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LARGE-EDDY SIMULATION OF ROADSIDE DISPERSION AND CHEMICAL TRANSFORMATION OF NITROGEN OXIDES IN AN URBAN ENVIRONMENT

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Abstract: The objective of this work is to present a high-resolution, urban scale large-eddy simulation (LES) framework for modelling dispersion and chemical transformation of nitrogen oxides (NOx = NO + NO_2) from urban traffic. The control-volume based computational fluid dynamics (CFD) simulation platform OpenFOAM has been adopted for LES transport and reactional modelling. A rudimentary chemical kinetic mechanism for NOx and tropospheric ozone (O_3) has been introduced as a non-limiting implementation. All urban structures are fully resolved in the solution domain, with dynamic grid refinement allowing local spatial resolutions to reach 10 m and below. A k-way Boolean operation and a reduced convolution Minkowski sum algorithm are used to automate the conversion of available geographical data, such as two-dimensional urban footprints and object heights, into three-dimensional geometrical entities. Said methodology is applied to urban regions in the City of Berlin of up to 2 km × 2 km around active roadside air quality measurement stations from the BLUME (*Berliner Luftgütemessnetz*) network. Particular emphasis is placed on the period in July 2014, where emission observations from measurement campaign and WRF regional model simulations are available.

Key words: *Large Eddy Simulation (LES), Dispersion, Chemical Transport, Urban-Scale Simulation, OpenFOAM, Weather Research Forecasting (WRF),*

INTRODUCTION

Scientific data derived from detailed and accurate urban scale modelling can be used directly as relevant guidance information for environmental policy makers at municipal and regional levels. Such models must be conducted at sufficiently high spatial and temporal resolutions in order to satisfactorily resolve flow structures around urban entities and surface topologies. Due to the associated increase in computational effort, however, urban-scale models are typically applied on a small geographical region of interest (Jeanjean et al, 2015 & 2017). Meteorological conditions can be supplied to the urban model as boundary conditions, usually by way of coupled regional scale models (Zhang et al, 2015). Both off-line (Churchfield et al, 2010) and on-line (Leblebici and Tuncer, 2016) coupling approaches have been contemplated. Further, as the model resolution increases, the range of explicitly resolved turbulence also increases accordingly. This justifies the use of the large eddy simulation (LES) modelling approach (Maronga et al, 2015; Moeng et al, 2007; Smolarkiewicz and Charbonneau, 2013).

For the present study, a urban scale LES modelling framework is being developed based on off-line coupling between OpenFOAM 5.0 (Weller et al, 1998) and WRF 3.9.1 (Skamarock et al, 2008) to simulate dispersion and chemical transformation of urban traffic nitrogen oxides (NOx) emissions. Existing works on regional scale and urban scale coupling, such as those cited above, are focused on meteorology; chemical transport processes have so far not been considered. Further, in light of similar urban-scale modelling framework for large-eddy simulations, OpenFOAM provides a higher degree of flexibility in domain discretization. The computational grid can be locally adopted according to topological requirements, while preserving the surface normal of the original geometry. Further, an automated method is available to assimilate urban structure footprints, such as those supplied by urban geographic information systems (GIS), into simulation ready three-dimensional entities.

The methodology is to be applied to the City of Berlin, where a focus is placed on the period of July 2014, in light of previous modelling and observational studies already made (Kuik et al, 2018; von

Schneidemesser et al, 2018). In particular, the WRF-Chem model study of Kuik et al (2018) reported an average of 30% underestimation of NO_2 levels (~ 8 $\mu g \cdot m^{-3}$) from observations. This could possibly be attributed to an underestimation in traffic emissions. The present study aims to resolve possible sources of bias by modelling the immediate region(s) of interest, around a measurement station, for instance, through explicit representations of urban geometry and turbulent mixing.

GENERATION OF THREE-DIMENSIONAL URBAN GEOMETRY

Modelling urban-scale transport phenomena requires as input a seamless 3D representation of urban structures in the region of interest. Traditionally, these geometries are constructed manually based on city planning information, which heavily restricts the quantity of such structures that can be included in the simulation. However, GIS data containing digitized 2D footprint and elevation of individual urban structures are readily available in a format commonly known as *shape files*. An extrusion-based algorithm is thus developed to automate generation of simulation-ready urban geometries using said GIS data, as outlined in Lu et al (2012).

Each geometric entity present in the incoming shape files can be represented by layers of disjoint polygons in the vertical direction. These comprise *invariant polygons*, that is, those whose topology do not change for a given extruded elevation, and *transitional polygons*, which serve as interface between consecutive but distinctive invariant polygons. These polygonal profiles can be constructed directly from the corresponding 2D footprints and elevations stored in the shape files. A k-way Boolean operation is then invoked to merge contiguous entities, such as city blocks, by determining their intersection. This is done by identifying all nested boundary loops, termed *boundary orientatble loops*, of all the elements, instead of the conventional binary comparison, which improves computational efficiency. The merged boundaries, where invalid geometric features – namely, manifolds, degeneracy and gaps – are filtered using a reduced convolution operation based on the Minkowski sum of the boundary orientable loops. The resulting geometries are then tessellated to form the 3D urban structures.

The algorithm is used to process urban GIS data for the city of Berlin (Poznańska, 2013). All structures of height 3 m and below are discarded, reducing the number of incoming entities to approximately 394,000. The process takes 160 minutes, and produces about 131,000 contiguous structures. Figure 1 shows the original 2D urban footprint and the processed 3D geometries for Ernst-Reuter-Platz and its immediate vicinity in Berlin.

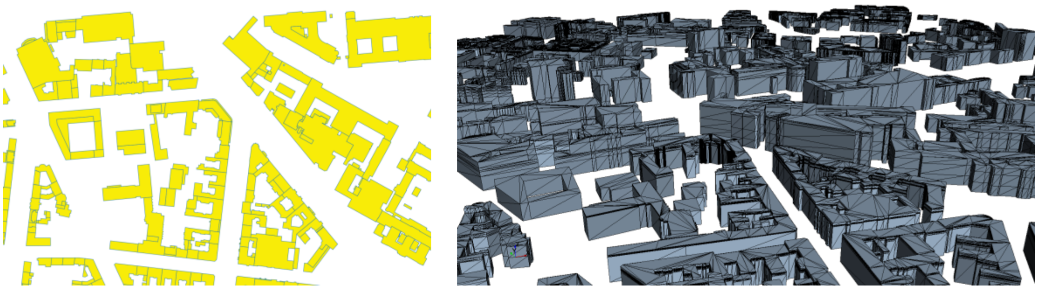

Figure 1. (Left) Urban footprint according to GIS data (Poznańska, 2013) for the region around Ernst-Reuter-Platz in Berlin and (right) the corresponding tessellated 3D representations used for the urban simulation.

REGIONAL SCALE MODEL SETUP

The meteorological conditions, namely, wind velocity, temperature and humidity for the coupled urban simulation domain have been produced with WRF region model and subsequently introduced as boundary condition to the urban-scale model. A one-way nested domain approach is employed. Data exchange with the urban domain takes place at the innermost domain, which as a horizontal resolution of 100 m × 100 m covering an area of 15 km × 15 km. The outermost domain covers a region of 1875 km × 1875 km at a horizontal resolution of 12.5 km × 12.5 km. The vertical direction contains 64 layers, with a ceiling pressure set to 15 kPa. The simulation covers the period of July 2014 as well as spin-up from June 24th to 30th 2014. Re-analysis data from ECMWF are used as initial meteorological conditions. The CORINE land use data (EEA, 2006), remapped to the USGS land use classes, including three urban classes, are used in conjunction with the NOAH land surface model with a single layer urban canopy representation (Kuik et al, 2016). Results from the nested WRF model for the two-meter temperature (T2) and ten-meter horizontal wind (U10) at different times in the diurnal cycle are illustrated in Figure 2. The horizontal resolution for this intermediate domain is 500 × 500 m.

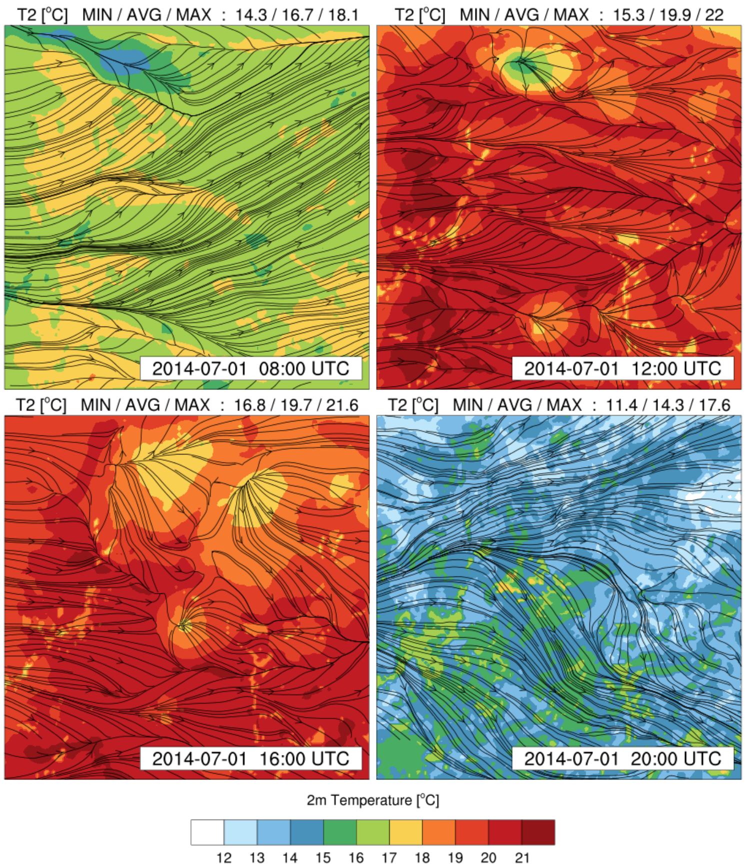

Figure 2. Two-meter temperature (contours) and ten-meter horizontal wind (streamlines) of nested WRF domain (horizontal resolution 500 m) at 8:00, 12:00, 16:00 and 20:00 UTC on July 1st, 2014.The city of Berlin is located roughly at the center of the domain.

A 4th-order spatial polynomial interpolation is used extract relevant field data from inner most regional model domain to the urban model. Latitudes and longitudes are converted to UTM coordinates using the WGS84 ellipsoid datum. A direct solver based on LU decomposition is implemented to determine the interpolation coefficients. This approach allows data pertinent to the grid geometry to be processed separately from the scalar variables, significantly reducing storage and computational requirements. Further, this method can be generalized to solve for interpolation coefficients at an arbitrary order of accuracy, including closest neighbor (i.e., zeroth order), which can be used for discontinuous variables such as sea surface temperature and land-use categories.

URBAN MODEL SPECIFICATIONS

A non-hydrostatic, compressible flow solver is used to model dispersion. A partially stirred reactor approach is used to model chemical transport (Bartulucci et al, 2018). Chemical kinetic mechanisms can be introduced at runtime such that the chemical species and reactions can be modified without recompiling the source code. As a non-limiting example a three-reaction mechanism for NOx photolysis and transformation (Saunders et al, 2003) is currently implemented and is presented below:

$$NO_2 + h\nu \rightarrow NO + O \qquad k = 0.1165\cos^{0.244}(\theta_z)\exp[-0.267\sec(\theta_z)] \quad ; \quad \theta_z \in [0, \pi/2) \qquad [1]$$

$$M + O + O_2 \rightarrow O_3 + M \qquad k = 2.3827 \times 10^{9}\exp(-510.0/T) \qquad [2]$$

$$O_3 + NO \rightarrow NO_2 + O_2 \qquad k = 2.59 \times 10^{10}\exp(-1598.0/T) \qquad [3]$$

where k is the reaction rate constant, θ_z is the solar zenith angle, and T is the local temperature. Note that the concentration for use with the Arrhenius rate constants is expressed in kilomoles.

Background concentrations of O_3 and NOx ($NO + NO_2$) can be obtained from observational data provided by urban background stations in the BLUME network (*Berliner Luftgütemessnetz*; Berlin air quality measurement network), such as that shown in Figure 3. Nitrogen oxides emissions from traffic sources can then be introduced in the urban-scale model as a distributed source on the road surface. Further, the emission levels for the road segments of interest can be retrieved from inventory data (Leitão et al, 2019).

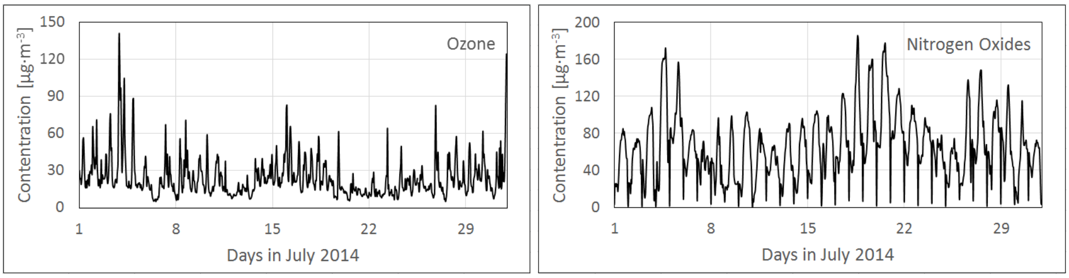

Figure 3. Concentrations of (top) ozone and (botton) nitrogen oxides at a BLUME urban background station for July 2014.

Preliminary run

A prototype simulation (RANS, decoupled) is set up for a 2 km × 2 km area around a BLUME station located at *Silbersteinstraße* (DEBE063, ϕ=52°28'3.04"N, λ=13°26'29.94"E) with a height of 500 m, as shown in Figure 4. A mean westerly wind of 4.5 m/s is prescribed, and the computation is assumed to be isothermal. Zero-gradient conditions are applied for temperature and pressure on all domain boundaries. Traffic emissions are represented by a passive scalar applied on selected road surfaces. The mesh consists of 1.06 million cells. A 1:2 grid refinement ratio is maintained, where the cell resolution is 50 m in the boundary regions, and gradually decreasing to 1.56 m at the finest level. In the immediate region surrounding the measurement station, the cell size is limited to 6.25 m and below.

Figure 5 shows the dispersion the urban traffic NOx (as a passive scalar) released on a road surface after spin-up over a 30 minute period. For reference, the mean wind flows from the bottom (west) to the top (east) of the figure. The plume depicted on the figure represents a mixing ratio for NOx of 0.5% and above. It follows the originating street canyon at the beginning. As it reaches the main intersection, it can be seen to preferentially disperse to the right (south) of the figure. There is no qualitative expansion of the plume between 15 minutes and 30 minutes.

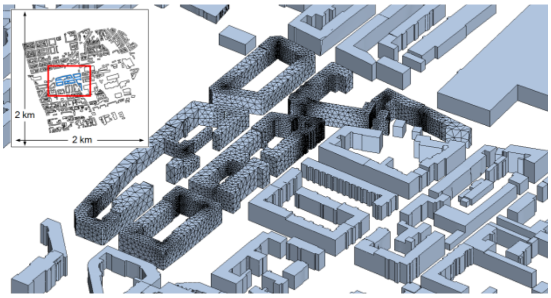

Figure 4. Close-up of the prototype run with region of interest highlighted (tessellated). Inset indicates horizontal extent (2 km × 2 km) of the urban model domain.

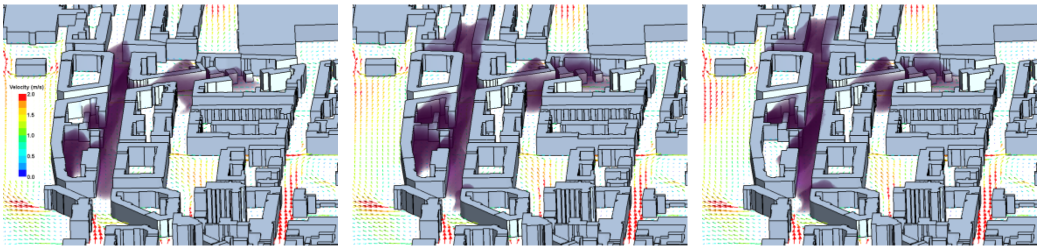

Figure 5. Dispersion of NOx passive scalar at (left) 5 min, (middle) 15 min, and (right) 30 min following spin-up from the prototype run. Mean wind travels from the bottom to the top of the figures.

OUTLOOK

The present study describes a simulation framework based on a coupled regional and urban model approach using large eddy simulation. While the treatments of transport and chemistry in the urban model are discussed and represented, particularly in the handling of arbitrary geometries, local mesh refinement, and the coupling of chemistry and transport, this methodology is still under active development. Additional models, such as long- and shortwave radiation, vegetation, and deposition, are next to be contemplated.

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