right\|\right),\ t \in \{1,\ldots,T\}$$

(b) Meteorological Encoder
performs two tasks in parallel:

- Extracts the wind channels
- Utilizes a 1x1 convolution to obtain meteorological features

Then, Wind Predictor and Meteorology Predictor are used to forecast future wind fields.

(d) ST Sequence Predictor
Although the Wind, Meteorology, and Pollutant Predictors serve different functions, their inputs and outputs all share the same dimensions: (T, C, H, W). The framework features a replaceable Spatiotemporal Sequence Predictor function, allowing for easy plug-and-play integration of models such as ConvLSTM[1], depending on the specific requirements.

[1]Xingjian Shi, Zhourong Chen, Hao Wang, Dit-Yan Yeung, Wai-Kin Wong, and Wang-chun Woo. Convolutional lstm network: A machine learning approach for precipitation nowcasting. Advances in neural information processing systems, 28, 2015

(c) Eulerian ADR Decoder
attempts to embed Chemical Transport Modeling (CTM) into neural networks, specifically represented by the following ADR equation:

$$\frac{\partial X}{\partial t} + \underbrace{\vec{W}\cdot\nabla X}_{Advection} = \underbrace{k_\theta \cdot \nabla^2 X}_{Diffusion} + \underbrace{R(X)}_{Reaction} + \underbrace{S}_{Source}$$

We numerically discretize the equation and incorporate the results as independent channels into the pollutant predictor.

Evaluation

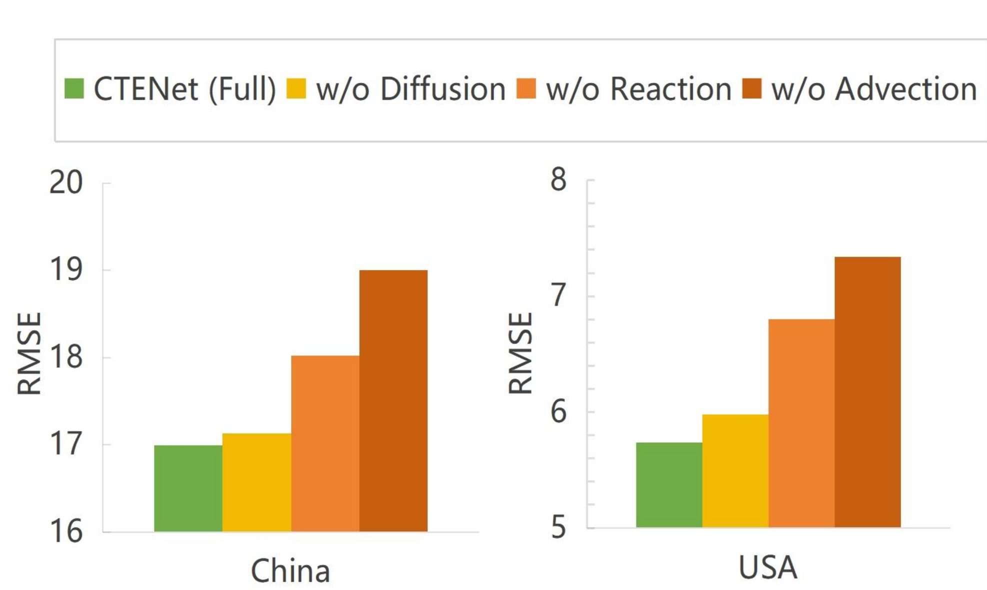
➢ Performance

RMSE improvement: **45.8%**(USA) and **21.0%**(China)

Methods	USA Data						China Data					
	24h		48h		72h		24h		48h		72h	
	MAE	RMSE	MAE	RMSE	MAE	RMSE	MAE	RMSE	MAE	RMSE	MAE	RMSE
HA	5.30	11.57	5.66	12.54	5.99	13.23	21.64	38.03	22.76	39.12	23.58	40.03
VAR	6.32	14.41	5.78	12.74	5.76	12.94	24.74	39.85	25.43	41.85	26.66	44.14
STGCN	4.29	9.03	4.51	9.03	4.63	9.08	31.43	43.72	31.91	44.06	32.69	44.75
DCRNN	5.40	14.50	5.42	12.81	5.38	13.48	28.14	49.81	27.45	47.36	27.39	47.63
GTS	5.57	14.65	5.60	14.32	5.61	14.18	23.46	41.70	23.50	42.53	23.85	44.41
AirFormer	4.05	10.44	4.40	10.74	4.60	10.89	19.09	36.08	20.89	38.42	21.85	39.61
AirPhyNet	4.47	11.36	4.79	11.40	4.94	11.48	18.75	36.35	19.97	37.16	20.74	37.64
$PM_{2.5}$-GNN	4.38	9.77	4.63	9.66	4.76	9.63	17.71	33.25	19.12	34.16	19.73	34.53
TAU	4.71	12.51	4.94	13.56	5.22	13.90	15.85	26.80	15.43	27.35	15.60	26.85
CTENet w/ ConvLSTM	4.12	8.46	4.31	8.66	4.43	8.84	13.79	23.14	14.44	23.79	**15.28**	**24.47**
CTENet w/ TAU	**2.66**	**4.86**	**2.99**	**4.86**	**3.10**	**5.00**	**10.90**	**16.99**	**13.28**	**22.60**	15.92	26.74
% Best Improvement	34.43	46.02	32.06	46.18	32.68	44.86	31.24	36.60	13.97	17.36	2.04	8.86

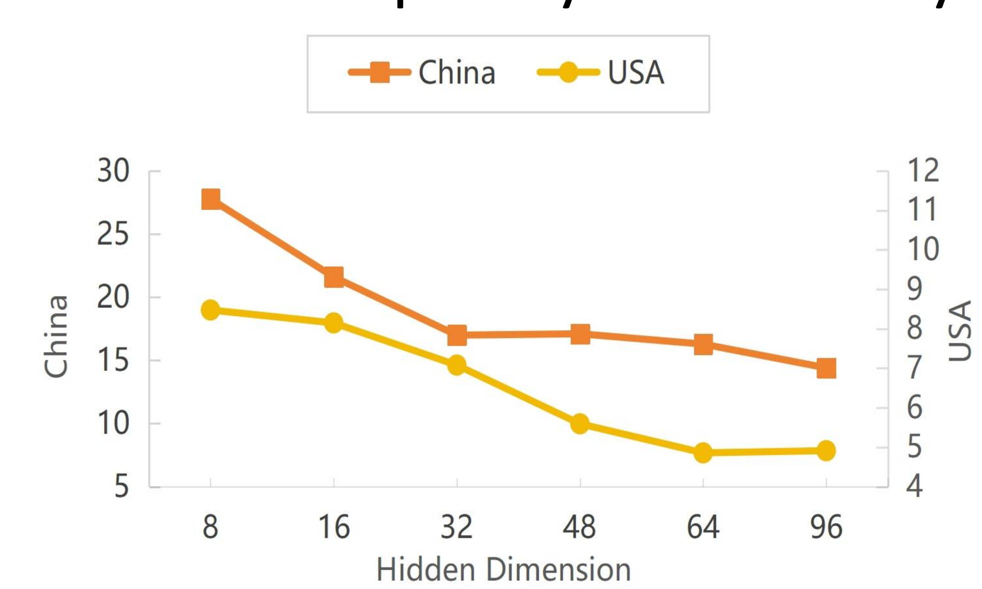
➢ Ablation Study

Effectiveness of the ADR terms



➢ Hidden Dimension Analysis

Model complexity and stability



➢ Case Study

Capture of Dynamic Pollutant Advection