

# Large eddy simulation and case study of reactive pollutant dispersion at a real intersection in downtown Montréal

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## SUMMARY

In order to fully characterize exposure risks to pollutants emitted by vehicles in a real-world scenario, we model their dispersion using highly detailed computational fluid dynamics (CFD) simulations of traffic conditions near the McGill University campus in downtown Montréal, Canada. We select a busy intersection often backed up with vehicles and significant amounts of pedestrian traffic. The CFD model includes important processes to the dispersion dynamics, including chemical reactions, vegetation and deposition effects, thermal effects, and vehicle induced turbulence. The large eddy simulations are validated with in-situ measurements of wind flow and concentrations of NO, NO<sub>2</sub>, O<sub>3</sub>, VOCs, PM<sub>2.5</sub>, CO, CO<sub>2</sub>, and CH<sub>4</sub>. The resulting distributions of pollutants and greenhouse gases are analyzed to identify the potential for hazardous air quality and characteristic dispersion patterns.

**Keywords:** *computational fluid dynamics, greenhouse gases, pollutant dispersion, air quality, vehicle emissions*

## 1. INTRODUCTION

Emissions of pollution and greenhouse gases (GHGs) from vehicles contribute significantly to hazardous air quality and anthropogenic climate change. Traffic-related air pollution includes nitrogen dioxide (NO<sub>2</sub>), volatile organic compounds (VOCs), particulate matter with diameter less than 2.5 μm (PM<sub>2.5</sub>), and carbon monoxide (CO), while further reactions in the atmosphere lead to the formation of ozone (O<sub>3</sub>). All of these, in high enough concentrations, have been linked to negative health outcomes in humans with long-term exposure, including mortality, heart disease, lung cancer, and the onset and worsening of asthma (Boogaard et al., 2022). Additionally, combustion of fossil fuels results in carbon dioxide (CO<sub>2</sub>) and methane (CH<sub>4</sub>) being emitted, two potent GHGs leading to anthropogenic climate change. Road transport is responsible for 15% of CO<sub>2</sub> emissions worldwide, representing a significant impact on the climate (Ritchie, 2020). Studying the dispersion patterns of these harmful species is critical in accurately separating background and local contributions and identifying exposure risks (Health Effects Institute, 2010).

This importance is even greater in cities and urban areas, which feature dense road networks and significant numbers of vehicles. Vehicle dispersion processes within urban streets are highly complex, as they are dependent on very local flow conditions, photochemical reactions, turbulence generated by moving vehicles, and buoyancy (Mei et al., 2023). These streets also often feature vegetation such as trees, which can both increase and decrease air quality (Salmond et al., 2013). Deposition onto vegetation, among other surfaces like buildings, serves as an important sink to these air pollutants. Due to the numerous factors impacting the dispersion of pollutants and GHGs, modeling their dispersion requires fully detailed simulations with high resolution. Computational fluid dynamics (CFD) with a large eddy simulation (LES) approach enables such an investigation.

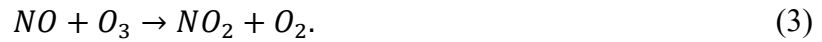
CFD, which is the process of solving the Navier-Stokes equations numerically, has many advantages over in-situ measurements or wind tunnel experiments, often being less expensive and allowing more control. Another significant advantage CFD provides is the ability to know field values at every point within a domain rather than at discrete measurement locations. CFD has already widely been used to study traffic pollutant dispersion. Early studies were often simplified to the case of a two-dimensional street canyon, which is a common feature found in cities of a road flanked on both sides by buildings. Baker et al. (2004) considered reactive pollutant dispersion of  $\text{NO}_x$  ( $\text{NO} + \text{NO}_2$ ) for such a case, using a LES approach. Kwak and Baik (2012) extended this to include VOC chemistry, showing reactions play a sizeable role in resulting pollutant concentrations. More recently, studies have moved to three-dimensional cases, however, most building geometries remain idealized. Crucial in any CFD study is the process of validating the model with actual measurements. Amorim et al. (2013) did so with a Reynolds-averaged Navier-Stokes CFD model of a real urban environment, including the effects of trees on dispersion. Their model found significant impact from the trees and high agreement between the predicted and measured concentrations. Still missing from the current literature using CFD to model traffic related pollutant dispersion is an LES model of a real, complex, urban environment, validated against in-situ measurements and including all important factors of detailed chemical reactions, buoyancy, vegetation and deposition effects, and vehicle induced turbulence. This study aims to do this for the case of a major street section in downtown Montréal, Canada, combining field measurements with CFD.

## **2. DATA AND METHODOLOGY**

The chosen measurement and modeling site is a 0.4 km section of Sherbrooke Street West, between Peel Street and University Street. This road frequently experiences heavy traffic, with vehicles often backed up at the multiple traffic lights along it. Being in the downtown of Montréal, many people walk within this area and are exposed to the dangerous vehicle emissions. This street section is also directly adjacent to the McGill University campus, which features an outdoor green space where students gather. For these reasons, it is an ideal case study location to analyze in detail the dispersion dynamics of traffic emissions and impacts on air quality.

Measurements were taken from 08:00–09:00 am local time on the day of 10 February 2026, which featured moderate winds and stable conditions. In the winter, temperature inversions are often present, which increase surface concentrations of harmful pollutants. A radiosonde launched upwind of the study area provided a profile of atmospheric conditions used to initialize the CFD model. Near the four streets within the region of interest (Sherbrooke Street West, Metcalfe Street, Rue Mansfield, and McGill College Avenue), three cameras were positioned to record the number and type of vehicles driving on each street to accurately model emission rates. The morning hour chosen represents the period of heaviest traffic congestion because of commuting.  $\text{NO}_x$ ,  $\text{O}_3$ , VOCs,  $\text{PM}_{2.5}$ ,  $\text{CO}$ ,  $\text{CO}_2$ , and  $\text{CH}_4$  were monitored at various locations along the street. At the main entrance to McGill University, a meteorological station was positioned to record near-surface wind velocities. Within the McGill University campus, a Doppler lidar measured wind profiles from atop Burnside Hall, which also was the location of a Picarro GasScouter recording concentrations of  $\text{CO}_2$  and  $\text{CH}_4$ . Finally, a weather station at the McTavish reservoir served as additional wind velocity validation.

Simulations of this period were carried out using the open-source CFD software OpenFOAM, with mesh generation performed by the utility SnappyHexMesh. A fully detailed computational domain including terrain, building geometries, and important vegetation was created, with the explicitly modeled features extending 0.4 km along Sherbrooke Street West and 0.7 km perpendicular (Figure 1). The full computational domain was constructed as a cylinder 4 km in diameter to account for varying wind directions and best practice guidelines specifying between buildings and boundaries (Franke et al., 2007). The compressible LES solver reactingFoam was selected to simulate the turbulent flow with thermal effects and chemical reactions, while the Smagorinsky subgrid scale model was used to achieve closure. The inlet profile of wind characteristics was assigned using the measurements of the upper air sounding. Vehicle emissions are modeled as line sources along the three roads, with emission rates calculated using the number and type of vehicles present at the time. Additional turbulence source terms are added in the street regions to model the effects of vehicle induced turbulence. The most important series of chemical reactions which traffic-related air pollution undergoes is the  $\text{NO}_x\text{-O}_3$  photochemical reaction (Baker et al., 2004):



This process is further affected by VOCs, with these chemical reactions accounted for in a coupled chemical mechanism model. Additionally, a vegetation model is included to include the impact on wind flow and deposition processes.

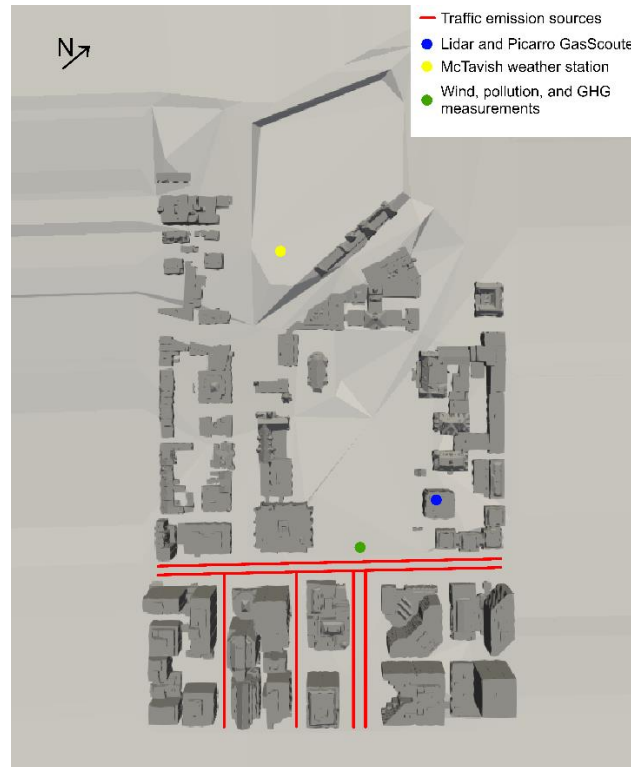


Figure 1: Section of computational domain with explicitly modeled buildings and measurement locations marked.

### 3. RESULTS AND DISCUSSION

First, the model's predictions of instantaneous and mean wind speed and direction are compared with the three wind velocity sensors. With the model's flow field validated, local wind conditions are investigated with a focus on the impacts on dispersion dynamics and air quality. Predicted concentrations of NO, NO<sub>2</sub>, O<sub>3</sub>, VOCs, PM<sub>2.5</sub>, CO, CO<sub>2</sub>, and CH<sub>4</sub> are then validated against measurements from the various instruments. The level of agreement between the modeled and measured concentrations of CO<sub>2</sub> points to the large contribution of vehicle emissions to overall GHG emissions in this downtown region. Locations of hazardous concentrations of various air pollutants are identified, with implications for pedestrians travelling within the area. The individual effects of each component of the model (chemical reactions, vegetation and deposition, buoyancy, and vehicle induced turbulence) on resulting distributions of pollution and GHGs are assessed. In the end, this model serves as one of the first neighborhood block-scale LES simulations of vehicle-related pollutant and GHG dispersion including multiple complex processes. With a study such as this, it is possible to estimate detailed exposure levels to traffic-related air pollution for use in risk assessment. It also allows for better attribution of city-scale GHG emissions and separation of background and local concentrations of both GHGs and pollution.

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