NUMERICAL SIMULATIONS OF POLLUTANT DISPERSION IN THE CENTRE OF A EUROPEAN CITY FOR DIFFERENT THERMAL TRANSFER CONDITIONS

Yongfeng Qu, Maya Milliez, Luc Musson-Genon and Bertrand Carissimo

Teaching and Research Center in Atmospheric Environment (CEREA) (ENPC/EDF R&D), 6–8 avenue Blaise Pascal, 77455 Champs-sur-Marne, France

Abstract: In order to estimate the complex urban environment on air pollution dispersion, numerical simulations are performed over a real urban area, modelled as detailed building geometries. Since urban radiative transfers play an important role because of their influence on the energy budget, to take into account atmospheric radiation and the thermal effects of the buildings in simulations of atmospheric flow and pollutant dispersion in urban areas, a three-dimensional (3D) atmospheric radiative scheme has been developed in the atmospheric module of *Code_Saturne*, a 3D Computational Fluid Dynamics (CFD) model. The full coupling of the radiative transfers and fluid dynamics models has been firstly validated with idealized cases. Then, the radiative-dynamics coupling is used to simulate a real urban environment and is validated with field measurements of a district of the city of Toulouse, in the South-West part of France, from the Canopy and Aerosol Particles Interactions in TOulouse Urban Layer experiment (CAPITOUL). The purpose of this work is to investigate passive pollutant dispersion from complex urban layout of Toulouse under different thermal transfer conditions for the street and the buildings surfaces: neutral and 3D radiative transfer heating. The presence of heat transfer continually modifies the airflow field while the airflow in the neutral case reaches a stationary stage. Compared to the neutral case, taking into account the thermal transfer enhances the turbulence kinetic energy and vertical velocity (especially at the roof level) due to buoyancy forces. The simulation results also showed that their effects considerably alter the plume shape.

Key words: Urban energy models, 3D Radiative transfers, CFD, Dispersion, Coupling

INTRODUCTION

The influence of the urban thermal environment has received more attention than in the past. In addition, a thermally comfortable environment is important for the inhabitants and commuters of urban areas. Current research concludes that emissions in buildings are one of the major sources of the pollution that causes urban air quality problems and green house gases that contribute to climate change. In that event, sustainable development requires the improvement of the interrelationship between buildings, their components, their surroundings and their occupants.

In order to improve the urban microclimate, various countermeasures have been proposed and researched, such as roof greening, use of high albedo paints, and water-retentive materials, etc. Then in order to better understand the phenomena occurring at neighbourhood scale and to study different scenarios, more and more realistic simulation tools are also developed, such as Computational Fluid Dynamics (CFD) analysis. However, many micrometeorological studies on flow and pollution dispersion assume a neutral atmosphere (neglecting thermal effects and stratification) and most building energy balance models neglect the three-dimensional (3D) local variation of the flow and air temperature fields. Moreover, many researches were performed on a simple model of an isolated urban block.

To address these issues, we propose a method for predicting microclimates within urban blocks, based on a coupled simulation using convection, radiation and conduction. Thus, we have developed a 3D microscale atmospheric radiative scheme in the atmospheric module of the 3D CFD code *Code_Saturne*. This numerical model is capable of simulating both the flow and the radiative-convective exchanges between the atmosphere and the buildings. For the ground surfaces, it can also take into account the humidity of the soil (latent heat flux). The code can handle general unstructured meshes with variable resolution, allowing to accurately simulate the complex geometry of the area of interest with a fine resolution and the surrounding area with a lower resolution.

In this study, the previously developed numerical method coupling convection, radiation and conduction was used to test the effects of the complexity of real urban geometries on the interaction between the airflow and the thermo-radiative exchanges with different surfaces. We choose the Canopy and Aerosol Particle Interactions in TOulouse Urban Layer (CAPITOUL) experimental dataset (Masson et al., 2008). The campaign is a joint experimental effort in urban climate which took place in the city of Toulouse in South-West France from 2004 to 2005 (Masson et al., 2008). Studying the energetic exchanges between the surface and the atmosphere was one of the objectives. The study area is mainly located in the city center around the corner of the two streets: Alsace-Lorraine and Pomme (yellow contour in Fig. 1a). In this neighborhood, vegetation is scarce and buildings are around 20 m height (Pigeon et al., 2008).



Figure 1. Aerial view of downtown Toulouse and Tetrahedral mesh: a) main study area, from Google Maps; b) Tetrahedral mesh on the central area zoom in the selected area a) (yellow contour); c) zoom in a center building wall. The north is indicated.

MODEL DESCRIPTION

Taking into account the larger scale meteorological conditions and the thermal stratification, the atmospheric module of *Code_Saturne* (Archambeau et al., 2003), described in Milliez and Carissimo (2007; 2008), uses a detailed representation of the surfaces allowing a complex 3D spatial representation of wind speed, turbulence, and temperature. A standard k- ε formulation is used in this work.

Detailed equations can be found in Milliez (2006) and Qu (2011). Our radiative model takes into account both short- and long-wave radiation. A hybrid method is used in this work to determine the surface temperature (Qu, 2011). Fig. 2 shows an algorithm outline. The inputs to the modeling approach are: date, location, urban configuration, meteorological conditions (velocity, temperatures), description of surface materials etc. From an initial flow field used to compute the convective fluxes, surface temperatures are computed using the thermoradiative model. Then the surface temperature is used as a boundary condition for CFD simulations, which are then performed.

Milliez (2006) first evaluated the model with idealized cases, using a constant 3D wind field. Then, Qu et al. (2011) have validated the full radiative-convective coupling by comparison with several surface wall temperatures from Mock Urban Setting Test (MUST) field campaign (Yee and Biltoft, 2004; Milliez and Carissimo, 2007; 2008). Furthermore, in order to assess the thermal impact on the flow fields in different thermal conditions, we extend the work of Qu et al. (2011) to lower wind speed and a higher building density than in MUST (Qu et al., 2012).



Figure 2. Algorithm outline of the modeling approach.

VALIDATION

From the experiment, we selected the day of July 15th 2004. The meteorological mast is located on a roof with its base at a 20 m height, and the top at 47.5 m above the road. It provided data including heat fluxes, air temperature, wind speed and direction etc. Detailed model-observation comparisons can be found in Qu (2011). Considering Alsace-Lorraine and Pomme roads as the center of interest in the computational domain (Fig.1a), the dimension of the 3D simulation domain is 891×963×200 m. The generation of the CAPITOUL complex mesh requires an important preliminary work to optimize the geometry (Qu, 2011). The buildings along Alsace-Lorraine and Pomme streets in the center of the area under study are modeled with fine details (Fig.1b). Then, the surrounding buildings are simplified as urban blocks. Finally, the buildings in the region outside are treated with a high roughness value of 1.5 m. The volumetric mesh used here is an unstructured grid of about 2 million tetrahedral cells. The grid resolution varies from 0.8 m near the center to 24 m far from the center zone (Fig. 1c).

In addition, we have separated 4 classes of albedo value depending on wall painting colors. Through the comparison with the Thermal InfraRed airborne images from two flights in the day of 15th July 2004, we demonstrate the importance of taking into account heterogeneities in materials and geometry to reproduce the spatial variability of the temperatures in complex urban areas. Moreover, the full coupling is tested against in situ observation during the same day. The results show that the coupling performs well overall in terms of the brightness temperature. The model predicts a good daytime sensible flux and outgoing infrared flux, but shows a night-time underestimation. Regarding the outgoing solar flux, the result shows an excellent model-observation agreement at the mast position. In the statistical study, some significant differences between the predicted and observed statistics of brightness temperatures, the analysis provides an interesting and different approach to evaluate the model performance (Qu, 2011).

DISCUSSION: THERMAL EFFECTS ON POLLUTANT DISPERSION

In this section, we investigate the thermal effects of buildings on pollutant dispersion. The meteorological initial and inlet boundary conditions are taken from a neutrally stratified wind profile blowing westward with a reference 47.5-m wind speed $U_{ref} = 3 \text{ m s}^{-1}$, associated with a neutral potential temperature profile of 22 °C (Fig. 1a). We consider a passive emission sources on the ground, starts at 1000 UT for a period of 3 hours as shown in Fig. 1a (yellow point).

In order to study the contribution of atmospheric radiation on the airflow, we performed two cases: a reference case without heat transfer, i.e. with a neutral stratification of the atmosphere, called hereafter "neutral case", and a case with the 3D atmospheric thermo-radiative model coupled to the dynamical one, called hereafter "thermo-radiative transfer case".

The numerical simulation results are analyzed at the end of the release, when the mean flow in the entire simulated urban canopy reaches a quasi-steady state in the neuter case. Airflow in the urban canopy is composed of very complicated vortices rotating in the horizontal and vertical directions. Figure 3a and b shows the Turbulent Kinetic Energy (TKE) fields on the vertical and horizontal cross sections of respectively the neutral and thermo-radiative cases. Compared to the neutral case, production of turbulence by the building is complex (Fig. 3a), the presence of heat transfer (Fig. 3b) enhances the TKE in the whole domain due to a large thermal production, in particular near the roof level.



Figure 3. Comparison of the mean Turbulent Kinetic Energy (TKE) (m²s⁻²) distribution on the vertical- and horizontal cross sections: a) neutral; b) thermo-radiative transfers. The wind direction and north are indicated.

Figure 4 shows hot spots of dimensionless pollution concentration near the ground for two thermal conditions. From the neutral case (Fig.4a), emission from ground obviously disperses by the dominated wind along the westeast direction. Since the wind velocities are reduced dramatically inside the canyons, stagnation areas are formed there. This kind of uneven distribution of wind velocities will definitely influence the pollutant dispersion. Hence in the yard pollutants were likely both less diluted and more entrapped than on the roof (higher yard pollutant concentrations).

With thermal transfer condition (Fig. 4b), a lower concentration is found downstream, compared to the neutral case, surface heating induces greater dispersion. Inside-yard concentration is lower.



Figure 4. Comparison of the concentration distribution on the ground level at the end of the release: a) neutral conditions; b) thermo-radiative transfer conditions. The wind direction and north are indicated.

To clarify the change in the dispersion characteristics with changes in thermal condition, we plot the concentration distribution on a vertical cross section at the released source position in Fig. 5. With thermal transfer conditions (Fig.5b), the air temperature is increased which results in an upward motion. Buoyant forces are dominant in this low-wind scenario, as the plume is seen to trend upwards from the point of emission. Moreover, the chosen thermal conditions do lift the plume sufficiently away from the surrounding buildings. Therefore, higher concentrations are found above the road in comparison with the neutral case (Fig. 5a).



Figure 5. Comparison of the concentration distribution at the end of the release on a vertical cross section where the emission released: a) neutral conditions; b) thermo-radiative transfer conditions. The wind direction and north are indicated.

CONCLUSIONS

We have investigated airflow and thermal exchanges in a real city during the CAPITOUL campaign, using new atmospheric radiative and thermal schemes implemented in *Code_Saturne*. A pre-processing is performed including the optimization of the complex geometry and creation of a high quality tetrahedral mesh for this study. It also requires determining the complex thermal parameters which take into account the actual variability of materials in the district. During the same day, the full radiative-dynamics coupling is tested against in situ observation including brightness temperature and heat flux etc. The simulation results show the importance of modeling in detail while doing local model-observation comparison. In particular we test the thermal influence on pollutant dispersion. The simulation results show not only the interest of using a CFD code for predicting the dispersion within complex geometries and but also that the thermal effects considerably alter the plume shape.

This type of tools can be applied to detailed studies of local urban climate, to the study of present conditions and future scenario, such as the densification of housing and the introduction of green area or green/white roofs. It can be used to further assess the street canyon ventilation potential, the possible shading strategies on building surfaces and the influence of both aspects on indoor thermal comfort and air quality. This tool is also well suited to the study of "hot spots" in the air quality of urban centers where the emissions are particularly concentrated and to evaluate the alternatives to mitigate them. It can also contribute to future research and applications in the field of wind engineering in the urban environment, when the thermal stratification is of importance. The model results are encouraging and give insight into local surface-atmosphere processes, but further testing has to be performed with other datasets.

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