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Mechanical Engineering / Applied Mechanics and Energy conversion

Carbon Dioxide Transport in the Stable Boundary Layer over Heterogeneous Surfaces: A Large-Eddy Simulation Study

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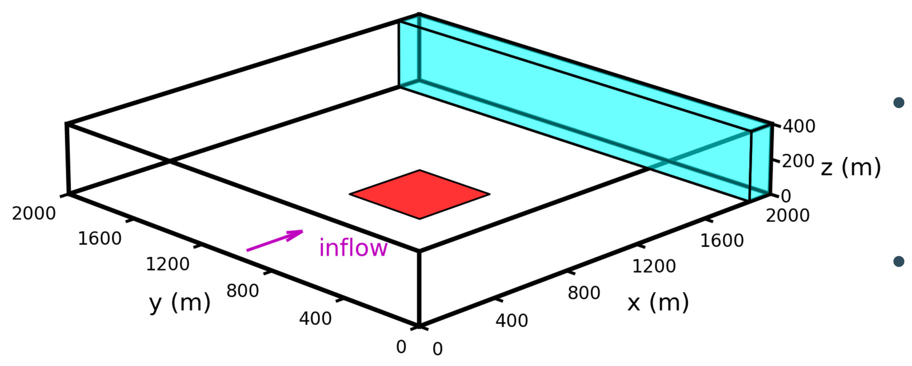
1. Introduction

- CO_2 fluxes in the nocturnal stable boundary layer are strongly influenced by surface heterogeneity
- Nine idealized LES cases are simulated to study the effects of thermal and flux heterogeneity
- Focus on dispersive motions and CO_2 budget closure

2. Numerical Aspect



- Stably stratified flow (≈ 2.2 K potential temperature difference)
- Heterogeneous surface patch (400 × 400 m²)
- Subject to atmospheric subsidence
- Concurrent precursor and fringe regions are applied

Simulated cases

$$T = \frac{T_{patch} - T_{ground}}{T_{top} - T_{ground}}$$

$$Q = \frac{Q_{patch}}{Q_{ground}}$$

Q / T	1	0.5	0.25
1	Q1T1	Q1T05	Q1T025
2	Q2T1	Q2T05	Q2T025
4	Q4T1	Q4T05	Q4T025

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

$$\frac{\partial \tilde{u}_i}{\partial t} = -\frac{\partial}{\partial x_j}\left(\tilde{u}_i\tilde{u}_j + \tau_{ij}^{sgs}\right) - \frac{\partial p^*}{\partial x_i} + f_c\epsilon_{ij3}\left(\tilde{u}_j - G\delta_{j1}\right) + \frac{g}{\theta_r}\left(\tilde{\theta}_\delta - \langle\tilde{\theta}_s\rangle\right)\delta_{i3}$$

$$\frac{\partial \tilde{\theta}_\delta}{\partial t} = -\frac{\partial}{\partial x_j}\left(\tilde{u}_i\tilde{\theta}_\delta + q_j^{sgs}\right) + \Gamma_w x_3 \frac{\partial\langle\tilde{\theta}_\delta\rangle}{x_3}$$

$$\frac{\partial \tilde{c}_\delta}{\partial t} = -\frac{\partial}{\partial x_j}\left(\tilde{u}_i\tilde{c}_\delta + q_{cj}^{sgs}\right) + \Gamma_w x_3 \frac{\partial\langle\tilde{c}_\delta\rangle}{x_3}$$

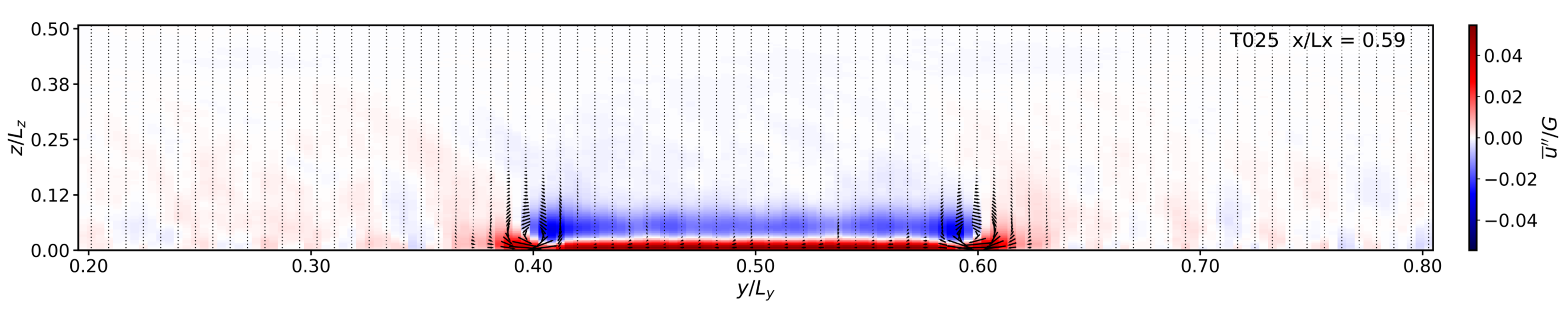
The Navier–Stokes and transport equations are solved using the SP-Wind solver

- In-house DNS/LES solver for atmospheric boundary layer flows
- Pseudo-spectral scheme in horizontal directions and 4th-order finite-difference scheme vertically
- Efficiently parallelized up to 10,000 CPUs on the high-performance infrastructure of the Flemish Supercomputer Center

3. Results

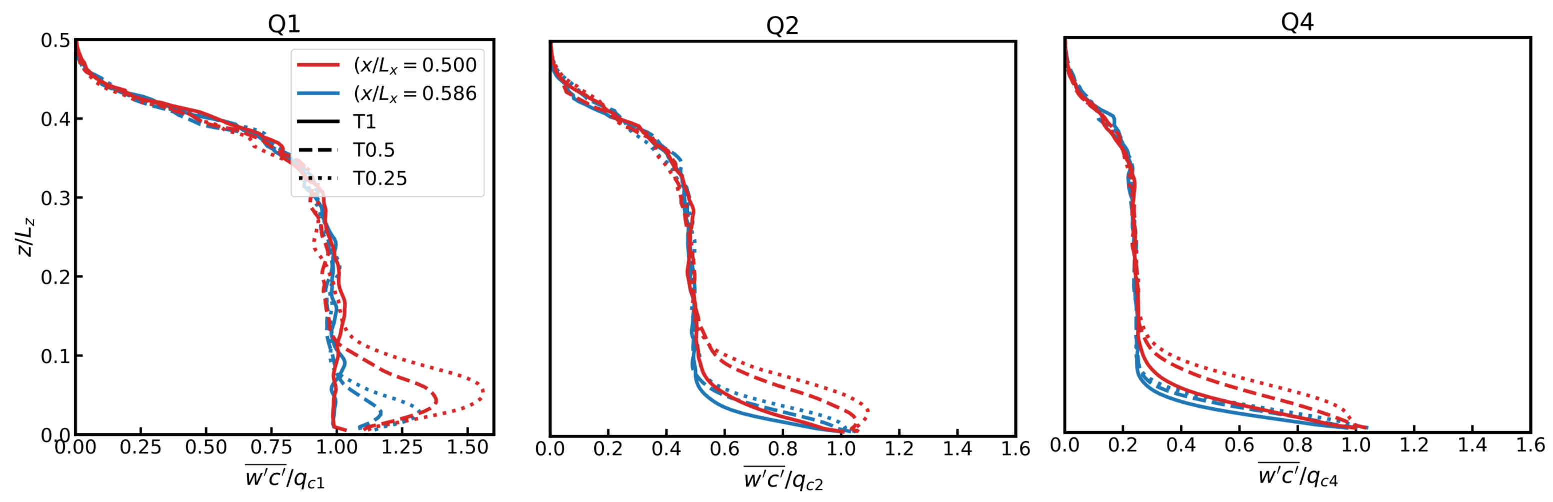
3.1 Dispersive velocities

$$\phi(x,y,z,t) = \langle\overline{\phi}\rangle(z) + \overline{\phi}''(x,y,z) + \phi'(x,y,z,t)$$



- Buoyancy effects at the edges generate swirls, resulting in LMP–HMP structures
- A second pair of LMPs-HMPs in vertical direction due to turbulent vertical momentum mixing

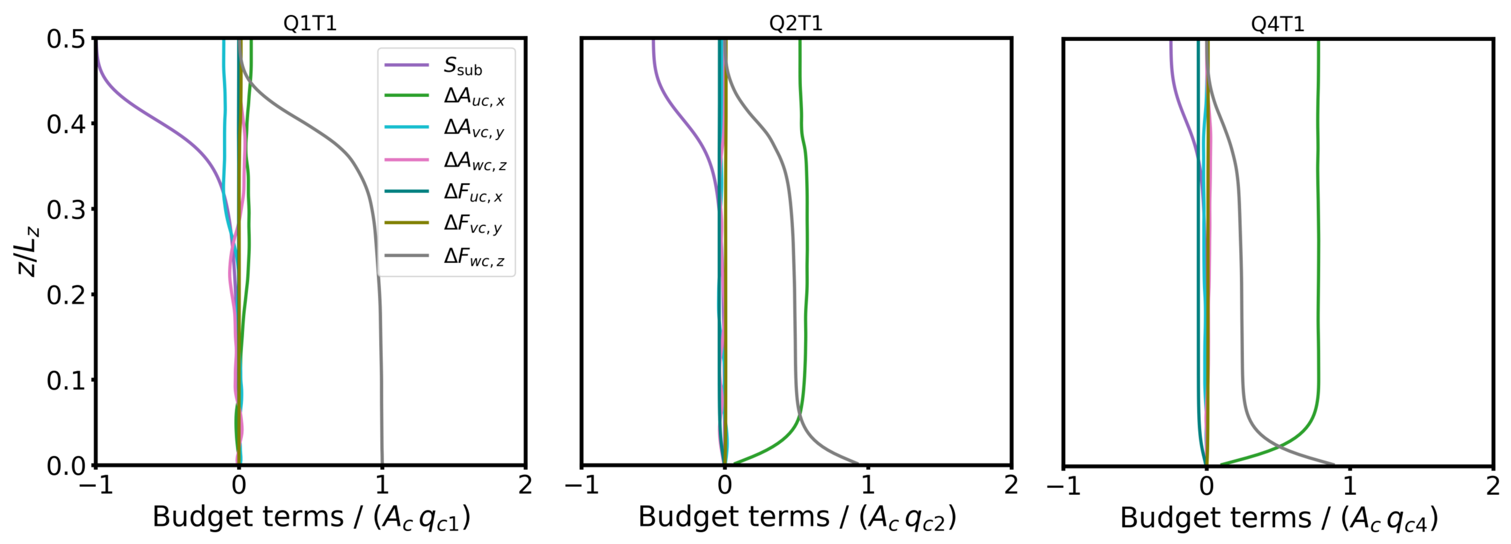
3.2 CO_2 turbulent vertical transport



- Both higher CO_2 flux and higher temperature increases vertical turbulent transport

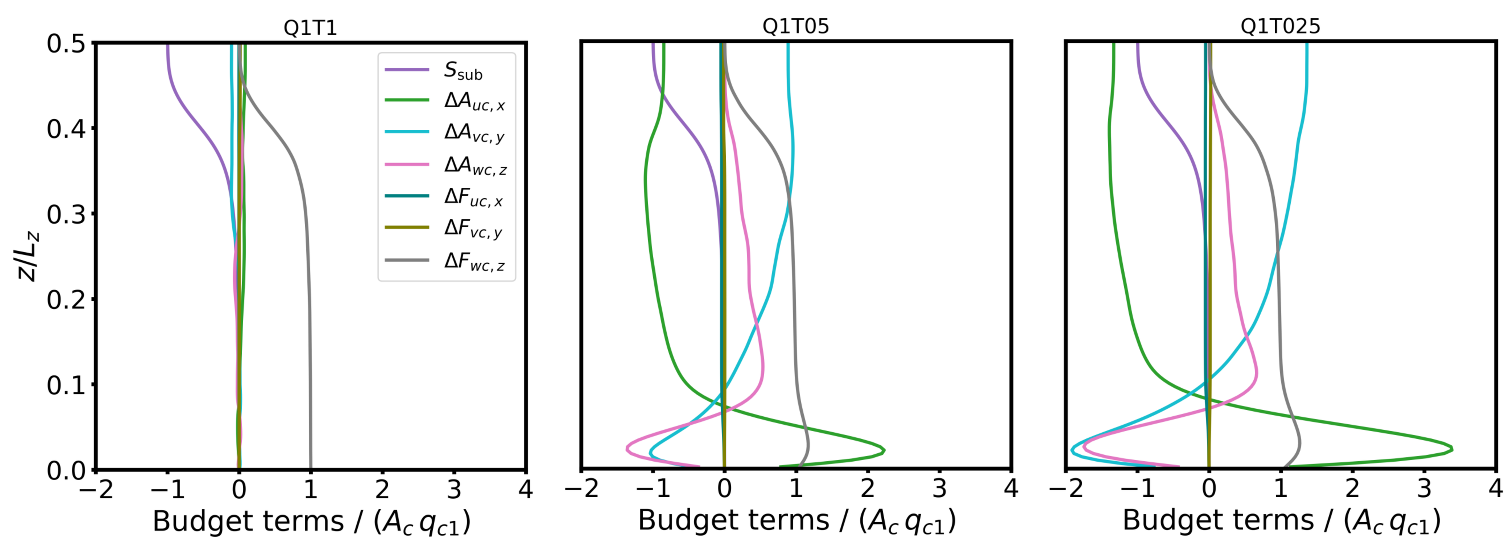
3.3 CO_2 Budget Analysis

3.3.1 Homogeneous T heterogeneous Q



- Under homogeneous condition, subsidence balances with vertical turbulent CO_2 transport
- When CO_2 flux is heterogeneous, balance is reached among subsidence, vertical turbulent transport and subsidence

3.3.2 Heterogeneous T homogeneous Q



- Heat-induced dispersive motions strongly alter local CO_2 balance components
- Clear edge effects when using control volumes right above the patch

4. Discussion

Surface heterogeneity reshapes CO_2 transport through coupled dispersive and turbulent processes, with their relative importance depending on thermal and flux contrasts.

However, Quantifying the relative contributions of dispersive and turbulent fluxes remains challenging. Case-by-case evaluation is needed under different atmospheric stability conditions.

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