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Parameterization Study of Chemically Reactive Pollutant Dispersion Using Large-Eddy Simulation

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Background & Objective

- Dispersion & transport of pollutant emitted from vehicles over urban areas largely affect pedestrian-level air quality. Poor ventilation inside street canyons often results in accumulation of pollutants which is harmful to human health.
- Most vehiclar exhausts are chemically reactive that evolve to their secondary counterparts in the atmospheric boundary layer (ABL). The conventional Gaussian plume model, which assumes inert pollutants, should be used with caution.

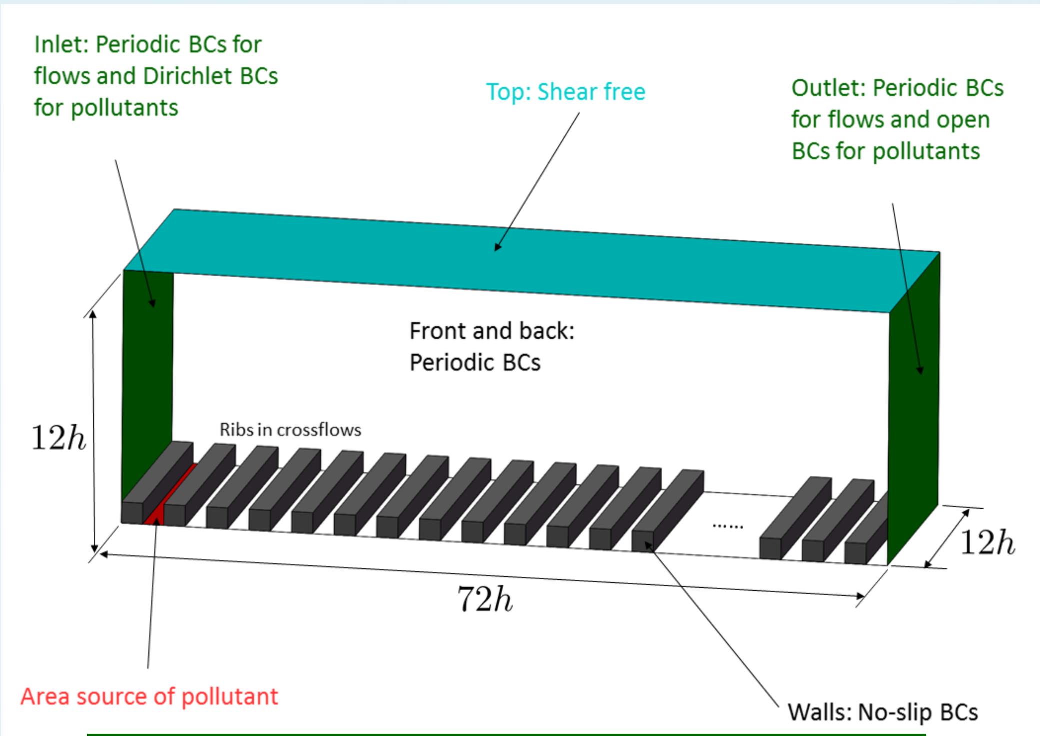

Fig. 1. Computational domain.

Methodology

- Large-eddy simulation (LES) with the one-equation subgrid-scale (SGS) model.
- Chemical reactions are included to handle the irreversible ozone titration (Fig. 1).

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

- The Gaussian plume model using depleted source:

$$C(x,z) = \frac{Q}{(\pi/2)^{1/2} U \sigma_z(x)} \exp\left[-\frac{1}{2}\left(\frac{z-h}{\sigma_z(x)}\right)^2\right]$$

Major Findings

- The current LES data in flow structure are validated by wind tunnel experiments, showing a good agreement with existing results available in literature (Fig. 2).
- The current LES-calculated passive scalar concentration over hypothetical urban areas shows that the theoretical solution is Gaussian shape independent from the streamwise location *x*.
- The far-field LES-calculated NO concentrations agree reasonably well with the Gaussian source depletion model over the near-wall region (Fig. 3).
- Budget analysis shows that the inaccuracy of Gaussian plume model near the roof level is mainly attributed to the chemistry term (Fig. 4).

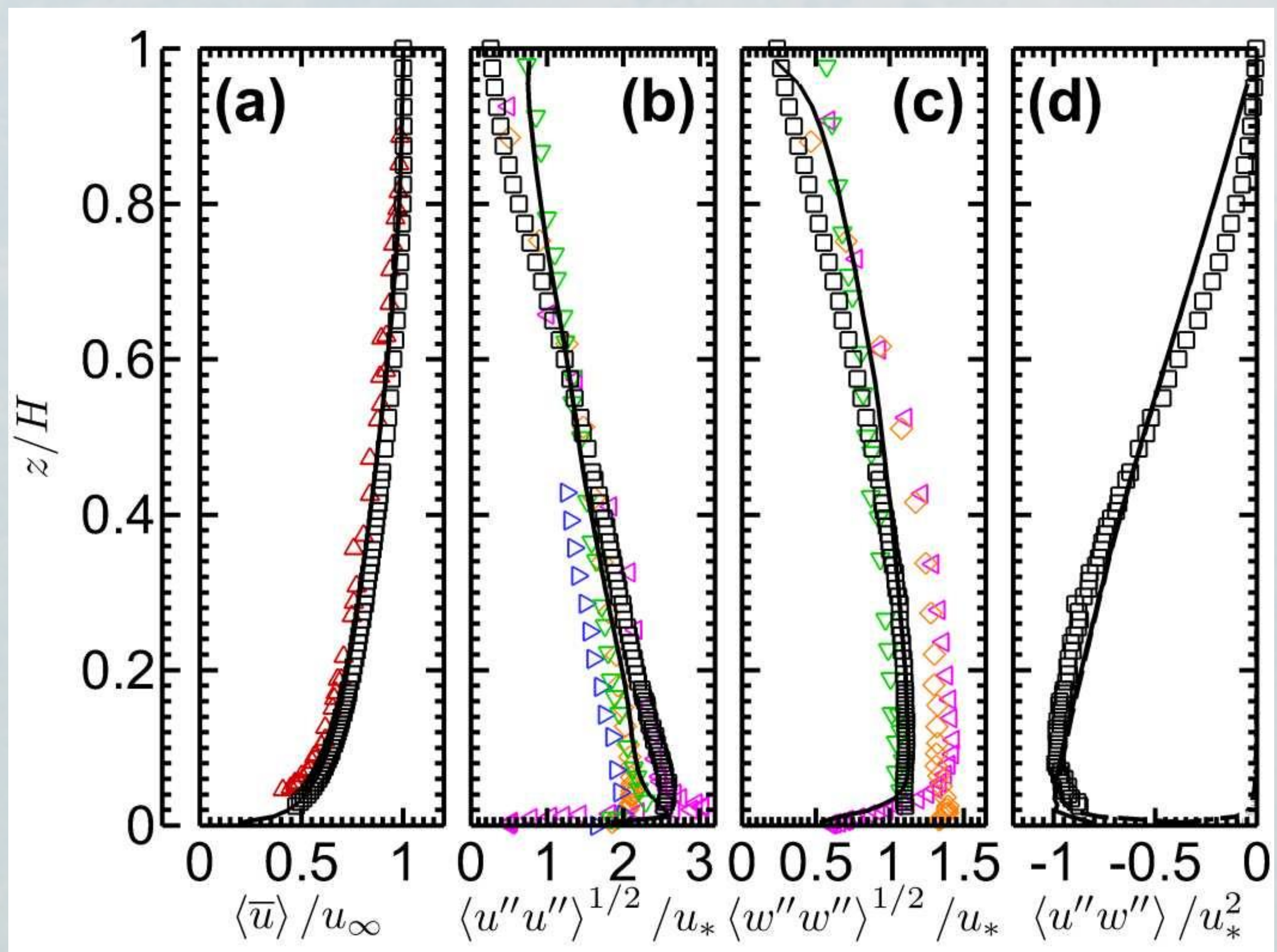

Fig. 2. Dimensionless profile of flows.

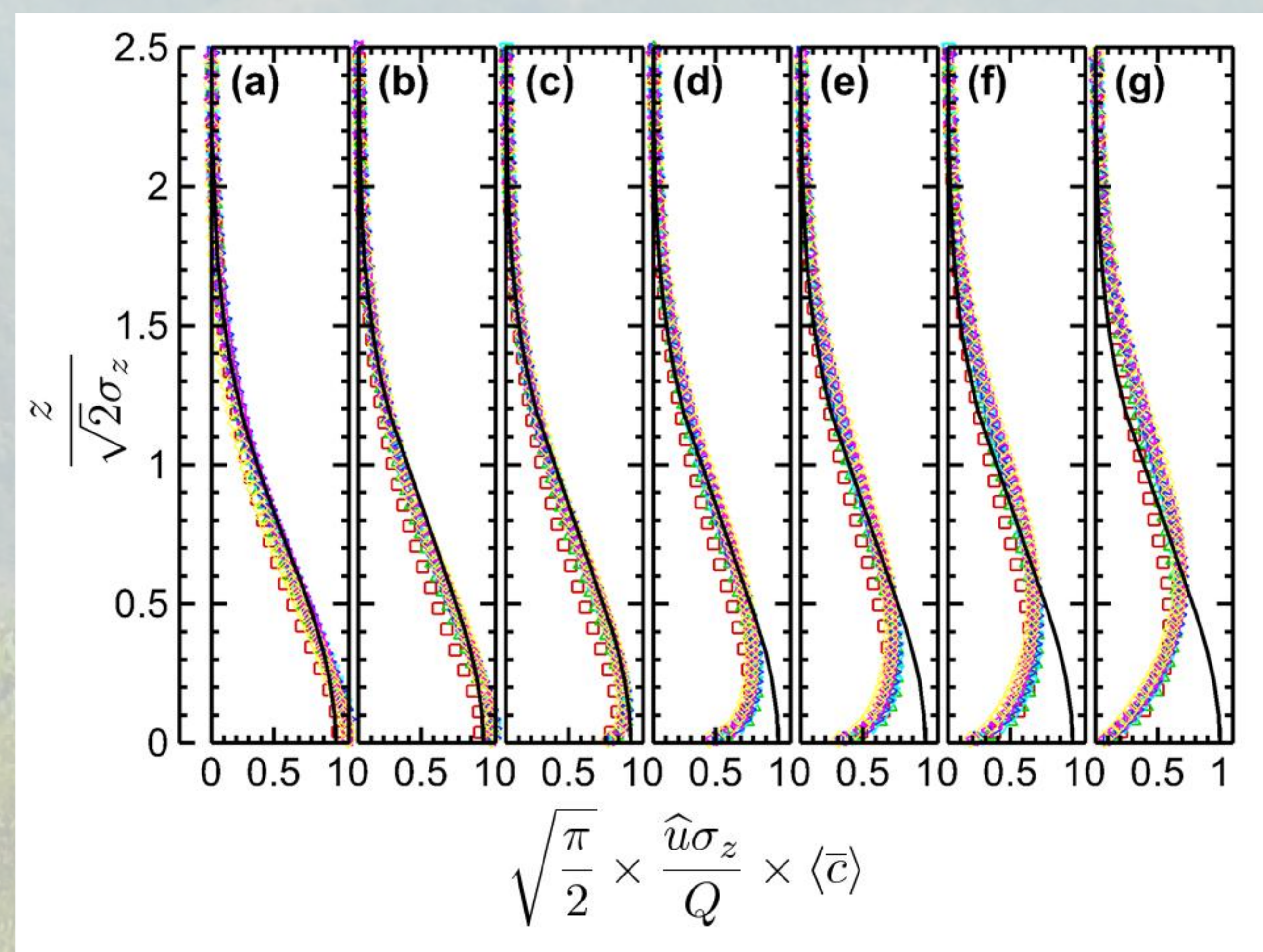

Fig. 3. Dimensionless profiles of passive scalar (a) & NO concentration with background ozone concentration $[O_3]_0$ of (b) 1 ppb; (c) 10 ppb; (d) 50 ppb; (e) 100 ppb; (f) 200 ppb and (g) 500 ppb. Black line : Gaussian form.

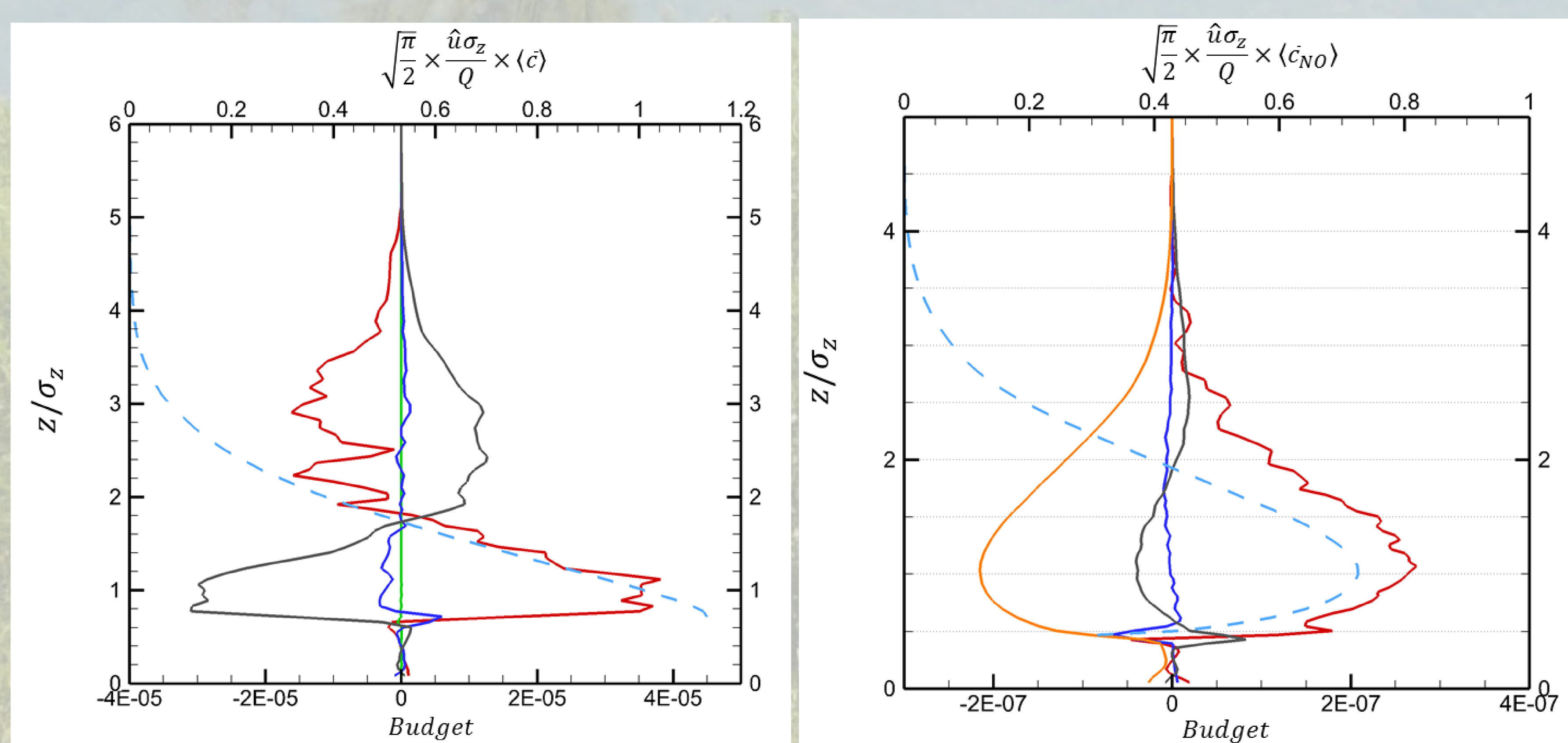

Fig. 4. Budget analysis for passive scalar & NO

Dash line: NO profile; red line: advection; orange line : chemistry; black and blue line: diffusion

References

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