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A GLOBAL SENSITIVITY STUDY OF PREDICTED NO_2 CONCENTRATIONS IN AN URBAN STREET CANYON

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Abstract: The prediction of NO_2 concentrations ($[NO_2]$) within a street canyon involves the coupling of several complex processes: traffic emissions under different levels of congestion; dispersion via turbulent mixing; chemical processes of relevance at the street scale. This paper presents an analysis of $[NO_2]$ predictions from such a complex modelling system applied to a street canyon within the city of York, UK. The model system consists of a micro-scale traffic simulation and emissions model, a Reynolds Averaged turbulent flow model coupled to a reactive Lagrangian particle dispersion model. In particular the analysis focuses on the sensitivity of predicted $[NO_2]$ at different locations in the street to uncertainties in the model inputs. These include physical characteristics such as background wind direction, temperature and background ozone concentrations; traffic parameters such as overall demand and primary NO_2 fraction in the exhaust; as well as model parametrisations such as roughness lengths, turbulent time and length scales and chemical reaction rates. The sensitivity analysis was performed using a global sensitivity method based on random sampling high dimensional model representations (RS-HDMR). Nonlinear responses to parameter changes and parameter interactions could therefore be shown. Predicted $[NO_2]$ was shown to be relatively robust with respect to model parametrisations, although there were significant sensitivities to the activation energy for the reaction $NO+O_3$ as well as the canyon wall roughness length. Under off-peak traffic conditions, demand was the key traffic parameter. Under peak conditions where the network saturates, road-side $[NO_2]$ was relatively insensitive to changes in demand and more sensitive to the primary NO_2 fraction. The most important physical parameter was found to be the background wind direction, which with an input uncertainty of only 20°, could contribute to over 40% of the variance in predicted $[NO_2]$. The study highlights the key parameters required for reliable $[NO_2]$ estimations and suggests that accurate reference measurements for wind direction should be a critical part of air quality assessments for street canyon locations.

Key words: *street canyon, dispersion model, primary NO_2, sensitivity analysis, HDMR, wind direction*

INTRODUCTION

Although European directives to reduce NOx emissions from vehicles have been in operation for over a decade, many urban areas across Europe are still failing to meet the NO_2 air quality standards set by the EU First Daughter Directive. Within the UK there are a large number of Air Quality Management (AQM) Areas which have been declared on the basis of NO_2, a large proportion of which are in highly trafficked urban areas. Strategies must therefore be put in place to address potential reductions in NO_2 concentrations, particularly focussed on traffic sources. To aid in this AQM process, models can be developed which aim to predict roadside NO_2 as a function of important features of the urban environment such as traffic characteristics, wind speed and direction and street topology. The latter feature should be included since it is well understood that urban buildings interact with background winds to modify the turbulent flow structures within the street network, often restricting the dispersion of traffic related pollutants (Boddy *et al.*, 2005, Tomlin *et al.*, 2009). A number of computational fluid dynamics (CFD) approaches have been developed which address dispersion phenomena within street canyon environments (Ketzel *et al.*, 2000, Dixon *et al.*, 2006). Few models however, have attempted to couple this modelling of dispersion at the micro-scale with high resolution traffic emissions models and chemical transformation processes. The current work aims to present such an integrated system which couples a micro-scale traffic emissions model with a turbulent reactive dispersion model based on a combined CFD and reactive Lagrangian particle dispersion approach (Dixon and Tomlin, 2007, Ziehn *et al.*, 2009). The use of such models within the AQM framework requires understanding the confidence that can be placed in their predictions. Lack of confidence, or uncertainty, can result from a lack of detailed knowledge of the model parameterisations. It follows that model evaluation will benefit from the inclusion of sensitivity studies that highlight the impact of uncertain input parameters on predicted output concentrations. The use of Reynolds Averaged models in particular has raised questions as to their suitability for accurately describing turbulent chemical interactions when they contain only averaged representations of turbulent length and time-scales. It is worth considering how robust the model simulations are to parametrisations chosen within these averaged approaches. We attempt to address some of these questions here and present an approach for the assessment of sensitivities for a complex model aiming to predict roadside concentrations of NO_2 as a function of street topologies, background meteorology, traffic characteristics and chemical parametrisations.

METHODOLOGY

Case study and dispersion model structure

The location modelled in this study is that of Gillygate, York, UK, the site of an extensive measurement campaign (Boddy *et al.*, 2005) that has provided observations used in previous evaluations of some of the model components used here (Dixon *et al.*, 2006). Gillygate is a relatively narrow street with an aspect ratio (building height to street width) of approximately 0.8, leading to cross-street recirculating flow under a range of background wind directions, restricting the dispersion of pollutants out of the street. The traffic flow along Gillygate is quite high with significant periods of congestion, and it therefore represents a potential pollution hot spot. Figure 1 shows the grid and the building configuration of Gillygate and the surrounding area that were used for the simulations in this study. The building heights in meters are indicated in the legend. The basis for the underlying flow and turbulence model under consideration is the k-ε Reynolds-Averaged Navier-Stokes (RANS) model MISKAM (Eichhorn, 2004). This model was chosen on the basis that it is commonly used as an operational model (Ketzel *et al.*, 2000) and has undergone previous evaluation for street canyon case studies, e.g. Dixon *et al.* (2006). A non-equidistant grid was used to enable a higher resolution within the area of interest. Marked on Figure 1 are the two

locations G3 and G4 that were used in the original measurement campaign. We use these locations here for investigating output predictions, as well as three other sites on each side of the street at 20m intervals to the South of G3 and G4. A wind direction of 0° represents channelled flow from North to South along the street canyon. The wind directions sampled in the case study represent oblique flow over the building adjacent to G3 towards the North of the domain and leads to a helical in-street recirculating flow with a northerly channelled component (Boddy *et al.*, 2005).

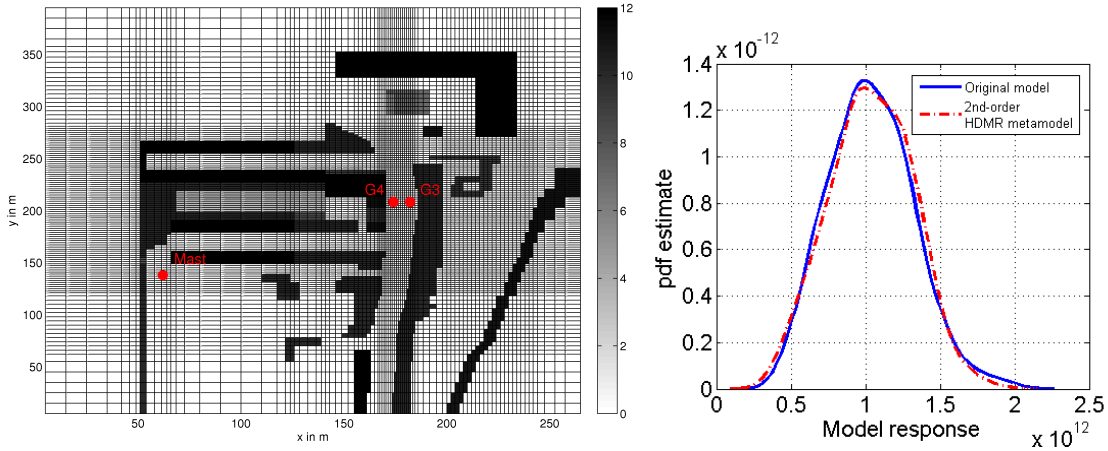

Figure 1. (left) Site schematic for the York Gillygate site showing the grid and building configuration as used in MISKAM (right) Example of predicted output NO_2 distribution based on 512 full model runs and a second order HDMR fit to the sample.

The output from MISKAM is used as the underlying turbulent flow structure for a dispersion model based on the Lagrangian stochastic particle dispersion approach with micro-mixing and chemical sub-models (for a full description and evaluation see Dixon and Tomlin 2007, Ziehn *et al.*, 2009). The complex dispersion modelling system was used previously (Ziehn *et al.*, 2009) to investigate a reactive plume of nitrogen oxides (NOx) released into an approximately homogeneous turbulent grid flow doped with ozone (O_3) for comparison against wind tunnel experiments. The chemical and micro-mixing sub-models used here are the same as those specified in the photolysis extended case described in Ziehn *et al.* (2009) and the reader is referred there for details. In summary, only simple reactions between NO, NO_2 and O_3 are included in the chemical model but these do include the photolysis of NO_2 and O_3. No organic reactions are included in the analysis. For the current study the coupled dispersion model is further linked to a traffic micro-simulation model.

Traffic micro-simulation:
Vehicle flows within the study area were modelled using an established, commercial traffic micro-simulation package AIMSUN 5.1.10 (TSS, 2010) which represents the movement of individual vehicles through a road network using discrete time intervals of the order of one second. Individual components within micro-simulation govern the interaction of vehicles with one another, the interaction of vehicles with traffic signals, how vehicles make lane-changing manoeuvres and how vehicles accept gaps in traffic streams. Within each time-step individual components are called, using information from the previous time step, to assign new kinematic information (speed, acceleration and position) to every vehicle. Vehicle and driver parameters which are considered static within a given run (e.g. maximum vehicle acceleration rates) are generated on vehicle entry to the network, and sampled from appropriate distributions. Given the fine spatial and temporal resolution of traffic micro-simulation, output statistics may be aggregated over a wide variety of scales, for use within appropriate environmental models. A substantial body of literature already exists on methodologies detailing such approaches, e.g. An *et. al.* (1997), Zallinger *et. al.* (2008).

Traffic emissions modelling:
NOx emissions were calculated using the polynomial emissions functions proposed by Int Panis *et. al.* (2006) based on vehicle type, instantaneous speed, and acceleration parameters. Calculated emissions were then linked by vehicle position to a particular 10 m section of road giving spatial-profiles of emissions along Gillygate via bespoke software external to AIMSUN (Goodman and Rhys-Tyler, 2008). The overall traffic network consisted of 4 kilometres of roads surrounding Gillygate and 8 intersections, including 2 signalised. Four categories of vehicles were considered: cars, vans, HGVs and buses, for compatibility with Int Panis *et. al.* (2006). The dynamic demand in the network (the number of vehicles desiring to travel through the network within the simulated hour) was varied over two sets of normalised ranges. The first is an "**off-peak**" case from 0.8-1.2 with the mean value of 1.0 representing 'typical' inter-peak demand. The second was a "**peak**" case with demand varying from 1.2-1.6. Each simulation run therefore represented 1 hr at a particular level of demand using a random sampling approach within the specified ranges. The normalised demand level was derived from a year of traffic flow data obtained from York's urban traffic control system equating to a two-way flow of ~880 veh h^{-1} along Gillygate. Additional to the dynamic demand, was a fixed level of demand from buses based on timetable information. At the base demand level, the network is considered as busy, but in an 'under-saturated' state, i.e. able to cope with the level of demand, with only transient queues forming at junctions. At demand levels above 1.1, modelled speeds begin to decline rapidly from ~20 kmh^{-1} to ~10 kmh^{-1} at a demand of 1.4. Substantial, over-saturated queues form as vehicles are unable to clear signalised junctions within a single signal period. For off-peak, under capacity periods, total emissions increase in a slightly non-linear fashion with the volume of traffic. Some of the non-linearity may be explained by the increasing relative fraction of HGVs present, whose contribution to NOx emissions starts to dominate those of passenger cars. This phase is followed by a transitional period as demand approaches and exceeds network capacity, where emissions stabilise at a high, overall level. The influence of these characteristics on modelled roadside NO_2 levels is discussed in the next section.

Overall model parametrisations

Close to a surface the turbulence in a RANS model needs to be modelled using boundary conditions that reflect the surface roughness. MISKAM represents these boundary conditions using an idealised log law based on surface roughness lengths for the incoming boundary flow, the urban surface and wall surfaces. It follows that parametrisations of these roughness lengths will be a possible source of uncertainty in the final output predictions. Within the Lagrangian particle model framework, the two important parametrisations are the Lagrangian structure coefficient c_0, and the mixing time-scale coefficient α. The Lagrangian structure function is defined as the ensemble average of the square of the change in Lagrangian velocity and the definition of c_0 is therefore important in determining the effective turbulent diffusion in velocity space. There is some debate within the literature as to whether its value can be universally defined for all types of turbulent flows with a range of values between 2 and 10 quoted from different studies (Anfossi *et al.*, 2000). It is interesting to establish therefore how sensitive concentration predictions are to the chosen value. Within the model tested, a simple particle mixing model is adopted, that of interaction by exchange with the mean (IEM) concentration (Sawford, 2004). In order to provide generality, the mixing model uses a coefficient α which defines the relationship between the turbulent time-scales (total turbulent kinetic energy and its dissipation rate) and the mixing time-scale at every point in the flow. The specification of α should also be considered to be uncertain. Uncertainties in the traffic emissions model have been adopted for the level of traffic demand as discussed above, and the NO:NOx ratio for the emissions source which determines the fraction of NO vs primary NO_2 assumed at source. The range adopted was chosen to reflect levels of primary NO_2 estimated for current UK vehicle fleets (Carslaw, 2005). The 26 model parameters varied within the sensitivity/uncertainty analysis can therefore be summarised as:

- velocity structure function coefficient c_o [4-6]
- mixing time-scale coefficient α [0.6-3]
- surface roughness z_0 for inflow, surface and wall [5-50, 0.5-50, 0.5-10, cm]
- temperature dependant rate parameters for $NO/NO_2/O_3$ reactions, photolysis rate parameters for JO_3 and JNO_2 [see Ziehn *et al.*, 2009 for details]
- background wind direction θ_{ref} [110-130°]
- temperature [273-298 K]
- background ozone concentration [$7.35x10^{11}$- $1.23x10^{12}$, molecules cm^{-3} or 30-50 ppb]
- NO:NOx ratio for traffic emissions [0.8-1]
- normalised traffic demand [off peak 0.8-1.2, peak 1.2-1.6]

where the ranges used are shown in the square brackets.

Global sensitivity method

The global sensitivity analysis has been achieved using the RS-HDMR (Random sampling high dimensional model representation) method introduced by Rabitz *et al.* (1999) to express the input-output relationship of complex models with large numbers of input parameters, and further developed into a user friendly Matlab package by Ziehn and Tomlin (2009). The mapping between input parameters $x_1,\ldots,x_n$ and output variables $f(\mathbf{x})=f(x_1,\ldots,x_n)$ in the domain R^n is written in the form:

$$f(\mathbf{x}) = f_0 + \sum_{i=1}^{n} f_i(x_i) + \sum_{1\le i<j\le n} f_{ij}(x_i, x_j) + \ldots + f_{12\ldots n}(x_1, x_2, \ldots, x_n) \quad (1)$$

where f_0 denotes the mean effect (or zeroth order term), which is a constant. The function $f_i(x_i)$ is a first order term (or first order component function) giving the effect of parameter x_i acting independently (although generally nonlinearly) upon the output $f(\mathbf{x})$. The function $f_{ij}(x_i,x_j)$ is a second order term describing the co-operative effects of the parameters x_i and x_j upon the output $f(\mathbf{x})$. The higher order terms reflect the co-operative effects of increasing numbers of input parameters acting together to influence the output $f(\mathbf{x})$. Due to its formulation as a set of hierarchical component functions, the HDMR expansion provides the possibility to determine sensitivity indices for each of the input parameters in an automatic way for selected model outputs. For given input parameter ranges, these indices indicate the relative contribution of each parameter to the predicted output variance. Thus they can be directly used to rank the importance of each individual parameter in determining the model output variance and to explore parameter interactions. The HDMR expansion is computationally very efficient if higher order input parameter interactions are weak and can therefore be neglected. For many systems a HDMR expression up to second order already provides satisfactory results and a good approximation of $f(\mathbf{x})$ (e.g. Benson *et al.*, 2008). In RS-HDMR, a number of model simulations are performed using a quasi-random set of input samples. This set of model simulations is then used to fit polynomial expressions for each component function in equation (1). The sensitivity coefficients for individual parameters or for interaction terms can then be easily calculated from the coefficients of the polynomial expansion (see Ziehn and Tomlin, 2009 for details). For the current studies, the 26 dimensional input space is sampled 512 times using a quasi-random approach from within the parameter ranges specified. The RS-HDMR meta-model fit is then generated where the output function $f(\mathbf{x})$ represents the NO_2 concentration at the 8 in-street locations discussed above.

RESULTS AND DISCUSSION

Accuracy of HDMR fits and overall uncertainty

In order to exploit the HDMR component functions for sensitivity analysis purposes, it is first important to establish that the HDMR meta-model gives a reasonable fit to the outputs from the full model runs. This test is especially important for the current example since the combined model simulation time was of the order of hours and therefore the sample size of 512 was limited by available computer resource. Figure 1 shows the modelled NO_2 distribution at G3 for the off-peak case, using the full and the HDMR meta-model illustrating that the second order meta-model gives a good fit despite the limited sample size. This provides confidence in the accuracy of the HDMR component functions and the sensitivity results derived from them. The output distribution suggests that given the broad ranges of input parameters adopted, the predicted [NO_2] at G3 can vary by at least a factor of 2. This suggests that more accurate parametrisation of the inputs is necessary to improve confidence in model

predictions. The peak [NO_2] at G3 is twice that at G4 confirming the influence of the in-street recirculation on the leeward in-canyon concentrations (data not shown).

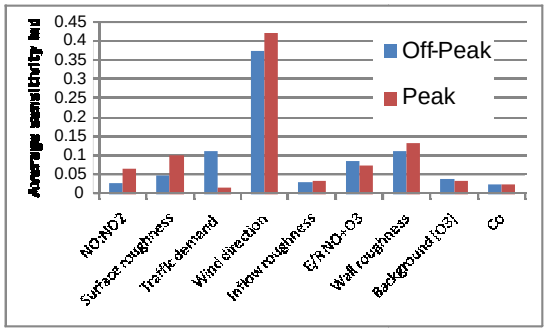

Figure 2. The average first-order sensitivity coefficients across all 8 sites for the peak and off-peak normalised traffic demand studies.

Sensitivity coefficients

The sensitivity coefficients calculated using HDMR provide the relative influence of each parameter on the variance within distributions such as that shown in Figure 1. They are scaled between 0 and 1 where 1 represents 100% contribution to the output variance. Figure 2 presents the average sensitivity coefficients across the 8 sample locations for predicted roadside [NO_2]. The mixing time-scale coefficient α and other unimportant parameters are not shown on the plot because [NO_2] shows only low sensitivities to their chosen values. The Lagriangian structure function coefficient c_o also exhibits a low sensitivity. This is an encouraging result and suggests that the simulated concentrations are not highly sensitive to the chosen turbulence model parametrisations. There are however sensitivities to the parametrisation of the velocity profiles at the model surfaces (i.e. to the chosen values of roughness lengths). The lowest sensitivity is to the inflow roughness, which indicates that the computational domain was large enough to reduce the influence of the inflow boundary. The wall roughness however, exhibits a mean sensitivity of over 10%. Detailed calculations show that for site G3, this can be as high as 30%. This suggests that predicted [NO_2] close to the street canyon walls (within 2 m in the case of G3) can be highly sensitive to the near wall flow parameterisations as was previously suggested to be the case by Benson *et al.* (2008) for velocity and turbulence fields in these locations.

Wind direction is the major physical parameter which dominates the prediction of [NO_2] at all locations. On average it accounts for around 40% of the variance in predicted [NO_2]. This implies that a reliable reference measurement of background wind conditions is an essential input for air quality modelling systems, particularly those aiming to represent recirculating flows within urban street canyons. Figure 3 demonstrates the nonlinear response of [NO_2] at a site 40m south of G3 to shifts in background wind direction. The higher concentrations are found at the oblique angle with the largest perpendicular wind component to the street (110°). The sensitivity to background O_3 is on average quite low, although a higher sensitivity to the activation energy for the reaction of NO with O_3 is seen. There is obviously some influence of chemical processes occurring at the street scale requiring better parametrisation of one of the rate parameters used within the scheme, using for example *ab initio* quantum calculations. These influences are greater (detail not shown) on the canyon windward side (G4), which due to the recirculation is not directly down-wind of the primary NOx traffic source and therefore more influenced by secondary processes. In terms of the influence of traffic characteristics, there are clear differences between the two modelled demand scenarios. For off-peak conditions, there is clearly a response to the levels of traffic demand with an average contribution of ~11% to the predicted [NO_2]. The HDMR component function shown in Figure 3 illustrates the non-linear response of [NO_2] at G3 to changes in the normalised demand level. The effect of demand appears to level off at the higher demand as the flow starts to reach congested conditions (see above discussion on emissions). Under peak conditions where the network saturates, road-side [NO_2] was relatively insensitive to changes in demand and more sensitive to the primary NO_2 fraction (see Figure 2).

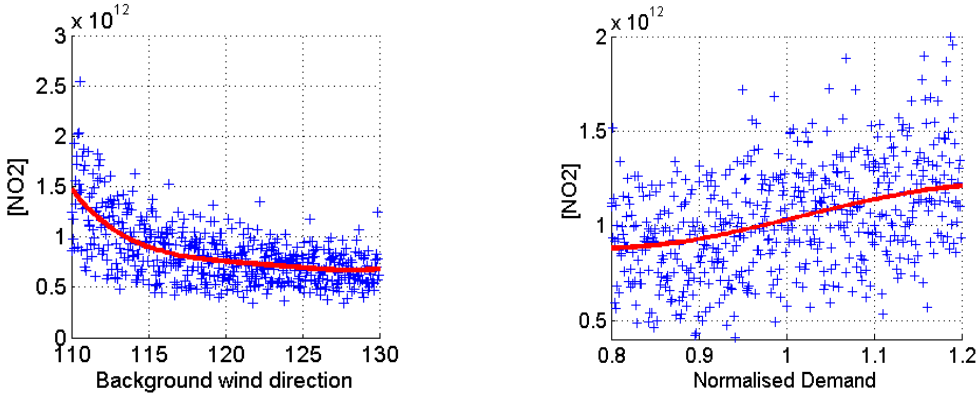

Figure 3. (left) HDMR component function (in red) of the response of [NO2] 40m south of G3 to changes in background wind direction (right) HDMR component function (in red) of the response of [NO_2] a G3 to changes in normalised demand. In both plots the scatter represents a projection of the outputs from the full model based on the quasi-random sample.

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