Street Canyon Atmospheric Composition: Coupling Dynamics and Chemistry

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1) Background

Atmospheric composition within urban street canyons (**Figure 1**), has a direct effect on the air quality of the environment in which a majority of people live and work. The study of atmospheric composition on the street canyon scale is important as increased vehicle emissions combined with poor ventilation can cause the build up of pollutants to levels that can have serious implications for health, vegetation and building materials (Vardoulakis *et al.*, 2003).

The composition of air within the street canyon is determined by:

1) **Background air mixed in from above the canyon**
2) **Advection of air into and out of the canyon**
3) **Vehicle and other emissions from within the street**
4) **Mixing and chemical processing of pollutants within the canyon**

At Birmingham a **Large Eddy Simulation (LES) model** has been developed that can accurately simulate the atmospheric motion and mixing, which result from background air flowing over a street canyon, and the chemical interactions between the various species present.

Figure 1: A typical street canyon formed by a road running between two rows of buildings.

2) Research Aims and Objectives

The main aim of this research is to develop the existing LES model by adding a more detailed chemical reaction scheme. A number of key questions relating to atmospheric composition can then be addressed using the enhanced model, for example:

- How different is the air quality in the street canyon from the overlying, background atmosphere? How does this depend upon the dynamics?
- To what extent are pollutants processed within street canyons before they escape to the wider atmosphere?
- What variability in pollutant levels is expected across a street canyon (e.g. comparing concentration at points A, B and C in **Figure 6a**). How do pollutant levels vary with time?
- What are the short term (second by second) pollutant levels experienced within street canyons?
- What are the potential impacts of emissions of nitrous acid (HONO) from traffic?
- How does changing the canyon geometry and characteristics affect the dispersion of pollutants?

3) Methodology

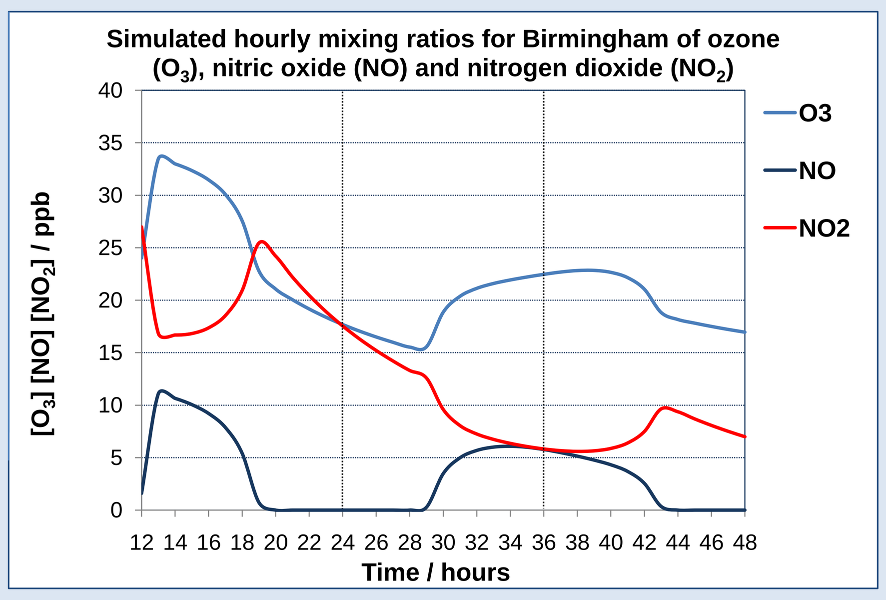
Chemistry

The Master Chemical Mechanism (MCM) is a near explicit chemical mechanism describing the degradation of 135 volatile organic compounds (VOCs). The MCM is too large to incorporate into the LES i.e. it is too computationally expensive. A "reduced" scheme must designed based on a subset of the MCM by reducing the number of species and reactions included.

Initially, a methane only mechanism was used within a box model to study changes in atmospheric composition (**Figure 2**).

In order to design the reduced chemical scheme, the Common Representative Intermediates Mechanism, CRI v2 –R5 which uses 19 non-methane VOCs to represent organic speciation will be evaluated and reduced further by removing unnecessary species and night time reactions (Watson *et al.*, 2008).The finalised scheme will then be applied to the box model and subsequently to the LES.

Figure 2



Box Model

A zero-dimensional box model of atmospheric chemistry (**Figure 3**) will be used to investigate chemical changes and a number of 'emission scenarios' that could be applied to the LES. The equation governing the change in concentration of species within the box over time is given below with each term in the equation numbered:

$$\frac{dC}{dt} = \frac{q}{h} + R - \frac{v_d}{h}C + \frac{u}{l}(C_b - C) + \frac{\omega_t}{h}(C_b - C)$$

1 2 3 4 5

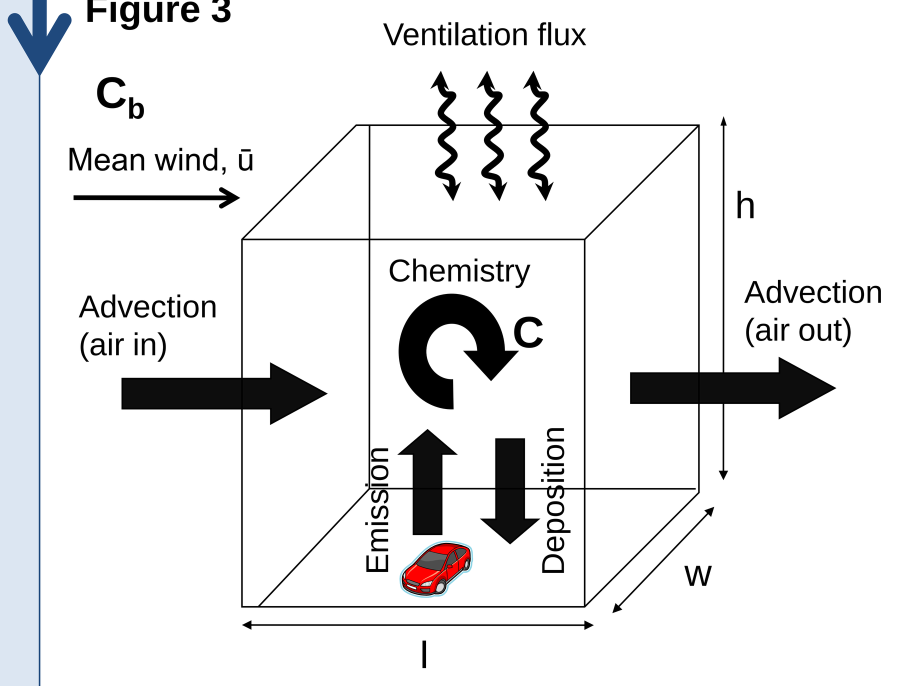
1) Emission term: q is the amount emitted per unit time and surface of the box (e.g. molecules $cm^{-2}\,s^{-1}$)

2) Reaction term: R is the net term of the reactions of production and consumption of species

3) Deposition term: represents the deposition of species within the box and is proportional to concentration

4) Advection term**:** represents the transport of species into the box from the surrounding environment and the transport of species out of the box

Figure 3



C is the concentration of atmospheric species within the box
C_b represents background concentration of species

5) Ventilation term: represents the exchange of air from within the box with air above the box

Assumptions:

- Air in box is well mixed
- Pollutant concentrations are homogeneous, therefore a function of time alone: C(t)
- Source of emissions is uniformly distributed
- Emissions mixed instantaneously

Emissions

Pollutant emissions in urban areas are primarily dominated by traffic (Vardoulakis *et al.*, 2003). Vehicle emissions are calculated using vehicle speed emission factors and vehicle fleet composition data taken from the National Atmospheric Emissions Inventory (NAEI).
Emissions (gkm^{-1}hr^{-1}) = Emissions Factor (gkm^{-1}veh^{-1}) x Activity (Volume of traffic (vehicles hr^{-1}))

Transport Emission Factors Representing the National Vehicle Fleet- 2009					
Vehicle type	NO_x / g km^{-1}	CO / g km^{-1}	Benzene / g km^{-1}	1,3 Butadiene / g km^{-1}	HC / g km^{-1}
Petrol Cars	0.1885	1.1723	0.0028	0.0014	0.119
Diesel Cars	0.4132	0.1571	0.0007	0.0004	0.044
Petrol LGVs	3.3500	0.6626	0.0015	0.0005	0.049
Diesel LGVs	0.6327	0.2946	0.0016	0.0008	0.081
Rigid HGVs	3.7543	0.7255	0.0002	0.0098	0.314
Arctic HGVs	8.0703	1.9388	0.0005	0.0251	0.842
Buses	4.4046	0.7343	0.0002	0.0074	0.257
All types	0.4862	0.9212	0.0023	0.0016	0.114

Figure 4

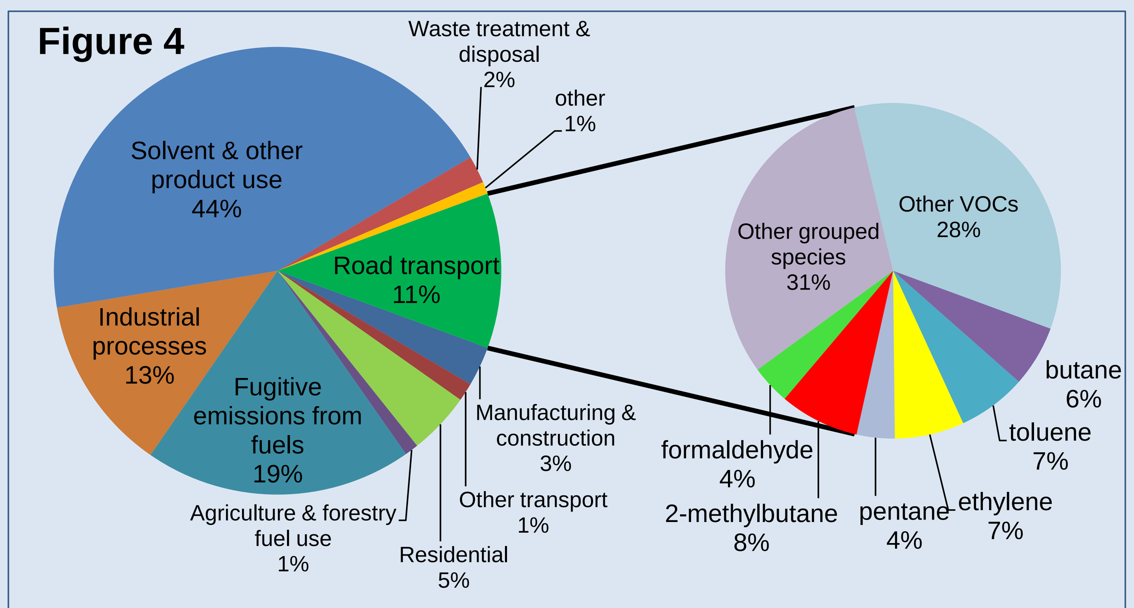


Figure 4: Sources of VOCs with species emitted from road transport 2006 Data: Department for Environment , Food and Rural Affairs (DEFRA), 2008

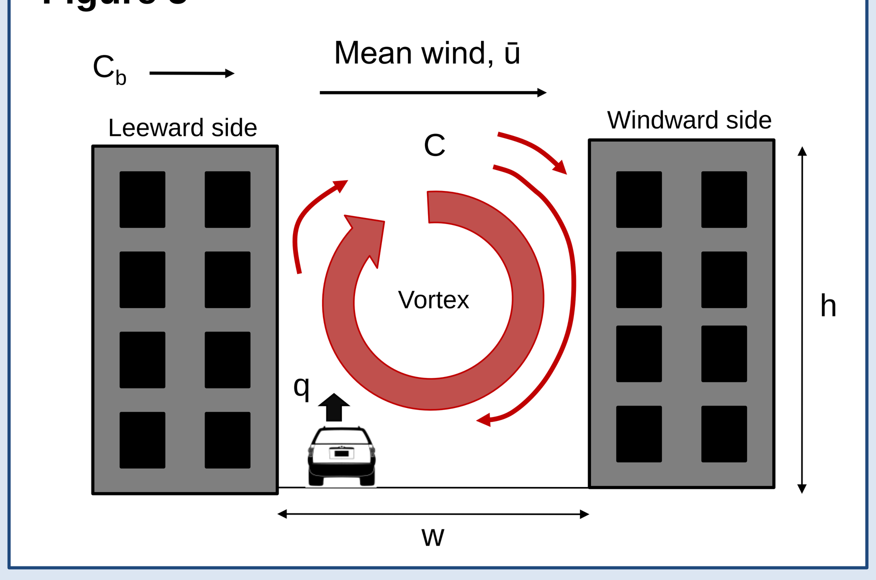
- q obtained by converting emissions in gcm^{-1}s^{-1} into molecules cm^{-1}s^{-1}, using molar mass of each pollutant and distance travelled by each car.
- Hydrocarbons (HCs) are total Volatile Organic Compounds (VOCs)- various sources (**Figure 4**).
- Most important VOCs to be included dependant on mass, Photochemical Ozone Creation Potential (POCP) and OH reactivity. Most abundant VOC is 2-methylbutane (**Figure 4**).

Canyon Dynamics and LES Modelling

Where canyon aspect ratio (h/w) ≈ 1, skimming flow is observed (**Figure 5**). Skimming flow, characterised by a single canyon vortex (Oke, 1987), gives a low level of ventilation and is relatively ineffective in removing pollution.

Pollutant dispersion within the canyon is dependent on the rate at which the street exchanges air vertically with the above roof level atmosphere and laterally with connecting streets (Vardoulakis *et al*., 2003). Ventilation of air in the box model is dependent on transfer velocity, ω_t. For h/w ≈ 1, $\omega_t \approx 0.0015 {*} U_{ref}$ (Cai *et al*., 2008). Using:

Figure 5



$$\bar{u} = U_{ref}\left(\frac{z}{z_{ref}}\right)^{0.25} \quad \text{where } \bar{u} = 5\ ms^{-1}:\ u_{ref} \approx 9\ ms^{-1} \therefore \omega_t \approx 0.0135\ ms^{-1}$$

LES has been previously used to investigate the dispersion and chemical reaction of NO_x and ozone and also the effects of shading on pollutant concentrations (Grawe *et al*., 2007). After incorporating the reduced chemical scheme into the LES, the transport and chemical reaction of species within and above the canyon will be studied. The enhanced model will provide a powerful tool to observe the effects of mixing and chemical processing on atmospheric composition.

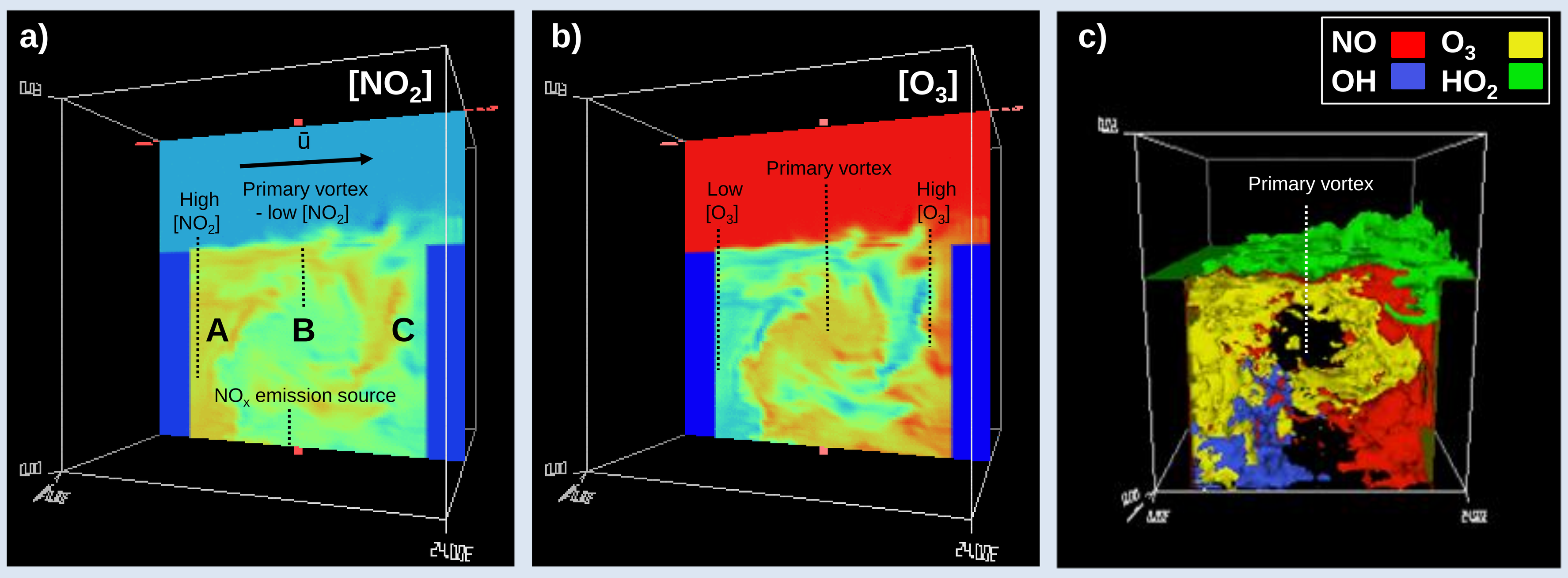


Figure 6: Variation in concentrations of a) NO_2 , b) O_3, and c) Iso-surfaces of several chemical species within the canyon cavity obtained using output from the LES

4) Further Work

- Design reduced chemical scheme using box model
- Add background concentrations, advection and ventilation to box model
- Investigate chemical changes (e.g. emission rates) and develop various emission scenarios
- Begin to address various questions relating to urban atmospheric composition using finalised model.

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MCM - The Master Chemical Mechanism v3.1 - http://mcm.leeds.ac.uk/MCM/; NAEI - Data warehouse - http://www.naei.org.uk/data_warehouse.php

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