9-12 May 2016 Budapest, Hungary
17th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
Harmo'17

Time Scale Analysis of Chemically Reactive Pollutants over Urban Roughness in the Atmospheric Boundary Layer

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Parallel Session 5, Star Auditorium

Topic 1: Model Evaluation & Quality Assurance – Model Validation, Model Intercomparisons, Model Uncertainties & Model Sensitivities

H17-002; 1750 to 1810; May 12, 2016 (Monday)

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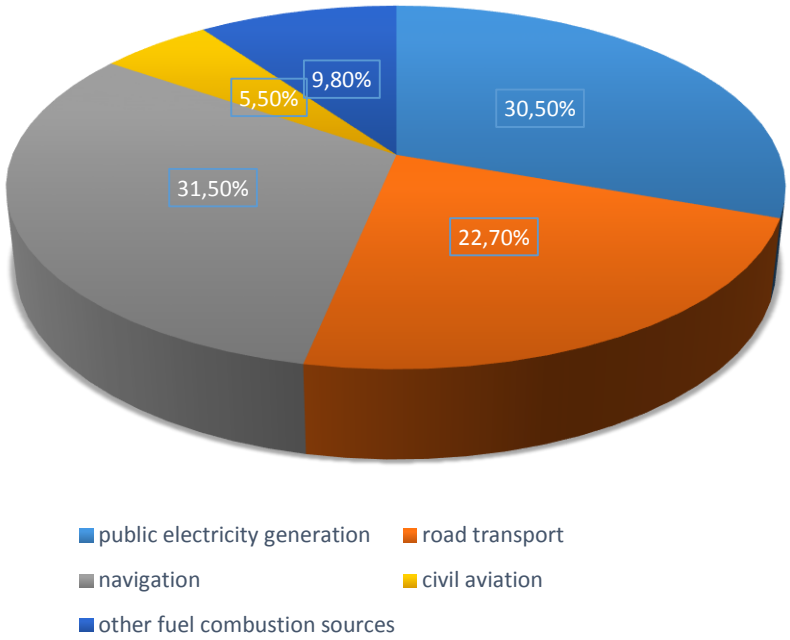
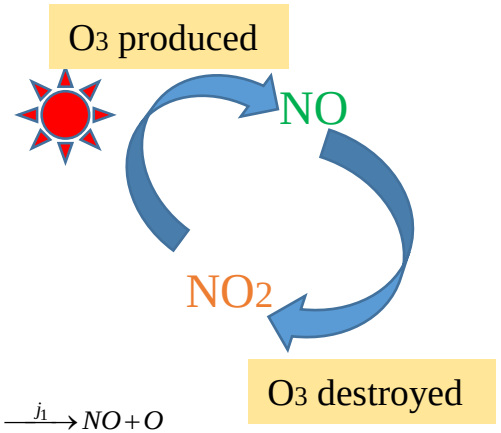
Background





$$NO_2 + h\nu \xrightarrow{j_1} NO + O$$

$$O + O_2 + M \xrightarrow{k_2} O_3 + M$$

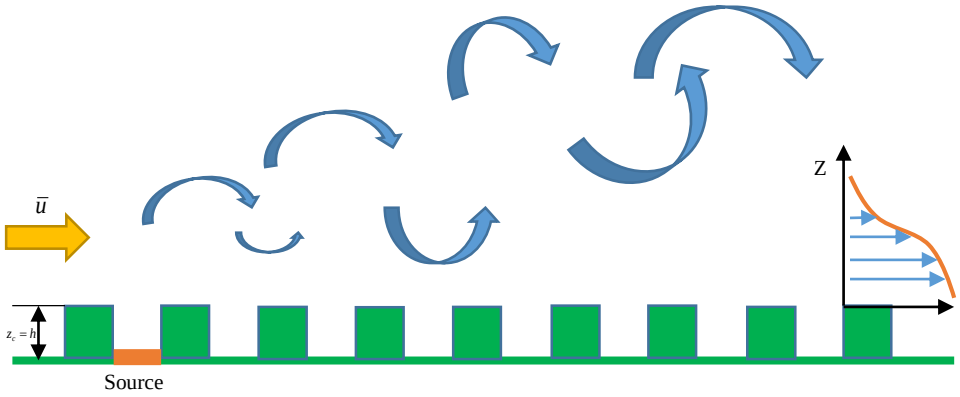
$$O_3 + NO \xrightarrow{k_3} NO_2 + O_2$$

- According to Hong Kong Environmental Protection Department (EPD), the total emission of NO_x in Hong Kong in 2013 is about 113,220 tonnes.
- The emission sources of NO_x in Hong Kong include power electricity generation, road transport, navigation, civil aviation, and other fuel combustion sources.
- Road transport is one of the major sources of NO_x.

- While most practical dispersion models assume inert pollutants, emissions from traffic exhaust are chemically reactive.
- NO can be oxidized by ozone (O_3) in the atmosphere.
- With sunlight, NO_2 can also decompose into NO and O_2
- Chemical reaction in the atmosphere is much more complicated than that.

Data Source: http://www.epd.gov.hk/epd/english/environmentinhk/air/data/emission_inve.html

Background



- Elevated pollutant concentrations are commonly observed in urban areas, such as street canyons, threatening human health.
- Dynamics are complicated by atmospheric turbulence, geometry/orientation of buildings, thermal stratification and chemical kinetics, etc.
- The oxidation rate of NO is affected by both physical process and chemical process. The physical process is mixing of the plume with the ambient air. The chemical processes are the molecular reactions of NO with species in the surrounding air.
- There exists a wide range of turbulent eddies which act on dispersing plume. Dispersion and mixing of material, which constitute the plume, are caused by eddies of all sizes in the atmospheric boundary layer.
    - Large eddies (larger than the cross-section of plume, in the order of tens to several hundreds of meters): cause meandering of the plume
    - Middle eddies (about the size of cross-section of plume or smaller): cause broadening and internal mixing of plume.
    - Small eddies (in the order of millimeters): important for chemical reaction

Street canyon

Building-height-to-street-width ratio

AR = h/b

Objectives

- Develop a CFD model for simple NO_x-O_3 chemistry
- Analyze the plume dispersion characteristics of passive scalar and chemically reactive pollutant.
- Analyze the plume characteristics in different cases with different O_3 concentration.
- Compare the time scales of diffusion and chemical reaction

Methodology

- Model
  Large-eddy simulation with one-equation SGS model

- Governing equations (filtered)

  - continuity equation

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0$$

  - momentum conservation

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j}\bar{u}_i\bar{u}_j = -\Delta P\delta_{i1} - \frac{\partial \bar{p}}{\partial x_i} + (\nu + \nu_{SGS})\frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j}$$

  - Transport equation for pollutant

$$\frac{\partial \phi}{\partial t} + u_j \frac{\partial \phi}{\partial x_j} = \frac{\partial}{x_j}\left(D\frac{\partial \phi}{\partial x_j}\right) + S(\phi)$$

- First step is to handle irreversible chemical reaction

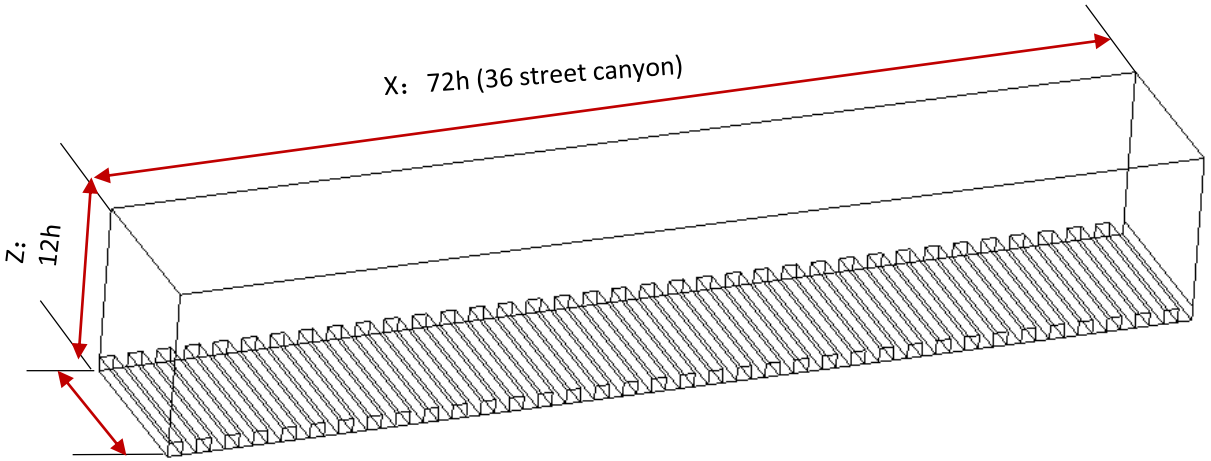
$$NO + O_3 \xrightarrow{k_3} NO_2 + O_2$$

- Source term for NO, NO_2 and O_3

$$\frac{d[NO]}{dt} = -k_3[O_3][NO] \qquad \frac{d[O_3]}{dt} = -k_3[O_3][NO]$$

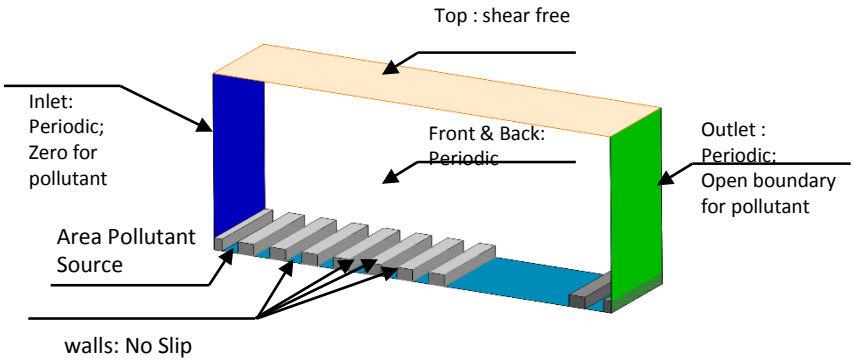
$$\frac{d[NO_2]}{dt} = k_3[O_3][NO]$$

Geometry and Boundary Conditions



Computational Domain

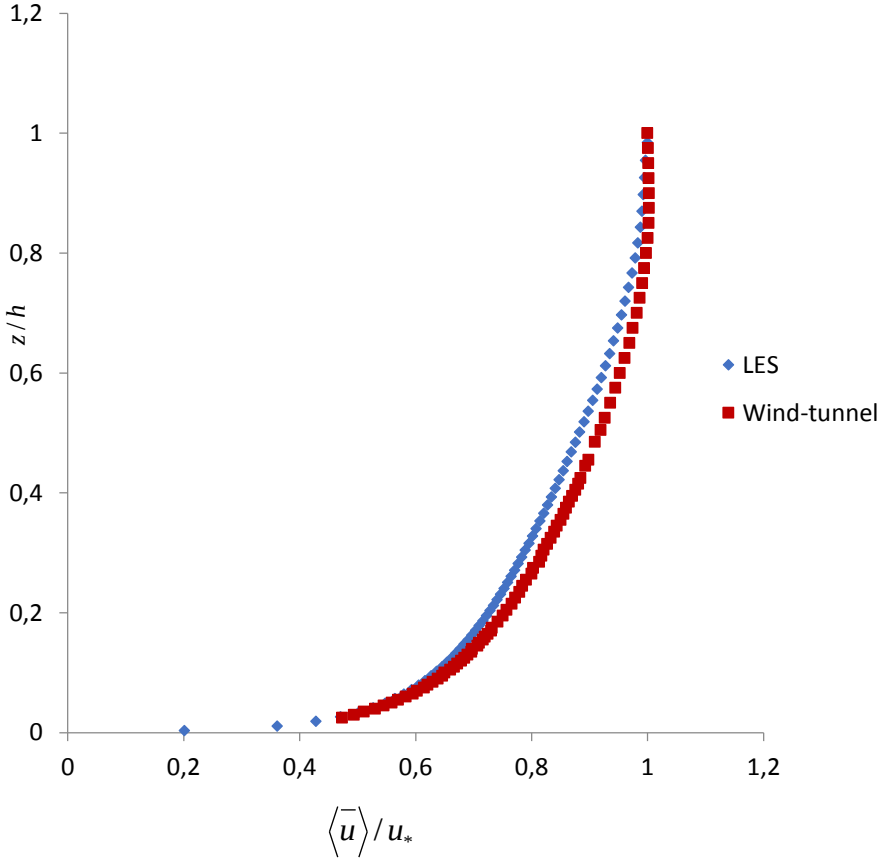
Description	Parameter	Value
Domain Length	X	72h
Domain Width	Y	12h
Domain Height	Z	12h
Building Height	h	1h
Street Width	b	1h
Number of Street Canyons	n	36

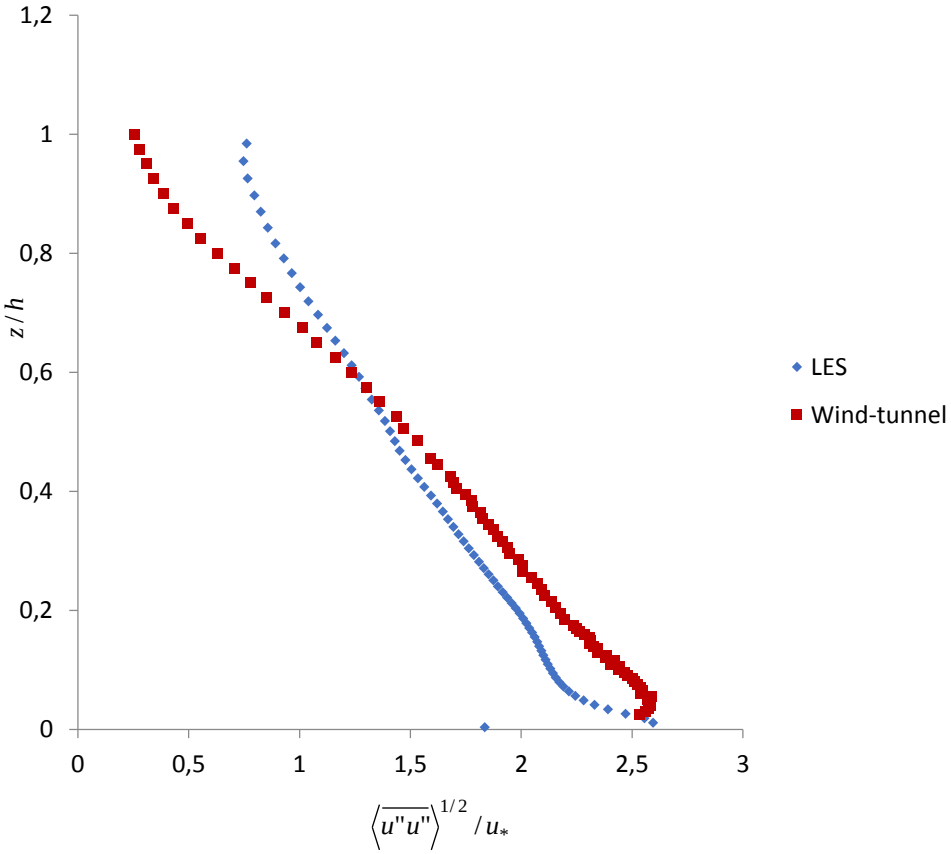


Boundary Condition

Case NO.	NO Concentration /ppb	O3 Concentration /ppb
Case 1	1000	1
Case 2	1000	10
Case 3	1000	50
Case 4	1000	100
Case 5	1000	500
Case 6	1000	1000

Results – Velocity Fields 1/3

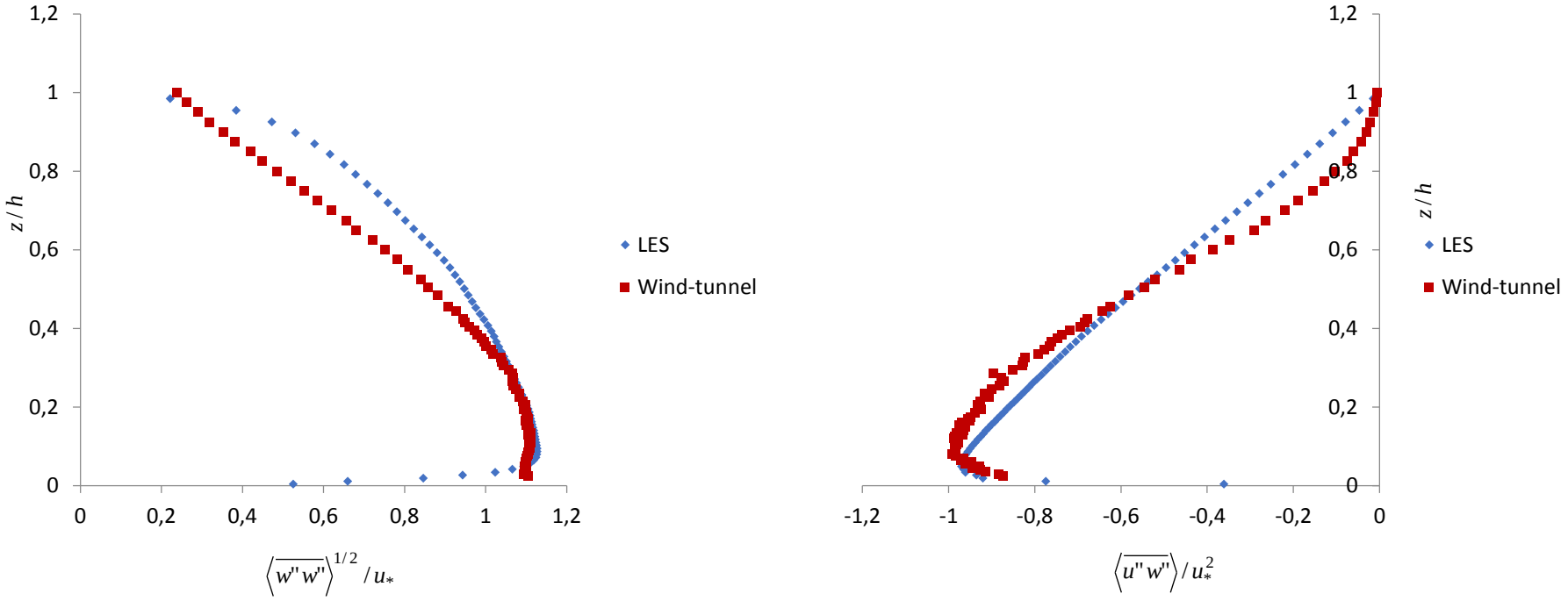




Velocity scale: friction velocity $u_\tau = \sqrt{\tau_w / \rho}$ τ_w is the wall shear stress.

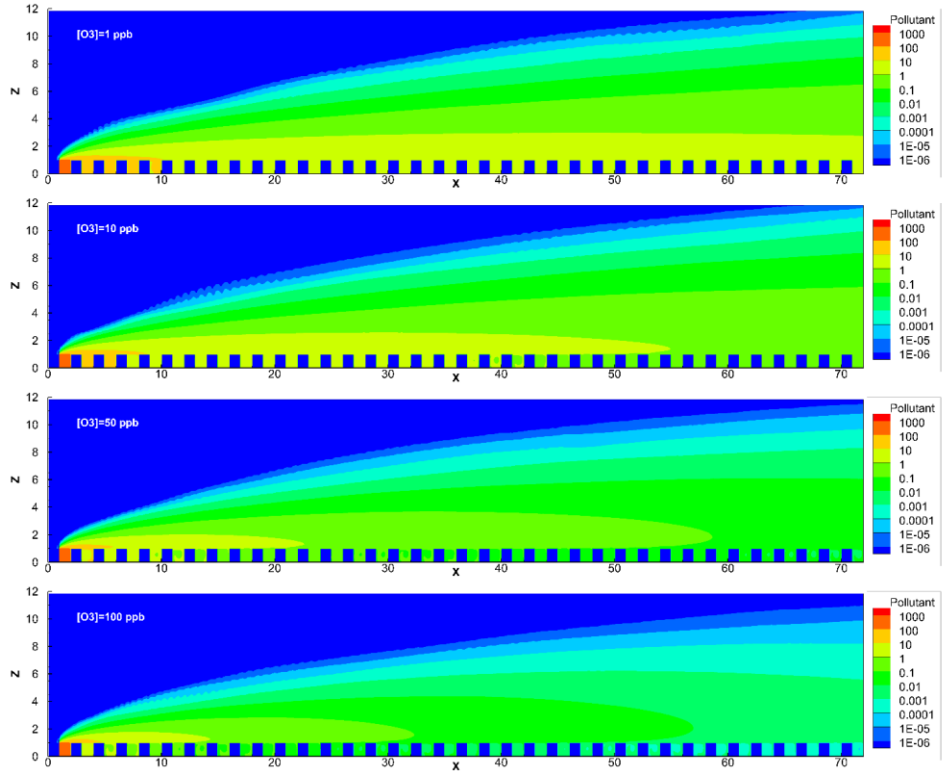
1. The vertical velocity profile fits well with that of the wind tunnel measurement.
2. The turbulence in LES is smaller than that of wind tunnel measurement for $z \leq 0.6h$. It is because the turbulence in the wind tunnel is not only generated from roughness but also from upstream.

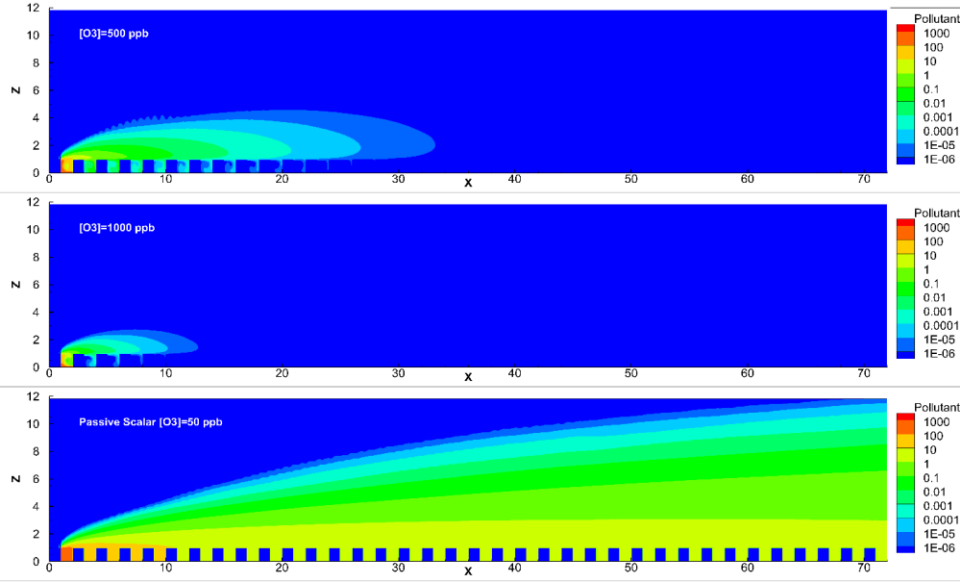
Results – Velocity Fields 2/3



1. *w”* is important in the momentum transport and pollutant transport in the vertical direction.
2. *w”w”* in LES fits well with the wind tunnel data especially in the inertial sublayer.

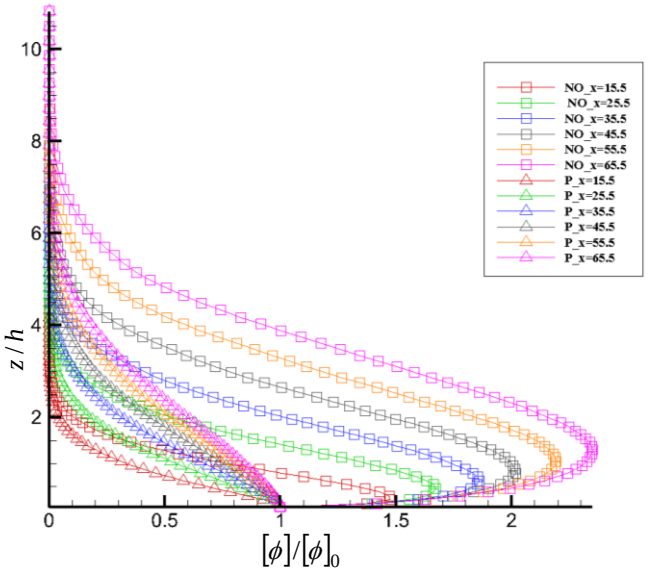
Results - Pollutant Contours

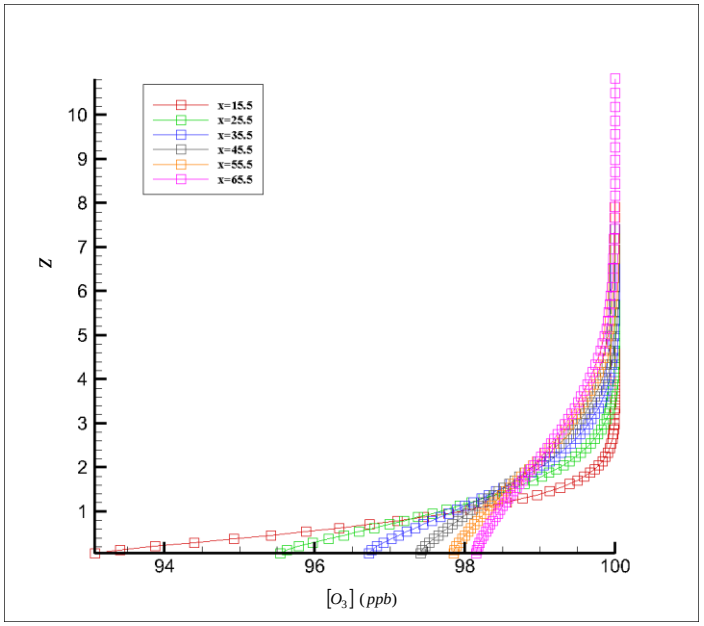


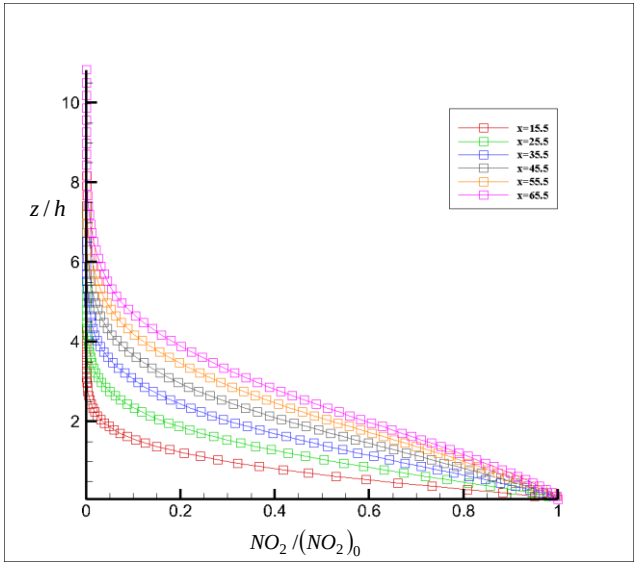


1. The background O_3 mixed with NO from the area source in a molecular scalar.
2. When background [O_3] increases, the plume of NO is compressed.
3. In case [O_3] = 500 ppb and [O_3] = 1000 ppb, almost all the NO is consumed by the background O_3

Vertical profile of Pollutant in case $[O_3]_0$ =100 ppb







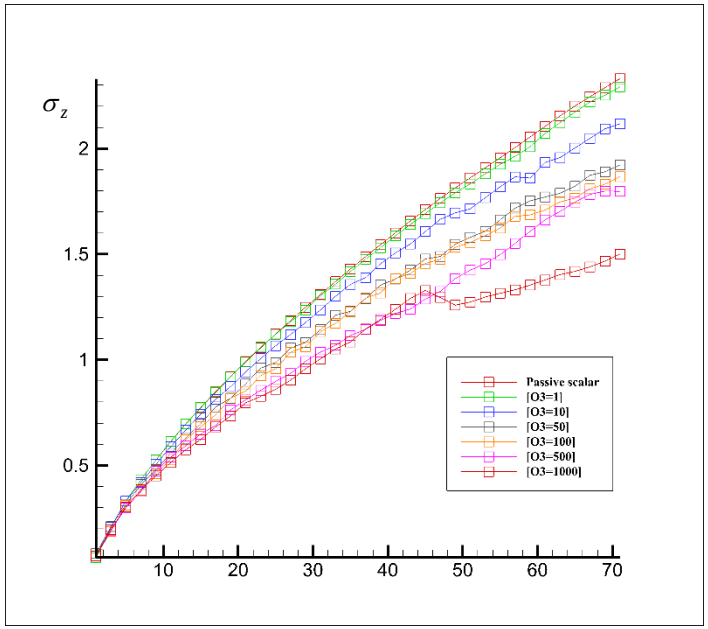
1. The concentration of pollutant is normalized by the pollutant concentration at the roof level.
2. Near the roof level, the characteristics of concentrations of NO and passive scalar are very different.
3.Perhaps it is because O_3 entrains below the roof level. Near the roof level, the chemical reaction is quite fast that consumes more NO.

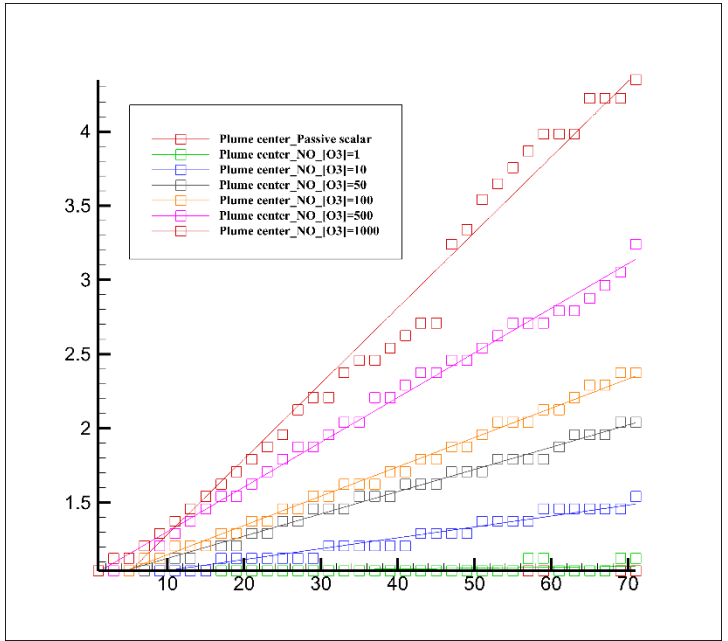
Dispersion coefficient

σ_z is the vertical dispersion coefficient. In the current study, it is calculated by the following equation.

$$\sigma_z = \sqrt{\frac{\iiint (z - z_c)^2 \phi dydtdz}{\iiint \phi dydtdz}}$$

z_c is the plume center height (the location of maximum concentration is used as the plume center height).





Time scale

Diffusion time scale

Molecular/turbulent transport and mixing processes are involved in the plume dispersion in the atmosphere. The time scale of dispersion reflects the effects of different processes taking place on a wide spectrum of scales.

- Diffusion time scale

$$\tau_d = \frac{\sigma_z^2}{4K}$$

- For passive scalar

$$\sigma_z = \left(\frac{2Kx}{U}\right)^{1/2}$$

- So we can derive the diffusion time scale

$$\tau_d = \frac{2Kx}{4KU} = \frac{x}{2U}$$

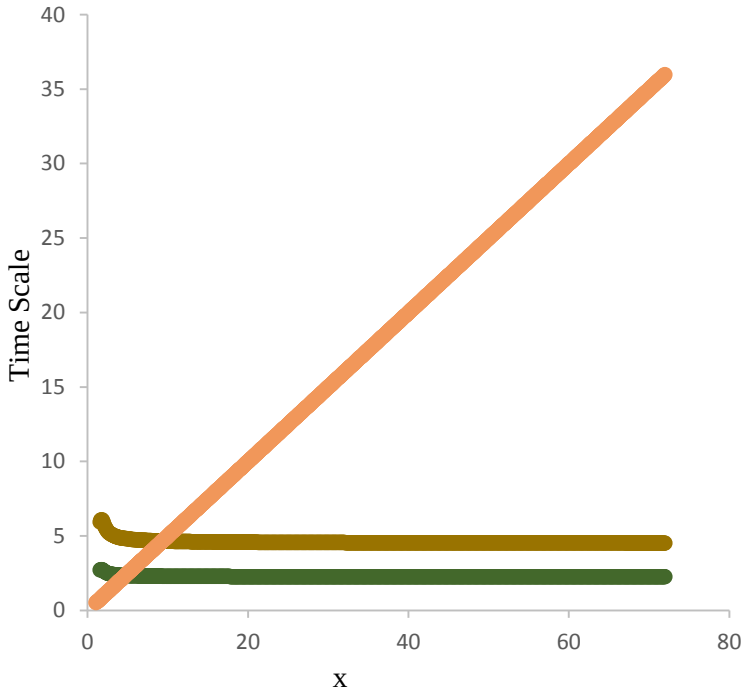
Reaction time scale

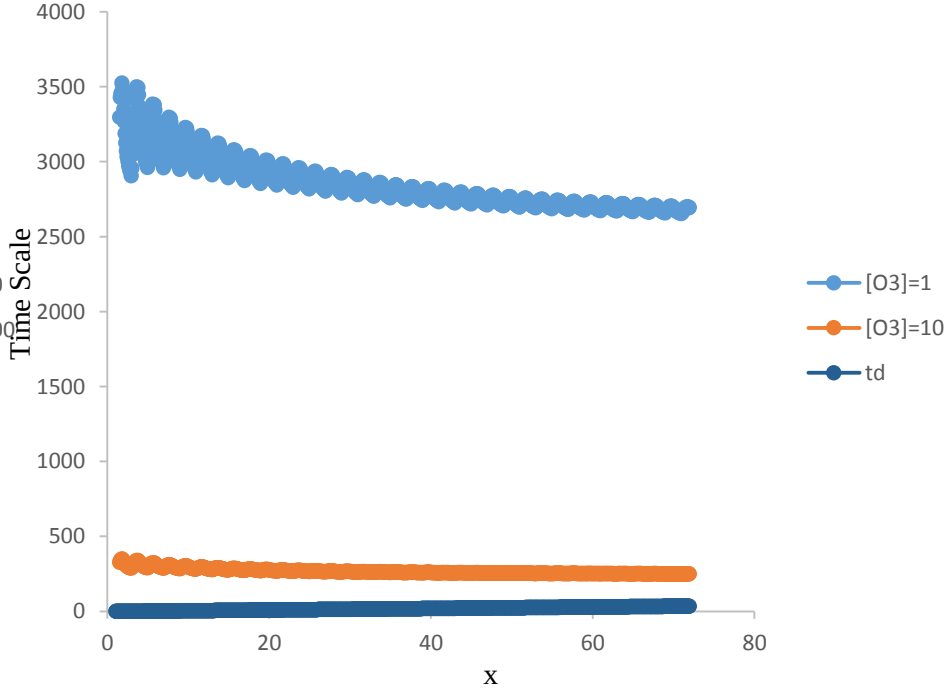
Reaction time scale is the time for the chemical reaction to take place.

$$\tau_{NO} = -\frac{1}{k_3 \left\langle [O_3] \right\rangle}$$

Time scale

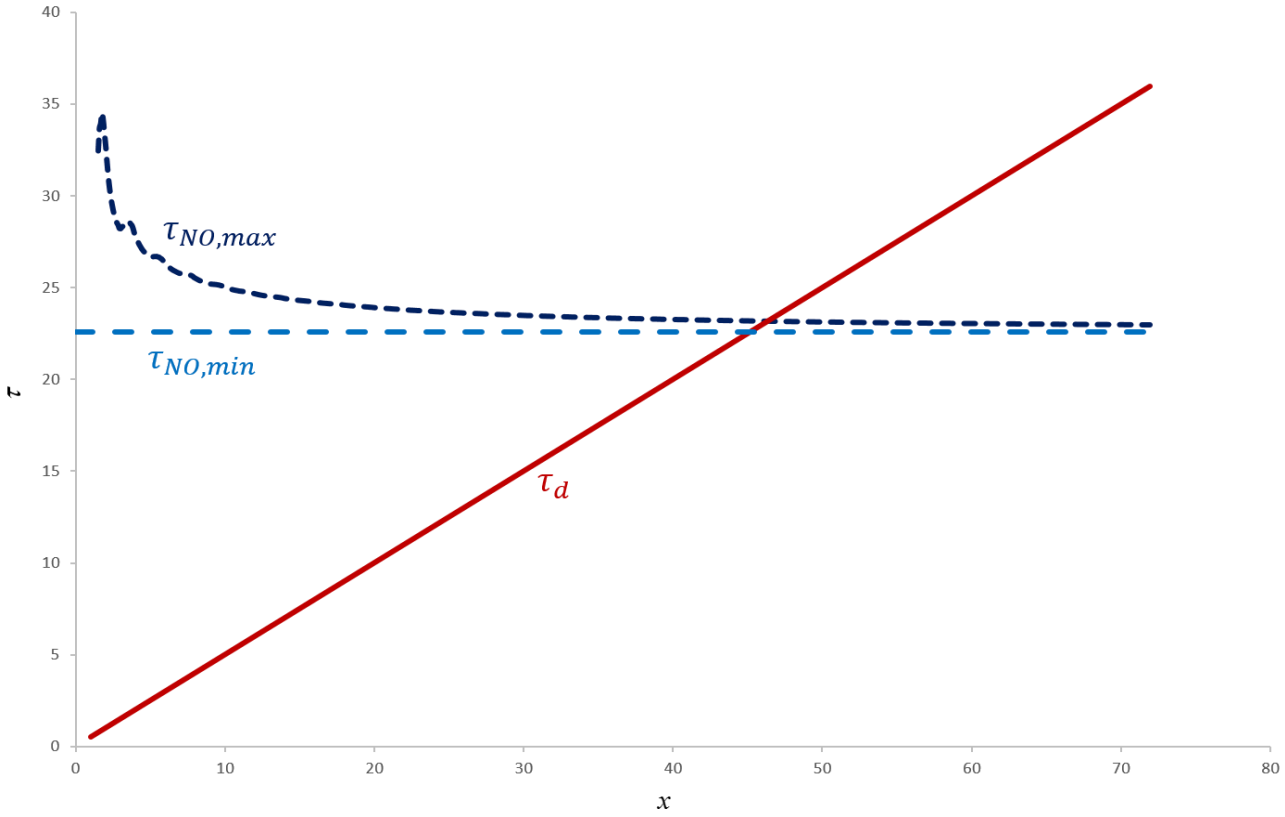
- In the cases $[O_3]_0$ = 1000 ppb and $[O_3]_0$ = 500 ppb, the minimum reaction time scale is 2.26 second and 4.53 second, which is much smaller than the diffusion time scale away from the pollutant source. The fast chemistry implies that most of NO is consumed by O_3 titration.
- In the cases $[O_3]_0$ = 1 ppb and $[O_3]_0$ = 10 ppb, the reaction time scale is much longer than the diffusion time scale. Physical dispersion thus dominates the pollutant removal.





Time scale

- In the cases $[O_3]_0$ = 50 ppb and $[O_3]_0$ =100 ppb, the reaction time scale and the diffusion time scale are comparable.
- In the case $[O_3]_0$ = 100 ppb, in the near field next to the pollutant source, diffusion time scale is smaller and diffusion dominates the pollutant removal. In the far field, the reaction time scale is smaller, thus chemical reaction dominates the pollutant removal.



Conclusion

1. The behavior of the passive scalar and NO is different. It shows that the chemical reaction has major effects on the dispersion behavior of pollutant.
2. The current LES model is validated with the wind tunnel experiments. The velocity data in LES fits well with that of the wind tunnel measurement.
3. The vertical concentration profile of reactive pollutant is different from that of passive scalar. The chemical reaction enhances the plume height and reduces the dispersion coefficient compared with that of the passive scalar. The dispersion coefficient of chemically reactive pollutant is weaker than its inert counterpart so pollution chemistry reduces plume width and coverage.
4. At a low level of $[O_3]_0$ (= 1 ppb), τ_{NO} is longer than τ_d so physical dispersion dominates pollutant removal. For $[O_3]_0$ at 100 ppb, the physical and chemistry timescales are comparable with each other.

Thank you !