# MK1　Analysis of roadside air quality using chemistry-coupled CFD model

## 化学反応モデルを組み込んだ CFD モデルを用いた沿道大気質の解析

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**Abstract:** In this study, a chemistry-coupled CFD (computational fluid dynamics) model was applied to assess the roadside air quality in a real situation. CBM-IV (Carbon bond mechanism IV) was used as the chemical reaction model coupled to the CFD. The performance of the chemistry-coupled CFD model was tested in Umeda-shindo, where roadside monitoring station is located. The boundary conditions were calculated by air quality model WRF-CMAQ (Weather Research and Forecasting - Community Multiscale Air Quality Modeling System). Results showed that comparing with the observation data, the chemistry-coupled CFD results showed better accuracy in $NO_x$ concentration than the WRF-CMAQ data. In a real situation, the building geometry and mobile emission were found to have great impacts on the urban air quality in the CFD simulation, emphasizing the importance to assess the roadside air pollution with high spatial resolution.

**Keywords:** Roadside air quality, CFD, Gas-phase reaction, Diurnal variation

### 1.　Background

In urban area, roadside air pollution is a serious environmental issue. In order to evaluate the roadside air pollution caused by pollutants emitted mainly from automobiles accurately, it is required to consider both chemical reaction and shape of buildings. Most of air quality models, however, use low mesh resolution such as 1 $km^2$ or coarser, which is not sufficient to consider shape of buildings. On the other hand, the conventional CFD (computational fluid dynamics) model which typically has not treated chemical reaction, can perform air quality simulation in city-block scale with high spatial resolution, but cannot consider chemical reaction. Hence, this study developed a chemistry-coupled CFD model and applied it to roadside air quality simulations.

### 2.　Methodology

In this study, air quality simulations were performed with a chemistry-coupled CFD model. The CFD model consisted of momentum, continuity, heat and mass conservation equations. The $k$–$\varepsilon$ turbulence model for the high Reynolds number turbulence was used as the turbulence model. CBM-IV was used to calculate the chemical reaction. The WRF-CMAQ was used to obtain the boundary conditions of air temperature, wind and air pollutants concentration. The total emission rate of vehicles in calculation domain was derived from the Japan Auto-Oil Program (JATOP) Emission Inventory-Data Base (JEI-DB) in the year 2010 developed by Japan Petroleum Energy Center. Then, in the realistic city model, each road emission rate of the total emission rate were decided by the number of cars data of each road from the Japan Ministry of Land, Infrastructure, Transport and Tourism (MLIT). The calculation area was in Umeda-shindo, where roadside monitoring stations is located. The calculation domain was within 600 m × 600 m × 150 m, mesh numbers were 93 × 93 × 51 in the x, y, and z direction respectively. The analysis domain includes 5 roads and 22 buildings. The pollutants concentration observation point location was based on the location of Umeda-shindo roadside monitoring station location.

## 3. Results

In the case of Umeda-shindo, compared with the observation data, the CFD results showed better accuracy in $NO_x$ concentration than the WRF-CMAQ data, obviously (Fig. 1). Fig. 2 shows the diurnal variation of concentration distribution in x-y view at 1.5m. Due to the vehicle emission, high $NO_x$ concentration remained in the street from 0800 JST to 1200 JST. Then, at 1600 JST, since the decrease of vehicle emission and occurrence of photochemical reaction, $NO_2$ concentration decreased. However, at 2000 JST, $NO_2$ concentration still remained a high level, because of the titration reaction occurred by the NO and $O_3$. Due to the titration reaction, $O_3$ concentration showed reverse contrasting distribution compared with $NO_2$ concentration during a day. Fig. 3 shows the diurnal variation of concentration distribution in x-z view (observation point A-A section). Due to the vehicle emission, high $NO_x$ concentration remained in low height from 0800 JST to 1200 JST. Because of the wind flow pattern, the concentration distribution shows higher value in the downwind area than upwind area. At 2000 JST, though the emission from the vehicles decreased, the $NO_x$ concentration in the street was still higher than the concentration above the building area.

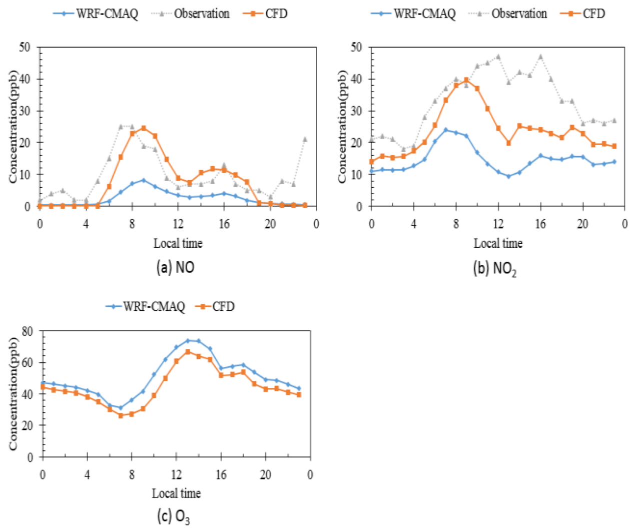


Fig. 1 Comparison among the WRF-CMAQ, observed data and CFD calculation results at the observation point in Umeda-shindo

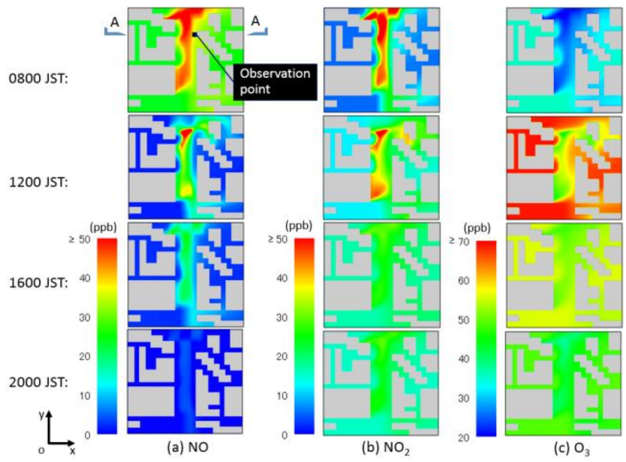


Fig. 2 Concentration distribution in x-y view in Umeda-shindo (z=1.5 m, observation point height)

## 4. Conclusion

In the case of Umeda-shindo, compared with the observation data, the chemistry-coupled CFD model showed better accuracy in $NO_x$ concentration than the WRF-CMAQ data, obviously. The results showed that in a real situation, the building geometry and mobile emission were found to have great impacts on the urban air quality in the CFD simulation, emphasizing the importance to assess the roadside air pollution with high spatial resolution.

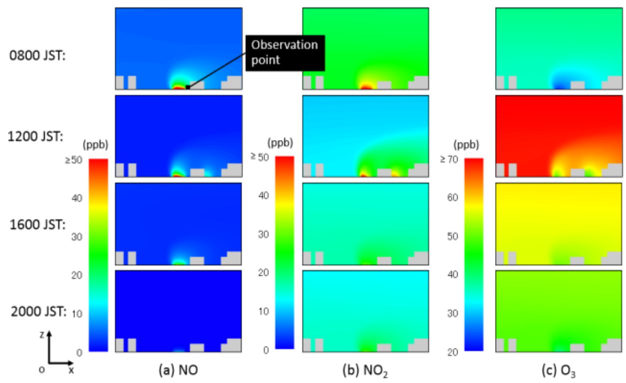


Fig. 3 Concentration distribution in x-z view (observation point A-A section)