Influence of Building Aspect Ratio and Traffic Volume on Reactive Pollutant Dispersion in Urban-like Street Canyons during Direct Ground Heating

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A&WMA International Specialty Conference:
Leapfrogging Opportunities for Air Quality Improvement

May 10-14, 2010
Xi’an, Shaanxi Province, China
Platform Presentation Session IVg
“Photochemical Studies and Analysis”
Thursday, May 13, 2010,
10:30-12:00pm
| CHAPTER 1 | INTRODUCTION |
| CHAPTER 2 | LITERATURE REVIEW |
| CHAPTER 3 | MODELING METHODOLOGY |
| CHAPTER 4 | MODEL VALIDATIONS |
| CHAPTER 5 | RESULTS AND DISCUSSION |
| CHAPTER 6 | CONCLUDING REMARKS AND LEAPFROGGING ASPECT |
CHAPTER 1 INTRODUCTION
Objectives

- Model the characteristics of **reactive pollutant dispersion** in urban-like street canyons;

- Investigate the **Building Aspect Ratio** and **Traffic Volume** contributing to the **evolution of reactive pollutant dispersion** in urban-like street canyons;

- Analyze how the **direct ground heating** affects **spatial distribution of reactive pollutants**; and

- Evaluate the **urban design optimization** of urban-like street canyons.
Tropospheric ozone ($O_3$) is a secondary air pollutant formed due to photochemical reaction between nitrogen oxides $NO_x$ [nitric oxide (NO) and nitrogen dioxide (NO$_2$)] and volatile organic compounds (VOCs) in the presence of solar radiation.

Most of the $NO_x$ and VOCs come from anthropogenic sources such as vehicles and factories but biogenic VOCs from vegetation also contribute at least much to tropospheric ozone formulation at a level as anthropogenic VOCs.
The causes of ozone episodes are complex and depend on various factors including emissions, meteorological parameters, topography, atmospheric chemical processes, and solar radiation.

The substantial weights of the urbanization related emission structure and street canyon design layout in exploring the relationship between ozone evolutions should not be overlooked.
A Schematic diagram of a typical passive pollutant dispersion in a regular street canyon

- Building aspect ratio $\sim 1$ refers to a regular canyon
- The synoptic wind conditions above the roof-top and local wind flow within the cavity of the canyon
- Under perpendicular flow for synoptic wind (free-stream velocity) over 1.5 m/s, the upwind canyon side refers to leeward and downwind canyon side windward.
- Wind vortices mainly depend on roof-top wind speed and local wind flow can be affected by vehicular mechanical turbulence, urban geographical features, atmospheric stability, and ground-wall thermal affections.
- Carbon monoxide (CO) is used as hypothetical vehicular exhaust due to its chemically inert and long-lasting residence in ABL

Hasson and Crowther (1998)
Vardoulakis et al. (2003)
Li et al. (2006)
<table>
<thead>
<tr>
<th>Topic</th>
<th>Effect</th>
<th>References</th>
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</thead>
<tbody>
<tr>
<td>Anticyclonic conditions (that is, clear skies, light winds and subsidence)</td>
<td>Enhance substantial thermal convective circulations with declining mixed-layer depths</td>
<td>Akkinson (1981); Stemman (1987); Loffler-Mang et al. (1997); Giza (1998); Bai and Wang (2001) and Ma and Lyons (2003)</td>
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<td>Cyclonic conditions</td>
<td>Enhancement of ozone concentration during the prevalent ocean wind by very weak ozone titration reaction and intrusion of regional ozone</td>
<td>Khan et al. (2007)</td>
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<td>2. Accumulate emissions in an airstream.</td>
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<td>Solar radiation</td>
<td>A favorable parameter over ozone formation</td>
<td></td>
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<td>Temperature (including ground surface and overlying air)</td>
<td>Affect the formation and dispersion of ozone and its precursors.</td>
<td>Silman and Samson (1995); Ellis et al. (2000); Vuleumier et al. (2001) and Sokhi et al. (2001)</td>
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<td>Circulation in relation to meteorological fields</td>
<td>Elevation of ozone.</td>
<td>Pirovano et al. (2007)</td>
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<td>Formation of an upper residual layer during nighttime</td>
<td>Carry over a fraction of the ozone from the previous day that contributes to the background concentration in surrounding regions</td>
<td>Velasco et al. (2008)</td>
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<td>High pressure contributed synoptic scale subsidence</td>
<td>Vertical momentum of transportation of pollutants and even accumulate pollutants in the lower atmospheric layers during daytime via meteor stagnation conditions</td>
<td>Banta et al. (1998) and Finardi et al. (2000)</td>
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<td>Surface water vapor mixing ratio</td>
<td>Monitor morning transition time which can lead to interaction among the photochemically aged NOx, VOCs as well as their reacted products in the residual layer and the pollutants emitted at night in the nocturnal boundary layer</td>
<td>White et al. (2002)</td>
</tr>
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<td>Boundary layer structure and dynamics (associated with weak synoptic conditions)</td>
<td>Ozone and its precursors.</td>
<td>Assimakopoulos and Helmis (2009)</td>
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<td>Bottom up and top down mixing processes of air pollutants.</td>
<td>Krautstrunk et al. (2000)</td>
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<td>Elevation of ozone.</td>
<td>Shafarian et al. (2000)</td>
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<td></td>
<td>Ozone could be characterized by high traffic conditions and the mixing layer was deep whilst ozone were relatively low.</td>
<td>Assimakopoulos and Helmis (2009)</td>
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<td>Removal of ozone along concentration gradient.</td>
<td>Chung (1977); Stull (1988); Reiter (1991)</td>
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CHAPTER 2  LITERATURE REVIEW

Reviewed studies which addressed on the relationship among climatic mechanisms, meteorological process, and ozone evolution (cont’d) (Tong et al. 2010)

<table>
<thead>
<tr>
<th>Inversion, (capping inversion layer)</th>
<th>Illumination of sunlight on the ground through the ozone layer.</th>
<th>Hantie et al. (1993); Wanner et al. (1993); Kleyman et al. (1994); Neuf et al. (1994) and Gustiel et al. (1998).</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Promotion of the ground-level pollutant exposures and regional pollutant mass budgets by storing pollutants in the nighttime residual layer.</td>
<td>Salmond and McKenzie (2005).</td>
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<td></td>
<td>Vertical exchange of ozone.</td>
<td>Ludwig and Darwic (1973); Fochesatto et al. (2001); Athanassiadis (2002) and Strothers et al. (2007).</td>
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<td>Elevated NOx concentrations scenario via prohibiting the vertical dilution.</td>
<td>Finardi et al. (2001).</td>
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<tr>
<td>Vertical mixing, (diurnal variation of both surface and upper air condition)</td>
<td>Ozone and its precursors trapped aloft in the nocturnal residual layer could affect the ground-level ozone concentrations on the next day.</td>
<td>Zhang and Rao (1999).</td>
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<td>Upward mixing of the precursor substances of photooxidants from the planetary boundary layer into the free troposphere.</td>
<td>Langmann (2000).</td>
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<td></td>
<td>Elevation of ozone (mixing of ozone and its precursors from the residual mixed layer aloft to the stable boundary layer below during nighttime).</td>
<td>Samson et al. (1978); McInerney et al. (1998); Stull (1989); Corrimeier et al. (1997); Corrimeier et al. (2006) and Reitseburg et al. (2000).</td>
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<tr>
<td>Vertical and horizontal mixing, Medium to long range transport of ozone.</td>
<td>Ozone distribution and exchange with urban surface.</td>
<td>Martilli et al. (2003).</td>
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<td></td>
<td>2a. Enhancement of surface ozone during episodic type. (indirectly after enrichment of the free troposphere and then vertical mixing).</td>
<td>Zmis et al. (1999) and Bithell et al. (2000).</td>
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<td></td>
<td>2b. Enhancement of ozone during episodic type. (directly during deep intrusions of stratospheric air).</td>
<td>Gerasopoulos et al. (2006a) and Zmis et al. (2003).</td>
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<td></td>
<td>Ozone patterns could be influenced due to a combination of meteorological features dominating downwind or urban or industrial agglomerations.</td>
<td>Monks (2000); Kalabokas et al. (2000) and Gerasopoulos et al. (2005).</td>
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<tr>
<td>Study</td>
<td>Description</td>
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<td>Kim and Baik et al. (2001)</td>
<td>Used $k-\varepsilon$ turbulence model to show the effects of street canyon bottom heating on flows within street canyons of different aspect ratios</td>
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<tr>
<td>Baker et al. (2004)</td>
<td>Investigated of the dispersion and transport of reactive pollutants in and above street canyons</td>
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<td>Baik et al. (2007)</td>
<td>Pointed out the characteristics of flow and reactive pollutant dispersion in an urban street canyon can vary depending on the degree of street bottom heating</td>
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*No Building Aspect Ratio- (BAR-) and Traffic Volume- (TV-) based reactive pollutant dispersion & transport in direct ground heating street canyons has been modeled*
CHAPTER 3  MODELING METHODOLOGY

A schematic diagram of (upper) computational domain, building configuration, and boundary conditions; and (lower) the discretized part of current computational domain [Garmory et al. (2008)]

- 7 identical evenly spaced street canyons (constant street canyon width but varying building height) ~ $10^6$ grid cells
- Total height of domain extends 50m upstream of roof
- $1/7$ the power law inlet boundary layer profile
- Bulk velocity, 5m/s & $d=50m$
- Turbulent boundary conditions, 10% turbulence intensity & 100m length scale
- Fully developed single vortex and boundary layer in the sixth canyon of the domain
- Area emission source is placed on a centre ground point of the sixth canyon
- Time-step of 0.1s & 1s are tested & used for performance check.
### Part I - Governing transport equations (Reynolds averaging rules applied):

- **Conservation equation 1 - mass**
- **Conservation equation 2 - momentum**
- **Conservation equation 3 - energy**

### Part II - Governing transport equations used for coupling photochemistry:

- **NO-NO$_2$-O$_3$ related**

### Computational domain:

- **Building aspect ratios [Building - Height - to- Street-Width-Ratio]:**
  - 0.5, 1, 2, 4, 8

### Initial conditions and boundary conditions:

- **Medium/Heavy Traffic Volume settings**
- **Direct ground heating**
CHAPTER 3  MODELING METHODOLOGY
Model Configuration
Employed Fluent 6.3.26 CFD solution parameters and configuration

- 2D, segregated, implicit solver
- The constants for $k - \varepsilon$ turbulence model are $C\mu = 0.09$, $C_1\varepsilon = 1.44$, $C_2\varepsilon = 1.92$.
- Constant density
- Standard discretization for pressure
- Simple pressure-velocity coupling
- 1st order upwind discretization for momentum, turbulent kinetic energy $k$ and its dissipation $\varepsilon$.
- In this model, unsteady-to-transient-to-steady is considered to be about 7200s flow time
CHAPTER 3  MODELING METHODOLOGY

Mathematical Model
(Part I: Conservation equations of mass, momentum, and energy)

**Mean streamwise and vertical velocity components (ms⁻¹)**

**Mass conservation (continuity) Equation**

\[ \frac{\partial \bar{u}_i}{\partial x_i} = 0 \]

\[ - \frac{u_j}{u_i} \frac{\partial \bar{u}_i}{\partial x_j} = - \frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j^2} - \frac{\partial}{\partial x_j} \left( \bar{u}_i \bar{u}_j \right) + \left( \frac{\rho - \rho_o}{\rho} \right) g_i \]

**Kinematic viscosity (m²s⁻¹)**

**Momentum conservation (Navier-Stokes) equation**

**Energy conservation equation**

\[ - \frac{\bar{u}_i}{u_i} \frac{\partial \bar{\theta}}{\partial x_i} + \frac{\partial (u_i \bar{\theta})}{\partial x_i} = 0 \]

**Density of air (kgm⁻³)**

**Reynolds stresses (m²s⁻²)**

**Air temperature (°C)**

**Reference density for air (kgm⁻³)**

**Acceleration due to gravity (ms⁻²)**

\[ \bar{u}_i : \text{Velocity components (} u, \nu \text{) in the X and Z directions (ms}^{-1}) \]
CHAPTER 3  MODELING METHODOLOGY
Mathematical Model
(Part II: Transport equations of NO, NO$_2$, and O$_3$)

**Molecular diffusivity**

\[
\frac{\partial [\text{NO}]}{\partial t} + U_j \frac{\partial [\text{NO}]}{\partial x_j} = D \frac{\partial^2 [\text{NO}]}{\partial x_j^2} + \frac{\partial}{\partial x_j} (K_c \frac{\partial [\text{NO}]}{\partial x_j}) + J_{\text{NO}_2}[\text{NO}_2] - k_1[O_3][\text{NO}] + S_{\text{NO}}
\]

**Eddy diffusivity**

Source term of NO

**Source term of NO$_2$**

\[
\frac{\partial [\text{NO}_2]}{\partial t} + U_j \frac{\partial [\text{NO}_2]}{\partial x_j} = D \frac{\partial^2 [\text{NO}_2]}{\partial x_j^2} + \frac{\partial}{\partial x_j} (K_c \frac{\partial [\text{NO}_2]}{\partial x_j}) - J_{\text{NO}_2}[\text{NO}_2] - k_1[O_3][\text{NO}] + S_{\text{NO}_2}
\]

**Transport Equations of NO**

\[
\frac{\partial [O_3]}{\partial t} + U_j \frac{\partial [O_3]}{\partial x_j} = D \frac{\partial^2 [O_3]}{\partial x_j^2} + \frac{\partial}{\partial x_j} (K_c \frac{\partial [O_3]}{\partial x_j}) + J_{\text{NO}_2}[\text{NO}_2] - k_1[O_3][\text{NO}]
\]

Temperature dependent
photolysis rate (s$^{-1}$)

\[
J_{\text{NO}_2} = 8.14 \times 10^{-3} \left\{ 0.97674 + 8.37 \times 10^{-4} \times (T - 273.15) + 4.5173 \times 10^6 (T - 273.15)^2 \right\}
\]

\[
k_1 = 44.05 \times 10^{-3} \exp\left(-\frac{1370}{T}\right)
\]

Temperature dependent
reaction rate constant (ppb$^{-1}$s$^{-1}$)
### Computational Domain

**Building aspect ratios** [Building - Height - to- Street-Width- Ratio]:

- 0.5, 1, 2, 4, 8

### Initial conditions for Medium/Heavy Traffic Volume settings

- **Background:** $[\text{NO}]=0.05\text{ppb}$, $[\text{NO}_2]=0.2\text{ppb}$, $[\text{O}_3]=30\text{ppb}$
- **Emission source:** $[\text{NO}]=1000\text{ppb}$, $[\text{NO}_2]=10\text{ppb}$, $[\text{O}_3]=0\text{ppb}$
  - (Medium: Corresponding $[\text{NO}]\sim 200 \text{ \mu gm}^{-1}\text{s}^{-1}$)
  - (Heavy: Approximately set to about 5 multiples as medium case, $[\text{NO}]\sim 1000 \text{ \mu gm}^{-1}\text{s}^{-1}$)

### Boundary conditions for direct ground heating

- **Direct ground heating with ground surface temperatures,** have been set to be 16K higher than that of ambient air, & both windward and leeward walls have been set to 4K higher simultaneously in different aspect ratio canyons.
CHAPTER 4  MODEL VALIDATIONS
Comparison between Current Model with Similar experimental works

- The profiles of concentration of insert scalar on leeward and windward faces, normalized by concentration at ground level on leeward wall (top)

- Vertical profiles of normalized potential temperature and horizontal velocity at the centre line of the target street canyon (bottom left and right respectively)

| Street canyon height | Difference between potential temperature and ground temperature | Temperature difference between surface and ambient air | Horizontal inflow wind speed m/s |
The current photochemistry coupled CFD model cannot be validated as no experimental data on reactive pollutant concentration in a street canyon are available so far. Nonetheless, the model developed for the passive pollutant dispersion was validated with experimental data published in the literature (Hoydsh Dabberdt, 1998), for wind flow and temperature fields in a street canyon with bottom heating was validated by comparing the modeling results accordingly (Uehara et al., 2000; Kim and Baik, 2001). These can be, in general, representative to argue the modelled results are numerically correct on an assumed basis.

The inert scalar concentration profiles followed the trends likewise.

The normalized potential temperatures matched similarly with both sets of wind tunnel data as compared.

The normalized horizontal velocity as validated and shown lying in a region between Uehera et al. (2000) and Kim an Baik (2001).
Under the same direct ground heating condition, the amount of intrusion of ambient ozone into the canyon has been increased. It is indicated that increment of building aspect ratio encourages the accumulation of ozone.

The contours of $O_3$ concentration under the increasing building aspect ratio, ranging from 0.5 to 8, [top: 0.5 (left), 1 (right) and bottom: 2 (left), 4 (middle), 8 (right)]
CHAPTER 5  RESULTS AND DISCUSSION
Under the same direct ground heating condition

- The amount of intrusion of ambient ozone into the canyon changes merely slightly or not much observable change under the same BAR 1 with increasing TV but increases sharply with the same BAR 8 and heavier TV.

- The contours of $O_3$ concentration under different building aspect ratio and traffic volume (starting from top leftmost to bottom rightmost: BAR=1 and TV=medium, BAR=1 and TV=heavy, BAR=8 and TV=medium, BAR=8 and TV=heavy). Note that here BAR and TV are recalled as previously and refer to Building Aspect Ratio and Traffic Volume.

- This also indicated that the dominant role of building aspect ratio can encourage the accumulation of ozone especially under the downwind region.
Based on a review of the literature on the ozone evolution in urban environments, the importance of reactive pollutant evolution under urbanization related emission structure and street canyon design layout have been identified;

As well as identified the leapfrogging aspect to achieve air quality improvement in sustainable urban living environments.

A photochemistry coupled CFD model based on existing modeling works was developed and evaluated by employing building aspect ratios and traffic volume under direct ground heating to predict the evolution of reactive pollutant gases in urban-like street canyons.
By performing calculations on the above aspects, this developed model reveals that the building aspect ratio play an important role in governing the ozone accumulation in a street canyon with heavy traffic condition and ground heated condition.

This study indicated that the dominant role of building aspect ratio can encourage the accumulation of ozone especially under the downwind region.

The current study can serve as a reference to the possible policy makers in urban planning and health control.
REFERENCES ARISING FROM THE PRESENTATION

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Acknowledgement

- Professor Dennis Y. C. Leung, for his sincere support and supervision throughout this project in the University of Hong Kong. His guidance and advice lead to the completion of current presentation.

- This project is supported by the Hong Kong Research Grant Council (HKU7146/06E).
End of Presentation

Sincerely thanks!