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Effect of stable stratification on dispersion within urban street canyons: a large-eddy simulation

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Abstract

This study employs a validated large-eddy simulation (LES) code with high tempo-spatial resolution to investigate the effect of a stably stratified roughness sublayer (RSL) on scalar transport within an urban street canyon. The major effect of stable stratification on the flow and turbulence inside the street canyon is that the flow slows down in both streamwise and vertical directions, a stagnant area near the street level emerges, and the vertical transport of momentum is weakened. Consequently, the transfer of heat between the street canyon and overlying atmosphere also gets weaker. The pollutant emitted from the street level 'pools' within the lower street canyon, and more pollutant accumulates within the street canyon with increasing stability. Under stable stratification, the dominant mechanism for pollutant transport within the street canyon has changed from ejections (flow carries high-concentration pollutant upward) to unorganized motions (flow carries high-concentration pollutant downward), which is responsible for the much lower dispersion efficiency under stable stratifications.

Keywords: Large-eddy simulation (LES), Urban street canyon, Pollutant dispersion, Stable stratification

1 1. Introduction

With the continuous global urbanization process, more and more research interests are directed to the interaction between human activities and the built environment. Special attention is paid to the roughness sublayer (RSL), the region at the bottom of the atmospheric boundary layer (ABL) where the presence of the canopy influences directly the characteristics of the turbulence and dispersion. The RSL extends from the ground to a height of about

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there times the canopy height and includes the canopy air space (Kaimal and Finnigan, 1994). 7 One of the basic roughness elements in urban areas is the street canyon, a relatively narrow 8 street in-between buildings that line up continuously along both sides. Models of urban street 9 canyons remain the basis of the urban canopy model (UCM) in numerical weather prediction 10 (NWP, e.g., Weather Research and Forecasting model) models to account for the effect of 11 exchange of momentum, heat and scalars between the urban area and overlying atmosphere. 12 It is therefore of practical importance to investigate the flow, turbulence and scalar transport 13 within and above urban street canyons. 14

The stratification of the atmosphere has great impact on the turbulence and dispersion in 15 urban areas. The nocturnal atmosphere is generally stably stratified, although in urban areas 16 this is sometimes not true due to the urban heat island and strong turbulence. Compared with 17 the convective boundary layer (CBL), theory and observations in the stable boundary layer 18 (SBL) are rather more complex. Turbulence production by shear is counteracted by buoyancy 19 forces, resulting in generally low turbulence levels, or in very stable conditions, intermittent 20 turbulence (van Dop and Axelsen, 2007). The numerical simulation of the SBL is more chal-21 lenging since the size of turbulent eddies is limited. Therefore, the resolution of the numerical 22 model should be much higher when studying the SBL. Under very stable stratification, turbu-23 lence can be intermittent and gravity wave may be generated, which further complicates the 24 problem and makes numerical simulations inapplicable. The numerical simulation using large-25 eddy simulation (LES) has demonstrated that LES can adequately capture the characteristics 26 of weakly to moderately stably stratified boundary layer (Jiménez and Cuxart, 2005). 27

Many numerical studies have been conducted for the urban street canyons under unstable 28 and neutral stratification (e.g., Sini et al., 1996; Kim and Baik, 1999; Xie et al., 2006; Li et al., 29 2008, 2010a, 2012; Dallman et al., 2014; Hang et al., 2016; Cui et al., 2016), while only a few have 30 been done under stable stratification (e. g., Cheng and Liu, 2011b; Xie et al., 2013; Boppana 31 et al., 2014; Li et al., 2015; Tomas et al., 2015). Although stable stratification conditions 32 occur less frequently in urban areas during nighttime than in their rural surroundings due to 33 anthropogenic heat release and the enhanced turbulence by urban structures, the research of 34 stable stratification is still very important from a practical point of view, since the reduced 35 turbulence can lead to strong concentrations of contaminants, and the reduced downward heat 36 flux can result in very low surface temperatures and eventual frost damage in cold regions (Flores 37 and Riley, 2011). Previous research has shown that later at night, when the rural SBL is deeper 38 than the building height, the city is then capped by a stable layer (Godowich et al., 1985). This 39

⁴⁰ paper therefore intends to explore the turbulence and dispersion characteristics within urban
⁴¹ street canyons under stable stratification, and we will try to investigate the mechanism behind
⁴² these characteristics, which makes this study distinct from previous studies listed above.

The urban street canyon geometry in this study is essentially a two-dimensional (2D) 43 due to the periodic boundary conditions prescribed in the along-axis direction (see Section 2). 44 According to Vardoulakis et al. (2003) and Li et al. (2006), street canyons might be classified 45 into short $(L/b \leq 3)$, medium (3 < L/b < 7) and long $(L/b \geq 7)$, where L is the street length 46 and b is the street width (see Section 2). When L is infinite, this corresponds to a 2D street 47 canyon; otherwise, a three- dimensional (3D) street canyon geometry must be considered. The 48 flow and pollutant dispersion in 3D urban-like models with thermal effects or under neutral 49 stratification have been investigated in the literature (e. g., Santiago et al., 2014; Hang et al., 50 2015). 51

The rest of the paper will be organized as follows. The numerical method and simulation setup will be described in Section 2. Section 3 will present the results of turbulence and pollutant dispersion, followed by a conclusion in Section 4.

55 2. Methodology

This study employs the LES code (Li et al., 2010a, 2012) developed for incompressible turbulent flow based on a one-equation subgrid-scale (SGS) model.

58 2.1. Governing equations

The equations for the evolution of the filtered velocity field are derived from the Navier-Stokes equations for incompressible flow, with the buoyancy effect taken into account by Boussinesq approximation. The reference length scale h (the building height of the street canyon), the reference velocity scale U (free-stream velocity) and the reference temperature θ_a (the ambient temperature) are used to make the governing equations dimensionless. The dimensionless, filtered (resolved-scale) conservation equations for momentum, heat and mass read, respectively

$$\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial \overline{u}_i \overline{u}_j}{\partial x_j} = -\frac{\partial \pi}{\partial x_i} - \frac{\partial P}{\partial x_i} \delta_{i1} - \frac{\partial \tau_{ij}}{\partial x_j} + \frac{1}{Re} \frac{\partial^2 \overline{u}_i}{\partial x_j \partial x_j} + \frac{gh}{U^2} \overline{\theta} \delta_{i3}, \tag{1}$$

$$\frac{\partial\theta}{\partial t} + \frac{\partial\theta\overline{u}_i}{\partial x_i} = -\frac{\partial\tau_{\theta i}}{\partial x_i} + \frac{1}{RePr}\frac{\partial^2\theta}{\partial x_i\partial x_i},\tag{2}$$

$$\frac{\partial u_i}{\partial x_i} = 0,\tag{3}$$

65 where

⁶⁶ \overline{u}_i is the resolved-scale velocity in the *i*-th direction, π is the modified pressure normalized ⁶⁷ by constant density ρ , $-\partial P/\partial x_1$ is the mean streamwise pressure gradient prescribed to drive ⁶⁸ the atmospheric flow, $\overline{\theta}$ is the resolved-scale (potential) temperature, g is the gravitational ⁶⁹ acceleration, and δ is the Kronecker delta. The Reynolds number is defined as $Re = Uh/\nu$ and ⁷⁰ Prandtl number Pr is taken as 0.72. The subgrid-scale (SGS) or residual momentum flux τ_{ij} ⁷¹ and heat flux $\tau_{\theta i}$ are modeled using the eddy-viscosity assumption as

$$\tau_{ij} = -2\nu_T \overline{S}_{ij}, \quad \text{and} \quad \tau_{\theta i} = -2\nu_\theta \frac{\partial \theta}{\partial x_i},$$

⁷² respectively, where

$$\overline{S}_{ij} = \frac{1}{2} \left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right)$$

The turbulent viscosity for momentum ν_T and diffusivity for heat ν_{θ} are modeled as $\nu_T = C_k \ell e^{1/2}$ and $\nu_{\theta} = (1 + 2\ell/\Delta)\nu_T$, respectively, where C_k is a constant (see below), ℓ is the length scale (or filter width), and $\Delta = (\Delta_x \Delta_y \Delta_z)^{1/3}$ is the local grid size.

The transport equation for SGS turbulent kinetic energy (TKE) e reads

$$\frac{\partial e}{\partial t} + \overline{u}_i \frac{\partial e}{\partial x_i} = \mathcal{P} + \mathcal{B} - \varepsilon + \frac{\partial}{\partial x_i} \left(\frac{2}{Re_{\rm T}} \frac{\partial e}{\partial x_i} \right),\tag{4}$$

77 where

$$\mathcal{P} = -\tau_{ij}\overline{S}_{ij}, \qquad \mathcal{B} = -g\nu_{\theta}\frac{\partial\theta}{\partial z},$$
$$\varepsilon = C_{\varepsilon}\frac{e^{3/2}}{\ell}, \qquad Re_{\mathrm{T}} = Uh/\nu_{\mathrm{T}}.$$

The $C_k = 0.03$ and $C_{\varepsilon} = 1.0$ are model constants (Li et al., 2010b). The length scale ℓ is defined as (Moeng, 1984; Saiki et al., 2000)

$$\ell = \begin{cases} \Delta & \text{for neutral and unstably stratified region,} \\ 0.76 \left(\frac{e^{1/2}}{N}\right) & \text{for stably stratified region,} \end{cases}$$
(5)

⁸⁰ where N is the Brunt-Väisälä frequency defined by $N^2 = \frac{g}{\theta_a} \frac{\partial \overline{\theta}}{\partial z}$.

The conservation equation for pollutant mixing ratio \overline{c} reads

$$\frac{\partial \overline{c}}{\partial t} + \frac{\partial \overline{u}_i \overline{c}}{\partial x_i} = -\frac{\partial \sigma_i}{\partial x_i} + \frac{1}{ReSc} \frac{\partial^2 \overline{c}}{\partial x_i \partial x_i} + S,\tag{6}$$

where $\sigma_i = \overline{u_i c} - \overline{u_i c}$ is the SGS flux, Sc is the Schmidt number (which is prescribed as 0.72 in this study), and S is the source term. Similarly, σ_i is modeled as

$$\sigma_i = -\nu_c \frac{\partial \overline{c}}{\partial x_i},$$

84 where $\nu_c = (1 + 2\ell/\Delta)\nu_T$.

The above equations are solved using the Galerkin finite element method. The detailed mathematical formulation of the above equations was discussed in Li et al. (2010b).

⁸⁷ 2.2. Computational domain and boundary conditions

Figure 1 depicts the schematic computational domain used in the current study, which represents a typical street canyon in an idealized manner. The spanwise-homogeneous computational domain consists of a street canyon of height h at the bottom and a free shear layer of depth 3h above the building. The width of the street is b and its length is L. In our study, a street canyon of aspect ratio (AR, h/b) 1 with h = b = L is considered. The inlet and outlet length $b_u = b_d = 0.5b$.

The background atmospheric flow is simulated in the form of a pressure-driven free stream in the free shear layer only. The approaching flow is perpendicular to the street axis, which results in a free-stream wind speed U in the streamwise direction. The air flow boundary conditions are set to be periodic in the streamwise and spanwise directions, and no-slip conditions are set at all rigid walls. At the top of the domain, a shear-free boundary condition $(\partial \overline{u}/\partial z = \partial \overline{v}/\partial z = \overline{w} = 0, \ \partial e/\partial z = 0)$ is assumed.

A line source of length L with emission rate Q is located on the ground along the street axis 100 at a distance x_s (= b/2 in this study) from the leeward building. At the inlet, the temperature 101 is set to θ_a and pollutant concentration is set to zero (free of pollutant). At the outlet, the 102 convective boundary conditions (Li et al., 2008) are prescribed for both the temperature and 103 pollutant to ensure that they are convected outside the domain and will not enter into the 104 domain again from the inlet. The air temperature at the top is set to the ambient temperature 105 θ_a and the ground level (bottom) maintains a constant temperature $\theta_f = \theta_a + \Delta \theta$. When 106 $\Delta \theta < 0$ the street is cooled and a stable stratification occurs. The temperatures at the rigid 107 walls can either be set to a fixed value (ambient temperature θ_a) or adiabatic (no heat flux at 108 walls); we take the former situation in the present study. The pollutant flux is set to zero at 109 rigid walls (including building walls and roofs). 110

111 2.3. Simulation conditions

In this study, three scenarios of thermal stratification (neutral, unstable and stable) will be investigated. The bulk Richardson number, which is used to characterize the stability, is defined as

$$Ri = -\frac{gh}{U^2} \frac{\Delta\theta}{\theta_a}.$$
(7)

The values of Ri studied here are -0.1 (unstable), 0 (neutral), 0.1, and 0.188 (stable). The Reynolds numbers based on building height h and free-stream velocity for these cases vary from about 8,000 to 11,000, all above 3000, the critical value for the flow within the street canyon to be independent of the viscosity effect (Hoydysh et al., 1974).

The grid used for the street canyon of AR 1 consists of $128 \times 64 \times 128$ and $256 \times 64 \times 216$ 119 elements inside and above the street canyon, respectively. The grid is stretched near the wall 120 to better resolve the near-wall turbulence. The minimum grid sizes are $2.632 \times 10^{-3} H$ in the 121 streamwise and vertical directions and $1.563 \times 10^{-2} H$ in the spanwise direction. This spatial 122 resolution is about twice higher as those for the neutral (Li et al., 2008, 2009) and unstable 123 stratification cases (Li et al., 2010a, 2012). The distance between the walls and the first grid 124 away from the walls, expressed in wall unit, is about 0.55, which is less than 1, satisfying the 125 requirement for the no-slip condition prescribed along the walls. 126

The simulation was first performed for neutral stratification condition ($\Delta \theta = 0$) and, when a turbulent flow was established, switched to unstable/stable stratification condition ($\Delta \theta < 0$ or $\Delta \theta > 0$). The time for the flow to reach pseudo-steady state was about 400h/U. Another 300h/U simulation results were collected to retrieve the statistical flow, turbulence, and scalar properties with a time step of 0.0025h/U, which is half of that used for the above-mentioned neutral and unstable stratification studies.

133 3. Model validation

The model described in the previous section has been validated against isothermal windtunnel data (Li et al., 2010a), and then was validated for an urban street canyon with ground heating (Li et al., 2012). The simulated thin thermal boundary layer near the ground agreed very well with wind-tunnel measurements (Uehara et al., 2000), which was not resolved in studies using RANS models.

To gain more confidence in the LES model under stable stratification, an additional model evaluation exercise is conducted using an experimental database obtained by the Japanese National Institute for Environmental Studies in an atmospheric diffusion wind tunnel (Uehara et al., 2000). Their experiment was carried out inside a target street canyon within a model building array and the entire wind-tunnel floor was heated, which is not exactly the same as the configuration described in the previous section. For comparison, the boundary conditions for temperature at the outlet in the LES model are changed to periodic. Thus, the thermal energy convected from the outlet enters the domain from the inlet.

Following Uehara et al. (2000), a bulk Richardson number Rb is introduced to quantify the thermal effects, and is defined as

$$Rb = \left(\frac{gh}{U_h^2}\right) \frac{\theta_h - \theta_f}{\theta_a},\tag{8}$$

where θ_h is the temperature at the roof level, and U_h is the streamwise velocity at the roof level.

The results from our LES for a street canyon of aspect ratio 1 at $Re \approx 8900$ and Rb = 0.33151 (which is the closest Rb value from a series of numerical experiments) are compared with the 152 experimental data at Rb = 0.43 (Fig. 2). It is clear that the agreement between the current 153 LES results and the experimental data is generally good. The well-simulated wind profile 154 indicates adequate grid resolution in the current LES, especially above the street canyon. In 155 previous studies (Li et al., 2008, 2010a), a vertical domain size of 2h was used and a large 156 difference was observed between the simulated and measured wind profile above the street 157 canyon. In present study, a domain height of 4h is used instead, signifying the impact of the 158 vertical domain size in simulating correctly wind profile. However, the normalized temperature 159 shows much discrepancy both within and above the street canyon (Fig. 2b). The simulated 160 temperature shows quite constant values both within and above the street canyon, while the 161 measured temperature gradually evolves towards the ambient value. 162

As demonstrated above, the LES reproduces reasonably well the flow and temperature 163 structure in urban street canyons under different stratifications. For the pollutant dispersion, 164 the LES model was validated against wind-tunnel measurement under isothermal conditions 165 and good agreement was also observed (Li et al., 2008). As no experimental data can be 166 found for pollutant dispersion under unstable or stable stratification conditions, no additional 167 validation is performed for pollutant dispersion here. In the upcoming sections, the validated 168 model will be utilized to study in detail the flow, temperature, and pollutant dispersion inside 169 urban street canyons with different atmospheric stability conditions. The boundary condition 170 for temperature at the outlet reverts to the convective type, as described in the previous section. 171

172 4. Results and discussions

In this section, the validated model will be used in this section to reveal the flow and pollutant dispersion characteristics in a stably stratified roughness sublayer. In the following discussions, brackets $\langle \rangle$ represent the spanwise and temporal averages of physical properties, while a prime represents the deviation from their averages.

177 4.1. Flow and Turbulence

Figure 3 depicts the normalized streamwise velocity $\langle \overline{u} \rangle /U$ in the centerline (x/b)178 (0.5) of the street canyon under different stabilities. The major difference between all the 179 vertical profiles lies within the street canyon $(z/h \leq 1)$. The reverse flow $(\langle \overline{u} \rangle / U < 0)$ 180 in the lower street canyon shows strong dependence on Ri: when Ri < 0 this reverse flow 181 has a much stronger maximum than that when Ri = 0, indicating an enhancement of in-182 canyon recirculation by unstable stratification (i.e., both vertical and horizontal velocities are 183 strengthened. See Li et al. 2010b); when Ri > 0, this reverse flow is weakened and the 184 location of maximum is shifted upward compared with the cases for $Ri \leq 0$. Near the ground 185 $(x/h \le 0.15)$, the streamwise velocities under stable stratifications are close to zero, showing a 186 stagnant region in the vicinity of street. This can be seen more clearly in Figure 4 which shows 187 the streamline under different stratifications. The stagnant areas near the ground are evident 188 and may make the pollutant released from the street level extremely difficult to disperse, as can 189 be seen in later sections. Also shown in Figure 4 are the Reynolds stresses, which demonstrate a 190 strengthened peak near the roof level under unstable stratification, while becoming weaker with 191 increasing Ri. Since Reynolds stress is responsible for the vertical transport of momentum, it 192 is clear that increasing Ri weakens this transport. 193

¹⁹⁴ The normalised spanwise mean vorticity

$$\omega_y = \frac{h}{U} \left(\frac{\partial \langle \overline{w} \rangle}{\partial x} - \frac{\partial \langle \overline{u} \rangle}{\partial z} \right) \tag{9}$$

¹⁹⁵ is shown in Figure 5. In the isothermal case (Fig. 5a), the LES results agree quite well with ¹⁹⁶ the spanwise vorticity measured by Caton et al. (2003, Fig. 5a therein). The layer of large ¹⁹⁷ negative vorticity at the roof level indicates a strong shear layer there, but under unstable ¹⁹⁸ stratification (Fig. 5b), this shear layer becomes weaker. Under stable stratifications (Fig. 5c, ¹⁹⁹ and d), the shear layer at the roof level is much stronger and almost covers the whole roof. ²⁰⁰ This characteristic may be the reason for better/worse pollutant removal under unstable/stable ²⁰¹ stratifications, as will be seen later. Since this shear layer is located where Kelvin-Helmholtz instability occurs (Louka et al., 2000; Letzel et al., 2008), the stable stratification may help
promote the growth of this instability.

In the core region in the street canyon, the spiral negative vorticity becomes larger in 204 magnitude under unstable stratifications, confirming the strengthened recirculation. Under 205 stable stratification, the vorticity magnitude is about the same as in the neutral stratification, 206 but the center of the recirculation is shifted towards the upper right corner of the street canyon. 207 Near the bottom, there is a local maximum under neutral stratification that is enhanced under 208 unstable stratification. However, under stable stratifications, this local maximum is lifted to 209 $z/h \approx 0.15$ with a much reduced magnitude. This fact signifies that the stagnant air near 210 the bottom is decoupled from the major vortex in the street canyon, and it will inevitably 211 negatively impact the pollutant dispersion from the line source located in the center at the 212 street level. 213

214 4.2. Temperature distribution

The normalized mean temperature $(\langle \overline{\theta} \rangle - \theta_a)/\Delta \theta$ (Fig. 6) distribution is very similar 215 under different stratifications. As explained by Li et al. (2010a), this is because the turbulent 216 and diffusive heat fluxes are both linearly dependent on resolved-scale temperature gradients 217 in this LES model, except that the diffusivity for heat ν_{θ} is not constant. Therefore, at pseudo-218 steady state, the temperature is roughly governed by an elliptic equation. Since the temperature 219 is fixed at the boundary in the cases studied, the solution to the temperature distribution 220 is basically fixed, and the slight variations of the temperature distribution are due to the 221 differences in advection and the non-constant diffusivity for heat ν_{θ} . 222

At the lee side of the street canyon (Fig. 6), the normalised temperature is higher than 223 at the windward side, which is a result of the reverse streamwise velocity near the ground. In 224 the core region of the street canyon, the normalized temperature was rather uniform for all Ri. 225 However, it must be noted that, under stable stratifications, $\Delta \theta < 0$ and smaller normalized 226 temperature corresponds to higher $\langle \overline{\theta} \rangle$. Therefore, $\langle \overline{\theta} \rangle$ is higher near the windward 227 side than that near the leeward side. Under stable stratifications, with the stagnant air near 228 the street to suppress the turbulent heat transfer, the temperature within the street canyon is 229 expected to get even lower and the stratification becomes more stable. However, this positive 230 feedback often found in SBL is not likely to occur here due to the fixed-temperature boundary 231 conditions used in this study. By fixing the walls' temperature to the ambient temperature, 232 there implicitly exists heat flux from the building walls to the air within the street canyon to 233

²³⁴ maintain this higher temperature.

Under stable stratifications, the vertical gradient of mean temperature near the roof level is much smaller compared with that under unstable stratification, suggesting that the heat transfer between the street canyon and overlying atmosphere decreases with increasing Ri. This will be quantified in Section 4.4.

239 4.3. Pollutant dispersion

240 4.3.1. Mean concentration and flux

The normalised mean pollutant concentration fields $\langle \bar{c} \rangle UHL/Q$ (Fig. 7) for the neutral 241 and unstable stratifications are generally similar, but the magnitude of the mean concentration 242 is markedly less for unstable stratification case inside the street canyon. On the other hand, 243 under stable stratifications, the stagnant air near the street level results in a 'pool' of high-244 concentration pollutant there. Otherwise, above $z/h \approx 0.15$, the pollutant concentration under 245 stable stratifications distributes quite similarly to that under neutral stratification, in terms 246 of both the spatial pattern and quantity. Table 1 contrasts the average pollutant within the 247 street canyon, and particularly $z/h \leq 0.15$. The average pollutant mass $\int \langle \bar{c} \rangle U/Q \, dx \, dz$ 248 within the whole street canyon increases greatly with increasing R_i , with the pollutant mass 249 at Ri = 0.188 almost 4 times that at Ri = -0.1. More strikingly, at Ri = 0.188, the pollutant 250 mass in the lower 15% street canyon takes up almost half of the total pollutant mass within 251 the street canyon. 252

The vertical pollutant concentration fluxes $\langle w'c' \rangle (HL/Q)$ for each case are depicted 253 in Figure 8 for comparison to further demonstrate the effect of stratifications. Under neutral 254 stratification, there is a strong vertical flux near the windward wall due to the mixing of the 255 pollutant re-entering the street canyon with pollutant-free air from the free stream. However, 256 under unstable stratification, this vertical flux weakens, and instead the vertical flux in the 257 wake of the line source becomes strengthened and strong vertical fluxes are observed along the 258 leeward wall, which is absent from the neutral stratification. These are speculated to transport 259 more pollutants from the line source to the roof level, which has been confirmed by Li et al. 260 (2010a, 2012). The change by stable stratifications (Fig. 8c, d) is even more prominent. The 261 flux near the leeward wall changes to negative from positive under unstable stratification. This 262 indicates that the turbulent transport of pollutant becomes downward rather than upward, due 263 to the reduced updraft there. In the lower corner near the windward wall, there is a strong 264 local maximum of pollutant flux between the interface of the main vortex and the 'pooling' 265

air near the bottom (see Fig. 8c, d). The magnitude of this maximum is higher than that at the roof level. This shows that there is substantial upward transport of pollutant, due to the slowed downdraft there, which consequently brings less relatively fresh (less polluted) air down. The mechanism of these changes under stable stratifications will be further examined in Section 4.3.2.

With the aforementioned drastic changes of the pollutant flux pattern, the pollutant transport at the roof level is expected to show significant difference under stable stratifications. To verify this, the pollutant concentration budget (by taking the average of the pollutant transport equation (6), see Li et al. 2009)

$$\frac{\partial \langle \overline{c} \rangle}{\partial t} = \underbrace{-\langle \overline{u} \rangle}_{\text{streamwise advection vertical advection streamwise turbulent transport}}_{\text{streamwise advection vertical advection streamwise turbulent transport vertical turbulent transport} \underbrace{-\frac{\partial \langle w'c' \rangle}{\partial z} - \langle \frac{\partial \sigma_z}{\partial z} \rangle}_{\text{streamwise turbulent transport vertical turbulent transport}} \underbrace{-\frac{\partial \langle w'c' \rangle}{\partial z} - \langle \frac{\partial \sigma_z}{\partial z} \rangle}_{\text{streamwise turbulent transport}} + \frac{1}{ReSc} \left(\frac{\partial^2 \langle \overline{c} \rangle}{\partial x^2} + \frac{\partial^2 \langle \overline{c} \rangle}{\partial z^2} \right) \tag{10}$$

molecular diffusion

along the roof level for different Ri is compared in Fig. 9. Since the molecular diffusion terms in this equation are negligible, they are not discussed below and shown in Fig. 9.

The pattern of each component of the concentration budget under stable stratification is 277 generally similar to their counterpart under neutral stratification. It is noteworthy that there 278 is a much larger vertical gradient of mean pollutant concentration ($\partial < \overline{c} > /\partial z$) at the lee-279 ward side of the roof level under stable stratification. Therefore the vertical advection term 280 has a comparable magnitude under stable stratification to that under neutral stratification, 281 despite that $\langle \overline{w} \rangle$ under stable stratification is rather small there. On the other hand, the 282 vertical advection under unstable stratification (Fig. 9b) has a large negative contribution to 283 the concentration budget at $0 \le x/h \le 0.17$, since $\langle \overline{w} \rangle$ in that interval is negative (due to 284 a small vortex developing at the upper corner near the leeward building, see Li et al., 2010a), 285 indicating that fresh air is entrained into the street canyon at this leeward corner, which dilutes 286 the pollutant there (Li et al., 2010a). Another notable point is the role of vertical turbulent 287 transport under different stratifications: under unstable stratification, the vertical turbulent 288 transport has a strong positive value at the leeward corner, while under neutral and stable 289 stratifications, this term shows a negative contribution, with the magnitude under stable strat-290 ification much larger. This demonstrates the different efficiency of turbulent transport under 291 different stratifications, which deceases with increasing Ri: less high-concentration pollutants 292 are transported to the roof level from the point source by turbulence when the atmosphere 293 becomes more stable. 294

295 4.3.2. Turbulence structure of pollutant flux

The turbulence structure (or coherent structure) plays an important role in momentum 296 and scalar transfer processes, and can often be deduced using quadrant analysis. For pollutant 297 flux w'c', the first quadrant (Q1: w' > 0, c' > 0) is called ejections, which are the 'ejection' of air 298 with high-concentration pollutant from the urban canyon into the RSL above, while the third 299 quadrant (Q3: w' < 0, c' < 0) is called sweeps, which are the replacement of ejected fluid with 300 air of relatively low-concentration pollutant from above the street canyon. These two quadrants 301 contribute positively to the pollutant flux and are called organized motions, while the other two 302 quadrants (Q2: outward interactions, w' > 0, c' < 0 and Q4: inward interactions, w' < 0, c' > 0) 303 contribute negatively, and are called unorganized motions. These definitions are depicted in 304 Fig. 10. Please note that the definitions of ejections and sweeps here for turbulent pollutant flux 305 are different from those for momentum flux due to the different transport processes of pollutant 306 and momentum. The ratio of turbulent pollutant flux contribution from Q1 and Q3 under 307 different stratifications in the street canyon is presented in Fig 11. Above the street canyon, 308 the ejections dominate regardless of the stability. At the roof level, the contributions from both 309 quadrants are roughly equal, while sweeps contribute slightly higher, which is in accordance with 310 the findings from field measurement of the urban roughness sublayer turbulence (Christen et al., 311 2007) and other numerical studies (Coceal et al., 2007; Cheng and Liu, 2011a) under neutral 312 stratifications. It is evident that, generally, near the leeward wall the ejections (Q1) dominate, 313 while near the windward wall the sweeps (Q3) dominate, corresponding to the updraft of 314 polluted air and the downdraft of fresh air, respectively. With the increasing R_i , the dominance 315 of Q1 near the leeward wall becomes weaker. 316

Another important phenomenon observed from Fig. 11 is that, under neutral stratifica-317 tion, there is a region near the leeward corner where Q3 (sweeps) dominates. This region 318 greatly shrinks under unstable stratifications, since the buoyancy enhances the vertical motion 319 there and makes the pollutant transport there much more efficient (see Fig. 8b). Under stable 320 stratifications, this region surprisingly shrinks compared with that under neutral stratification, 321 while we would expect this region to expand due to the reduced pollutant transport by negative 322 buoyancy. Although ejections near the leeward wall seem to dominate under stable stratifica-323 tions (Fig. 11c and d), the corresponding pollutant fluxes there are negative (see Fig. 8c and 324 d), indicating neither ejections nor sweeps dominate there. To explain these seemingly strange 325 observations, a further check of the ratio of contribution from Q1 and Q4 is performed (Fig. 12) 326 for Ri = 0.188. It is evident that, near the leeward wall, the magnitude of Q1 is much lower 327

than that of Q4 (unorganized motions, indicating that flow carries high-concentration pollutant downward, due to the lower-than-average vertical velocity), which actually dominates turbulent pollutant transport there. This signifies that stable stratifications have greatly modified the mechanism of the pollutant transport within the street canyon, resulting in a much worse dispersion efficiency.

333 4.4. Scalar transfer coefficients

The scalar fluxes from the street canyon are important quantities for the transfer processes 334 between the urban canopy layer and the overlying atmosphere. Mesoscale models or models 335 of urban energy balance require the parameterization of these transfer processes. Therefore, 336 many laboratory and numerical studies have been performed to quantify these processes. If 337 the spatio-temporal average of the scalar flux at the roof level is F and the "strength" of the 338 source is C_s (this can be temperature for heat flux and concentration for pollutant flux), and 339 the ambient (background) "strength" of the scalar is assumed to be zero, the transfer coefficient 340 is then defined as (Barlow et al., 2004; Cai et al., 2008; Cheng and Liu, 2011a) 341

$$\Phi = F/(UC_s). \tag{11}$$

³⁴² The exchange velocity is defined as

$$w_T = F/C_s. \tag{12}$$

When F is heat flux and C_s is surface temperature, Φ is often referred to as the Stanton number, 343 St, in the engineering community. Note that here the transfer coefficient is defined for either 344 the air within the street canyon or for a specific facet of the street canyon (e.g., walls, street, 345 and roofs). The scalar emitted from a facet will first be transferred into the air within the street 346 canyon and then be transferred into the RSL. Therefore, three kinds of transfer coefficients can 347 be defined (see, e. g., Cai, 2012): (i) between the RSL and a facet, Φ_{B0} ; (ii) between the RSL 348 and the canyon air, Φ_{BC} ; and (iii) between a facet and the canyon air, Φ_{0C} . Furthermore, F 349 can be split into parts due to advection and turbulence 350

$$F^{\text{total}} = F^{\text{adv}} + F^{\text{turb}},\tag{13}$$

and Φ can also be defined for each part. Previous studies have shown that the transfer coefficients and exchange velocities depend on the urban geometry (e. g., aspect ratio h/b), locations of sources, and atmospheric stability.

Figure 13 shows the transfer coefficients of the passive pollutant from a line source at the street level. Apparently the advective parts of the transfer coefficients are close to 0 for all Ri for both Φ_{B0} and Φ_{BC} . In addition, Φ_{B0} is generally two orders of magnitude lower than Φ_{BC} , indicating the bottleneck of transfer from the facet to the overlying atmosphere lies in the transfer between the facet and the urban canyon air. Both Φ_{B0} and Φ_{BC} decrease with increasing Ri, with Φ_{BC} declining faster than Φ_{B0} .

Figure 14 shows the transfer coefficients of the active heat (i. e., the heat will interact 360 with and change the flow field, rather than just following the flow field like a passive scalar, 361 e. g., pollutant) from an area source at the street level. Again the transfer due to advection 362 is close to 0 and the transfer due to turbulence overwhelmingly dominates. The most evident 363 difference between Figs. 14 and 13 is that Φ_{B0} for heat is approximately one order of magnitude 364 lower than Φ_{BC} . This shows that the transfer of an active, area source is much more efficient 365 than that of a passive, line source. With increasing R_i , both Φ_{B0} and Φ_{BC} decrease drastically, 366 showing the strong impact of stability on heat transfer. 367

368 5. Conclusions

In the present study, a validated large-eddy simulation (LES) code was employed to study the effect of atmospheric stability on the dispersion characteristics within the roughness sublayer (RSL). Four cases with different Richardson numbers, Ri = -0.1, 0, 0.1, 0.188 were investigated with very high spatio-temporal resolutions in order to better resolve the small turbulent eddies in stably stratified RSL.

The major effects of stably stratified atmosphere on the flow and dispersion can be summarized as follows.

The magnitudes of the mean streamwise and vertical velocities within the urban street canyon are lowered. The updraft near the leeward wall and downdraft near the windward wall are both reduced, as well as the reversed flow in the lower half of the street canyon. A stagnant area emerges near the street level, and seems decoupled from the main vortex.

- Under stable stratifications, the vertical gradient of mean temperature near the roof level is much smaller compared with that under unstable stratification. The calculated heat transfer coefficient decreases drastically with increasing stability.
- As a result of the marked changes of flow and turbulence characteristics, the pollutant dispersion exhibits evident differences from that under neutral or unstable stratifications.
 The pollutant emitted from the street level 'pools' within the lower street canyon, with

about half of the pollutant mass trapped in the lower 15% street at a Richardson number (Ri) 0.188.

• The pollutant concentration flux near the leeward wall becomes negative due to the reduced updraft there. Further quadrant analysis of pollutant concentration flux shows that the dominant mechanism for pollutant transport within the street canyon has changed from ejections (flow carries high-concentration pollutant upward) to unorganized motions (flow carries high-concentration pollutant downward), which causes the much lower dispersion efficiency under stable stratifications.

In summary, the various quantities investigated in this study all pointed to the low efficiency and changing dispersion mechanism under stable stratifications. It was shown that the exchange between the RSL and urban street canyons is strongly dependent on the atmospheric stability. The high near-surface pollutant concentration within street canyons under stable stratifications will increase pedestrians' exposure and exacerbate health issues.

It is worthy noting that the present study simulates the urban flow and dispersion using a 399 low-Reynolds-number model with smooth urban facets, which is different from the realistic sce-400 narios (higher Reynolds number with rough urban facets). While the upscaling of the simulated 401 flow and turbulence characteristics to realistic scenarios is guaranteed by the higher Reynolds 402 number than a critical Reynolds number, the upscaling of simulated scalars (temperature and 403 pollutant concentration) is not well understood yet. In addition, the passive scalar emitted at 404 the road surface is fundamentally different from a real traffic source due to an existing laminar 405 viscous layer between the road surface and the air in the street canyon, which causes a ?bottle-406 neck of transfer? of the pollutant. Therefore, cautions should be taken when interpreting real 407 situations in urban areas according to the model results. 408

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Ri	Average pollutant	
	Whole canyon	Lower 15% canyon
-0.1	45.6	10.1
0	89.5	19.6
0.1	145.8	59.6
0.188	187.3	90.0

Table 1: The time-averaged pollutant mass $\int <\bar{c}>U/Q\,dxdz$ within the street canyon.

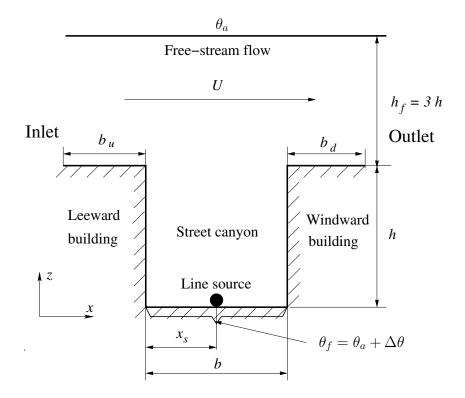


Figure 1: Schematic diagram of computational domain for the flow and pollutant transport in a street canyon.

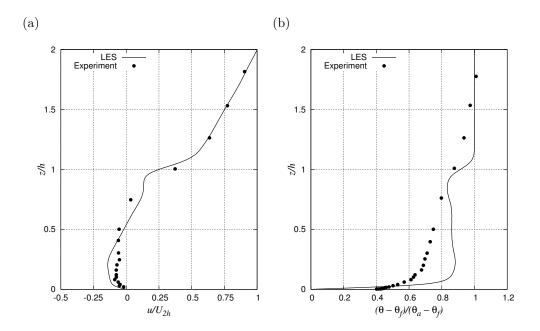


Figure 2: Vertical profiles of normalized (a) average streamwise velocity magnitude $\langle \overline{u} \rangle /U_{2h}$ and (b) temperature ($\langle \overline{\theta} \rangle -\theta_f$)/($\theta_a - \theta_f$) along the vertical centreline of the street canyon of aspect ratio 1, where U_{2h} is the average streamwise velocity at z = 2h. The experimental data of Uehara et al. (2000) was at Rb = 0.43 and the current LES results are at Rb = 0.33.

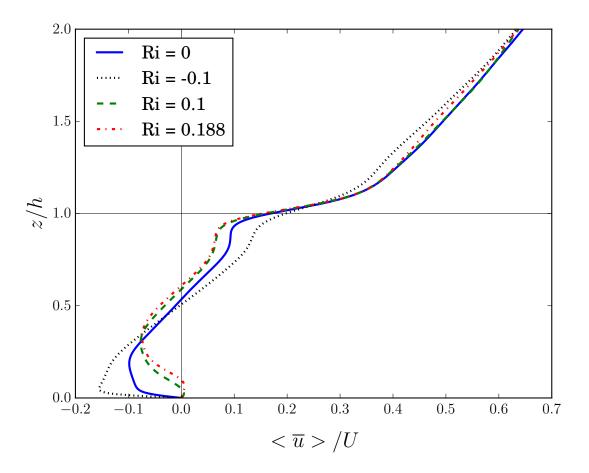


Figure 3: The normalized streamwise velocity in the centerline of the street canyon under different stratifications.

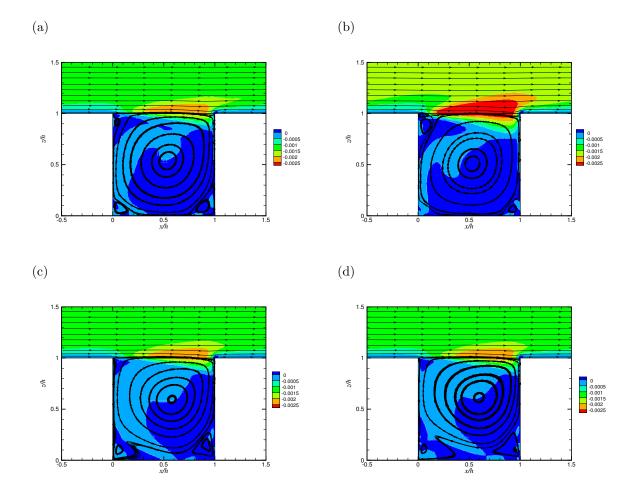


Figure 4: Streamline and normalized Reynolds stress $\langle u'w' \rangle /U^2$. Ri = (a) 0; (b) -0.1; (c) 0.1; and (d) 0.188.

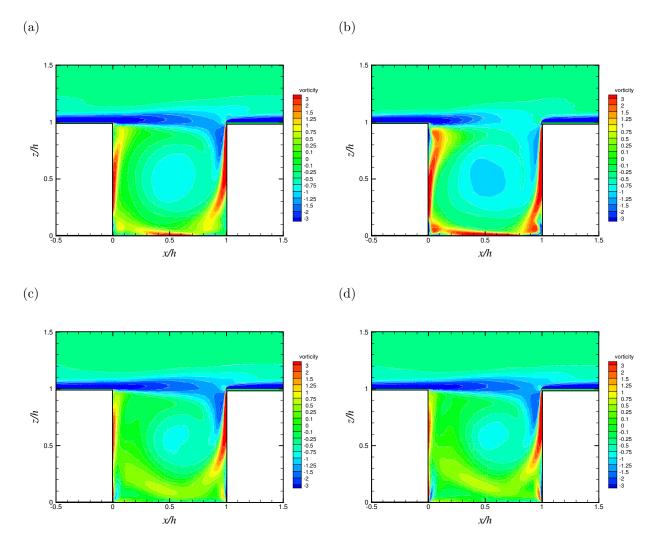
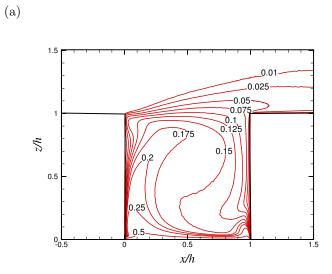
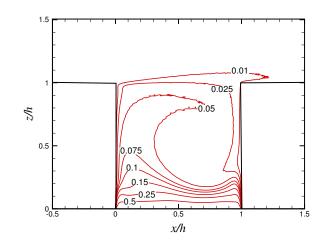


Figure 5: Normalized spanwise vorticity ω_y . Ri = (a) 0; (b) -0.1; (c) 0.1; and (d) 0.188.









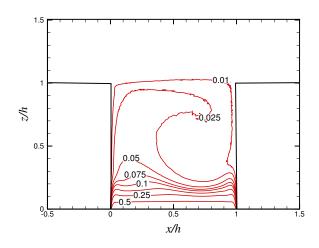


Figure 6: Normalized mean temperature $(\langle \overline{\theta} \rangle - \theta_a)/(\theta_f - \theta_a)$. Ri: (a) -0.1; (b) 0.1; (c) 0.188.

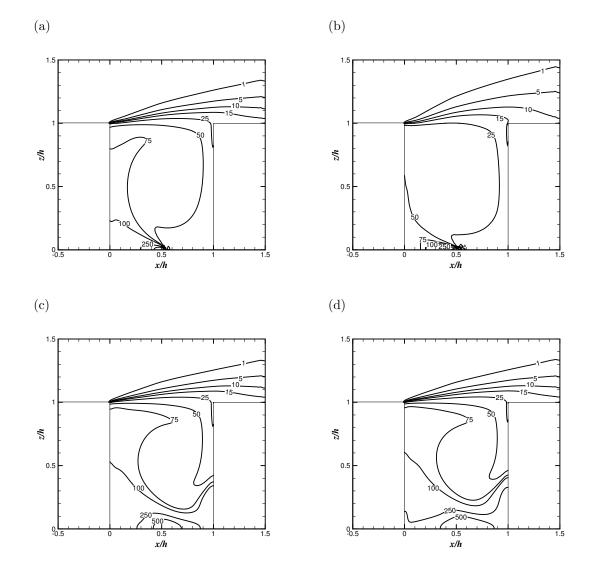


Figure 7: Dimensionless pollutant concentration $\langle \overline{c} \rangle UhL/Q$. Ri = (a) 0; (b) -0.1; (c) 0.1; and (d) 0.188.

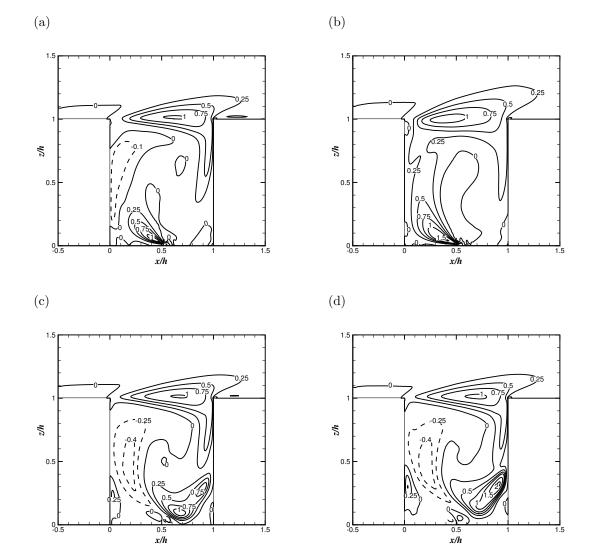


Figure 8: Dimensionless pollutant flux $\langle w'c' \rangle hL/Q$. Ri = (a) 0; (b) -0.1; (c) 0.1; and (d) 0.188.

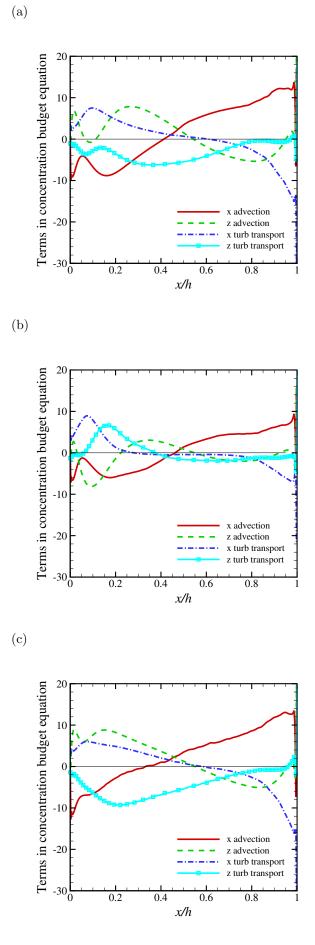


Figure 9: Horizontal distribution of the terms in the normalized pollutant concentration budget equation (10) along the roof level. Ri: (a) 0; (b) -0.1; (c) 0.1.

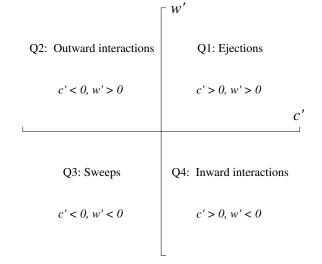


Figure 10: The schematic definitions of quadrants for turbulent pollutant flux.

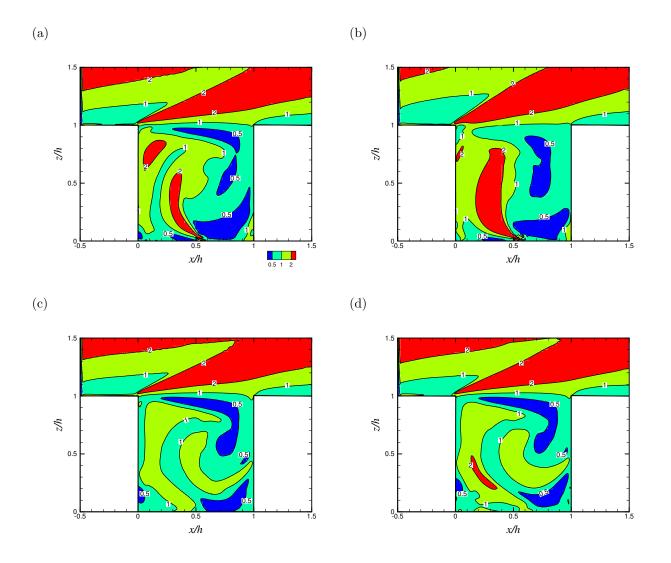


Figure 11: The ratio of pollutant flux contribution from ejections (Q1) and sweeps (Q3). Ri = (a) 0; (b) -0.1; (c) 0.1; and (d) 0.188.

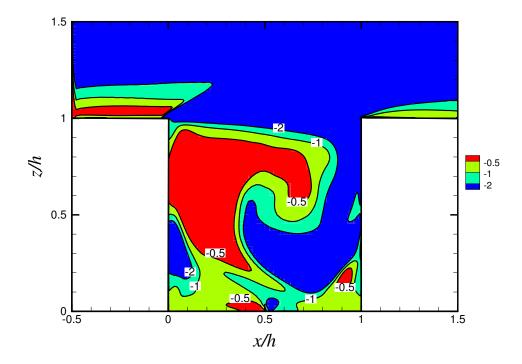


Figure 12: The ratio of pollutant flux contribution from ejections (Q1) and inward interactions (Q4) for Ri = 0.188.

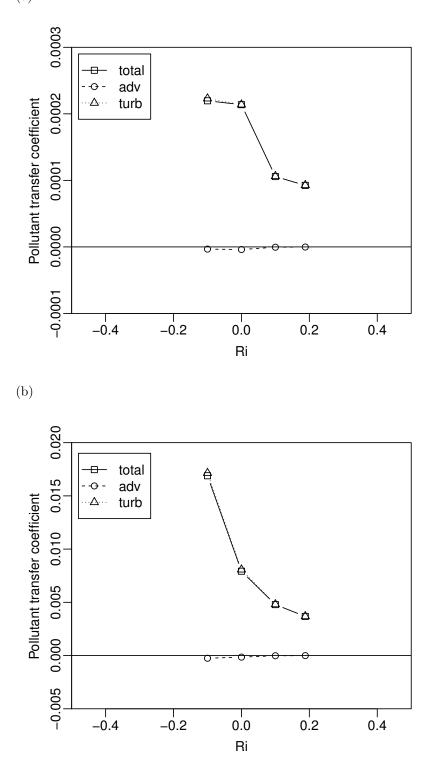


Figure 13: The normalized pollutant (passive, line scalar source) transfer coefficients by mean flow, turbulence, and in total between the RSL and (a) the street ground Φ_{B0} ; (b) the canyon air Φ_{BC} under different stratifications.

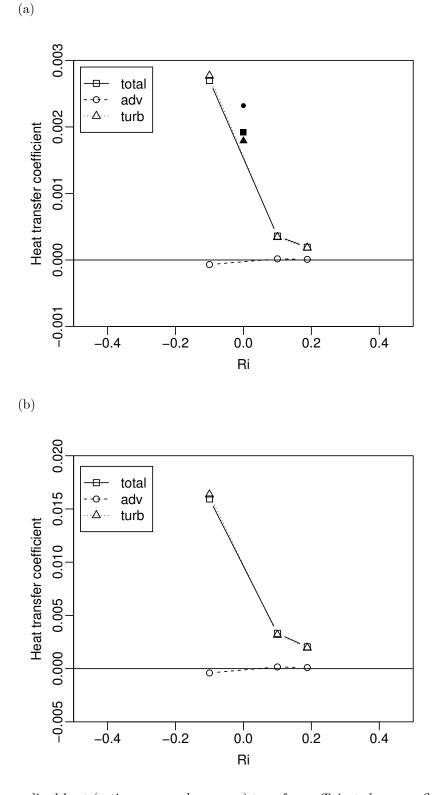


Figure 14: The normalized heat (active, area scalar source) transfer coefficients by mean flow, turbulence, and in total between the RSL and (a) the street ground Φ_{B0} ; (b) the canyon air Φ_{BC} under different stratifications. Also shown are the transfer coefficient of a passive scalar (area source) under neutral stratification (Ri = 0) from wind tunnel (Barlow et al., 2004): filled square; LES (Cai et al., 2008): filled triangle; and LES (Cheng and Liu, 2011a): filled circle.