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ANN-based physio-chemical prediction of the photochemical cycle and the reactive air pollutant dispersion in an urban environment

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SUMMARY:
This paper investigated the mechanism of the air pollutant's reactive dispersion in the ideal urban environment via a hybrid numerical intelligence model consisting of Architectural Institute of Japan (AIJ) wind tunnel data, k-ε model Computational fluid dynamics (CFD) simulation, and Artificial Neural Network (ANN) machine learning algorithms. The results showed that the normalized velocity distribution stay unchanged under different inflow speeds. The phenomenon of pollution accumulation on the rear of the building resulting from the turbulent kinetic energy (TKE) distribution was discovered. It was determined that the pollutant spreading region enlarges proportionally with the increase in Damköhler number of ozone ($Da_{O3)}$ number when it is close to 1. In contrast, the pollutant spreading region was unaffected by the Damköhler number of nitrogen oxide (Da_{NO}) number when it is far less than 1. Moreover, the ANN model showcased the strong advantage of characterizing the sophisticated nonlinear spatial diffusion and reaction of the air species by generating acceptably accurate predictions with significantly lower computational and time costs compared with CFD simulation.

Keywords: Reactive Pollutant Dispersion, Urban Environment, Artificial Neural Network(ANN)

1. INTRODUCTION

The increasing automobile exhaust brought by rapid growth in the number of vehicles exposes the residents in the metropolitan area to the great danger of respiratory diseases. A thorough investigation of pollutant dispersion mechanism and multi-pollutant interaction will be an indispensable reference to guide the improvement of a city ventilation system. In recent years, various machine learning algorithms have been implemented to investigate the sophisticated interaction between environmental parameters and pollutant distribution and reaction characteristics (Hossain, 2014; Lange et al., 2021; Weerasuriya et al., 2022). Although the previous studies rendered valuable insights into the single pollutant dispersion issue, the essential chemical reaction between nitrogen oxides and secondary pollutants remained blank. Thus, this paper aims to investigate the mechanism of the air pollutant's reactive dispersion via a hybrid numerical intelligence model consisting of the AIJ wind tunnel data, the k-ε model of CFD simulation, and the ANN model of the machine learning algorithm. Moreover, the impact of three different reference inflow speeds, four different Da_{O3} numbers, and 5 different Da_{NO} & Da_{NO2} numbers on

pollutant diffusion patterns were explored explicitly.

2. METHODOLOGY

2.1 CHEMISTRY MODELLING AND PHYSIOCHEMICAL COUPLING

In this simulation, the transportation of reactive pollutants: NO, NO_2, and O_3 with the chemical reaction are modeled as Eq. 1, 2 and 3.

$$\frac{\partial[NO]}{\partial t} + U_j\frac{\partial[NO]}{\partial x_j} = D\frac{\partial^2[NO]}{\partial x_j \partial x_j} + \frac{\partial}{\partial x_j}\left(K_c\frac{\partial[NO]}{\partial x_j}\right) + J_{NO_2}[NO_2] - k_1[O_3][NO] + S_{NO} \quad (1)$$

$$\frac{\partial[NO_2]}{\partial t} + U_j\frac{\partial[NO_2]}{\partial x_j} = D\frac{\partial^2[NO]}{\partial x_j \partial x_j} + \frac{\partial}{\partial x_j}\left(K_c\frac{\partial[NO_2]}{\partial x_j}\right) - J_{NO_2}[NO_2] + k_1[O_3][NO] + S_{NO_2} \quad (2)$$

$$\frac{\partial[O_3]}{\partial t} + U_j\frac{\partial[O_3]}{\partial x_j} = D\frac{\partial^2[O_3]}{\partial x_j \partial x_j} + \frac{\partial}{\partial x_j}\left(K_c\frac{\partial[O_3]}{\partial x_j}\right) + k_2[O][O_2][M] - k_1[O_3][NO] \quad (3)$$

where D denotes the molecular diffusivity of the pollutants, K_c indicates the eddy diffusivity of the pollutants. The S_{NO} and S_{NO2} represent the emission sources of NO and NO_2, and the square bracket ([ ]) denotes the mean concentration of pollutant species. J_{NO_2} indicates the photolysis rate of NO_2 in Equation (6). k_1 and k_2 represent the constant reaction rate in Equations (7-8), respectively.

The Damköhler number (*Da*), which is used to measure the rates of physical transportation and chemical reaction, is defined as the Eq. 4:

$$Da = \frac{\tau_d}{\tau_\gamma} = \frac{diffusion\ time\ scale}{reaction\ time\ scale} \quad (4)$$

2.2 CFD COMPUTATIONAL SETTINGS AND ANN DATA GENERATION

This paper displayed a standard k-ε model-based CFD simulation with coupled physical flow fields and chemical reactions, to study the influence of photochemical reactions on pollutant diffusion in an ideal urban environment. The dimension of the building, computational domain, boundary conditions, the hexahedral grid, and emission sources can be found in Fig. 1. The CFD simulation results matched well with wind tunnel data. The physiochemical coupling of the pollutant dispersion model is validated to support the following results and discussion.

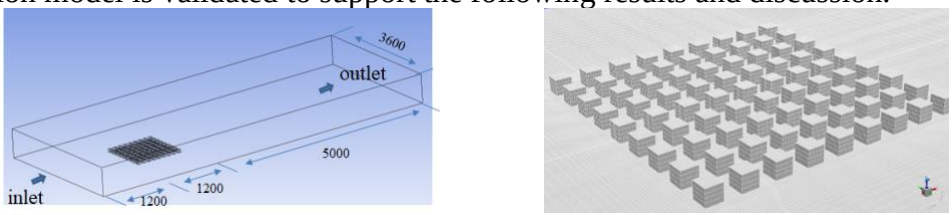

Figure 1. Dimensions of the building in the Computational domain (Left) and Boundary conditions, the hexahedral grid, and emission sources (Right)

Subsequently, an ANN-based machine learning algorithm was trained based on the results of the aforenoted CFD simulation. As shown in Fig. 2, the proposed ANN model was built with optimal

six neutrons, and 181 parallel independent sub-models to guarantee prediction accuracy while maintaining a reasonably accessible computational cost.

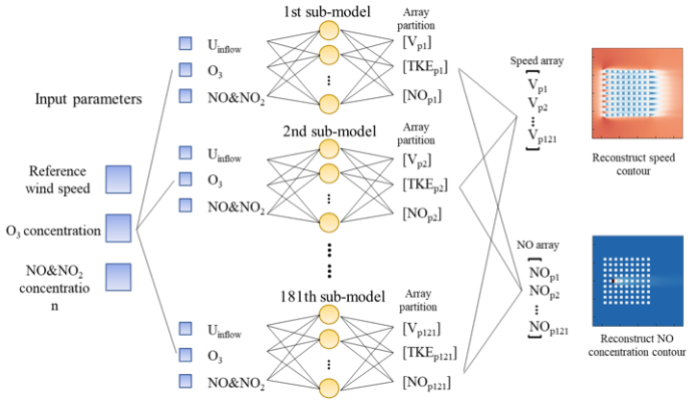

Figure 2. Architecture of the ANN model

3. RESULTS AND DISCUSSION

3.1 AIR SPECIES POLLUTANT ACCUMULATION ON THE REAR OF BUILDINGS

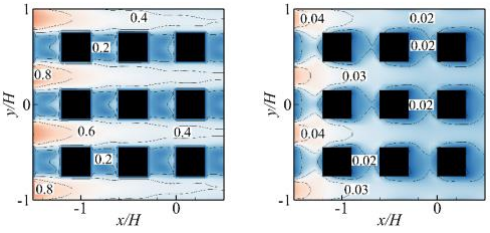

Figure 3. Comparison of velocity & TKE contour under normalized velocity contour with 3 m/s reference inflow speed at z=0.5H.

The normalized wind velocity contour remains almost unchanged under different wind speeds. There is a low-speed region at the rear of the building which results from the two flow separation areas, as shown in Fig. 3. As a result of lower TKE at the building leeward side, the air species pollutant is restricted in the back of the building.

3.2 IMPACT OF DA_{O3} AND DA_{NO} NUMBER ON POLLUTANT SPREADING REGION

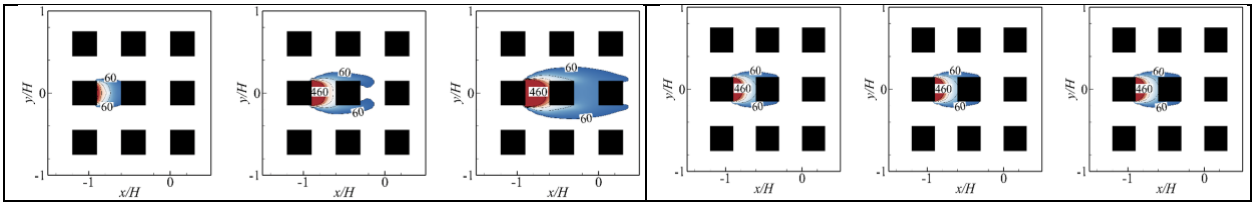

Figure 4. NO concentration contour with Da_{O3} numbers of 0.252, 0.756 and 1.259 (a), NO concentration contour with Da_{NO} of 0.0252, 0.0126, and 0.0063 (b)

The NO species diffusion region grows proportionally as the Da_{O3} approaches 1, as shown in Fig. 4. This is caused by the turbulence dispersion process overshading the chemical reactions during the process.

The NO species diffusion remained unchanged under the influence of *the* Da_{NO} number, while *the* Da_{NO} number is significantly lower than 1. This resulted from the turbulent dispersion process is much lower than the chemical reaction process, as shown in Fig. 4.

3.3 PREDICTION ACCURACY OF THE ANN MODEL

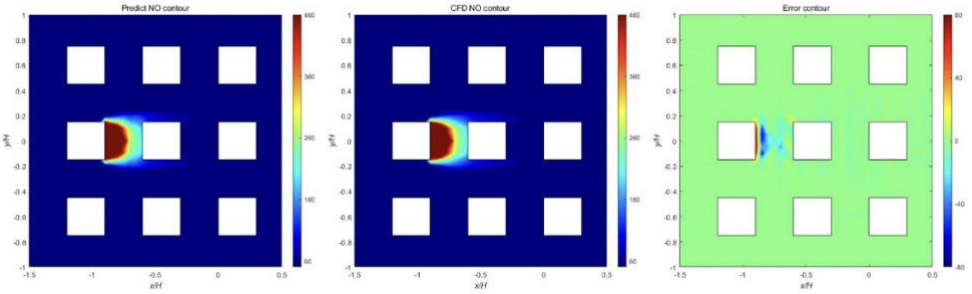

Figure 5. Comparison between the ANN model and CFD simulation results of non-dimensional NO concentration distribution comparison at z=0.03 m.

As shown in Fig. 5, the capability of the ANN model on characterizing the complex nonlinear spatial diffusion and reaction of the air species is demonstrated by the acceptably small relative error between ANN prediction results and the CFD simulation.

4. CONCLUSION

It was shown by the velocity & TKE contour plot that the normalized wind velocity distribution was unaffected by the variation in inflow speed, and the accumulation of pollution on the rear of the building resulted from the difference between the TKE at the leeward side of the building and the street. Moreover, there is an obvious proportional relationship between the Da_{O3} number and pollutant spreading region, while the Da_{O3} number is close to 1. Whereas this relationship cannot be found when the Da_{NO} number is much less than 1. Furthermore, the superior advantage of the ANN model is proved by predicting complex nonlinear spatial diffusion and reaction of the air species with an acceptable accuracy but dramatically higher computational and time efficiency compared with CFD simulation.

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