Modelling pollutant dispersion over a city in a hilly terrain under initially stable and neutral stratification

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Abstract - We present results of numerical modelling of dispersion of a passive pollutant over a middle-size city in complex hilly terrain under different initial thermal stratification conditions. The computations were performed in the time-dependent Reynolds-Averaged Navier-Stokes (T-RANS) framework, using an algebraic three-equation (AFM $k – ε – θ^2$) turbulence model for subscale heat and concentration fluxes. Considered are two scenarios that mimic relevant meteorological conditions. The first is a typical windless winter day with distinct potential temperature inversions (at 800m and 300m above the valley ground with a gradient of 4 K/km in the upper atmosphere) where the transport of pollutants is solely driven by thermal buoyancy effects generated by heat islands. A multi-zonal approach was used to define different levels of heat and concentration emissions within the city. The second case was forced and mixed convection with neutral stratification for the city centre at a neighborhood scale with pre-defined approaching wind. Here, a non-uniform building-resolving mesh (down to 3.5m) was used with traffic emissions along all major roads as the primary pollution sources. The simulations provided details of spatial and temporal evolution of flow and scalar fields over the city.

1. Introduction

Mitigation of ever increasing and alarming environmental pollution worldwide calls for comprehensive, multi-purpose prognostic tools that could provide reliable information on the outcome of a variety of natural and man-made scenarios and measures undertaken. Computer simulations, complemented by systematic field measurements and monitoring has been widely accepted as the only viable method to provide such information. However, the proper numerical modelling and simulations of spatial and temporal evolutions of flow, temperature and concentration fields in complex city-scale environment is a challenging task [1]. Combined effects of the localised time-dependent ground heating and pollutant emissions with initial vertical distributions of the air temperature (thermal stratification) for a real-scale terrain require advanced turbulence models and numerical methods.

In the present work, we focus on a real-scale city in a hilly terrain under different stratification conditions. The work is in essence a follow-up study of [2], [3], but with a more detailed multi-zonal approach in defining localised heat and concentration, as well as ground roughness regions.

2. Configuration, model and computational method

The simulations are performed using a time-dependent (“Transient”) Reynolds Averaged Navier Stokes (T-RANS) approach based on triple decomposition (time-mean, semi-deterministic (coherent) and stochastic motion). The assemble-averaged momentum, energy and species concentration equation are closed by the eddy-viscosity (for the momentum) and algebraic flux models, AFM, (for energy and concentration), which provide the turbulent
stress, heat and mass fluxes ($\overline{u_i u_j}$, $\overline{\theta u_i}$, $\overline{c u_i}$) respectively [2-4]. A specific feature of the AFM is the inclusion of the buoyancy production term which plays a crucial role in reproducing turbulent flux in highly mixed layers heated from below, where the average temperature and concentration are uniform and thus non-compliant with the common gradient diffusion hypothesis. The constitutive relations for the turbulent stress and fluxes are defined in terms of the turbulent kinetic energy ($k$), its dissipation rate ($\varepsilon$) and the temperature variance ($\overline{\theta^2}$), provided from their modelled transport equations, thus constituting the AFM three-equation $k$-$\varepsilon$-$\overline{\theta^2}$ model [4].

The above model was earlier tested in a number of relevant generic cases, as well in environmental flows including the here considered configuration for a similar, though simpler scenario [2-4]. It is noted that for environmental flows the Ra numbers are very high and the ground boundary conditions must be treated with Wall Functions to facilitate the use of affordable numerical grids. While in the earlier works [2], [3], the standard wall functions were used, the present computations employ the Simplified Analytical Wall Functions, SAWF proposed by [5], complemented with buoyancy-accounted modifications for specifying the turbulent properties, $k$, $\varepsilon$ and $\overline{\theta^2}$.

The equation set is solved numerically with a finite volume Navier-Stokes solver in a structured non-orthogonal domain, using collocated variable arrangement and Cartesian vector and tensor components [6]. The central difference scheme (CDS) is used for discretization of the diffusion terms and a second-order linear upwind (LUDS) scheme is applied for the convective terms for all variables. Then pressure-velocity coupling is ensured by the SIMPLE algorithm. Fully implicit second order three-time-level marching scheme is used for transient simulations.

Two cases are considered. In the Case 1 we consider a mesoscale solution domain of the total dimensions of $L_x \times L_y \times L_z = 18.5 \times 12.5 \times 3 \text{ km}$, bounded from below by the real terrain orography and covering the town region with the surrounding slopes. The domain was meshed by $N_x \times N_y \times N_z = 260 \times 176 \times 100$ ($\approx 4.57 \text{ M}$) control cells, clustered towards the ground in the vertical ($z$) direction. The Rayleigh and Prandtl numbers are $Ra = 4.2 \times 10^{17}$ and $Pr = 0.71$, based on the real values of the domain height, kinematic viscosity, thermal expansion coefficient, gravitational constant and the characteristic (ground – inversion-base) temperature difference.

![Fig. 1: A satellite view of the terrain. Left - a map of the city of Sarajevo, Bosnia and Herzegovina, 43°52'0"N, 18°25'0"E; right - the terrain orography of the simulated domain and specification of the urban heat islands, pollutant emission zones, and monitoring points](image-url)
In this case different ground conditions are defined for the three distinct zones, each with a sinusoidal temperature variation ($\Delta \theta_1 = \pm 1^\circ C$ – zone 1, $\Delta \theta_2 = \pm 0.75^\circ C$ – zone 2, $\Delta \theta_3 = \pm 0.5^\circ C$ – zone 3), all superimposed on the temperature variation of the surrounding ground of $\Delta \theta_s = \pm 1^\circ C$ during a diurnal cycle. Likewise, the non-dimensional concentration emission islands (active during the day and switched-off during the night) are defined as $C_1 = 1$, $C_2 = 0.75$, $C_3 = 0.5$ for each zone respectively, whereas all major traffic roads are treated as line sources with a constant line distributions of $C_0 = 1/100m$, on which a time variation can also be imposed for a full diurnal simulations. Finally, the surface roughness ($z_0$) per-zone is defined to be 2, 1 and 0.25m, respectively for the three zones and 0.1m for the surrounding. Two different initial stable stratifications are assumed with the base of the inversion layer at 800m and 300m above the valley ground with a gradient of 4 $K/km$ in the upper atmosphere, where the transport of pollutants is solely driven by thermal buoyancy effects generated by heat islands.

The second, Case 2, focuses on a urban microscale domain, a segment of the city downtown of 2.4×1.2×0.2km where realistic urban canopy is accounted for, including all major high-rise buildings that have caused public and environmentalists’ concern. The buildings were numerically resolved down to 3.5m mesh-cell size. Detailed time-dependent multiple-street pollution sources and different approaching wind conditions (under a neutral stratification) are mimicked, similarly as in [7], [8]. Preliminary simulations were earlier performed for a slightly smaller domain of 1.75×1.2×0.2 km with steady pollution (line) sources along the streets without thermal effects. To generate realistic conditions on the domain boundaries for the urban segment (Case 2), a precursor simulation was also carried out on a domain of 1.3×1.2×0.2km, covering a portion of the terrain with its orography, but without buildings, preceding the downtown in the upwind direction.

The Fig. 2. shows the domain used for Case 2, including orography, buildings (light green), river (blue stripe), different traffic-level streets (red: 100%, orange: 50%, yellow: 10%), overlaid with satellite image of Sarajevo. Several high-rise buildings can be easily identified in the domain. In the preliminary computations (reported in the short version of this paper, THMT’15 printed proceedings), the emissions per m$^2$ of street were constant over time and there were no thermal effects. The buildings were generated manually and the domain was meshed by the rectilinear, rectangular cells. For the realistic scenario of Case 2, covering a somewhat wider terrain area was covered, mainly to take into account the effect of
neighboring streets to the concentration levels. Here, the terrain orography is taken into account, which adds some complexity; the mesh was still rectilinear but the cells were no longer rectangular. An attempt to mimic a winter morning was made here, so the beginning of the simulation corresponds to 07:00h and the simulation covers a complete hour with temporal resolution of 7.5 seconds. This period was found interesting because the sun is already up and the heating process has started and the morning traffic was estimated to peak by the end of this interval. Because of limited resources, only one hour was simulated, although a full diurnal cycle would definitely be very interesting to observe/analyze.

In this case, concentration sources are turned into time-variable sources with somewhat more realistic levels of emissions achieved by approximately classifying the streets into three groups: 100%, 50% and 10% traffic-level streets, with concentrations again being defined per m² (red, orange and yellow lines in Fig. 2, respectively) with relative concentration of 1.0 corresponding to street segments in the 100% group at the peak of the emissions (at 08:00h). Also, time-variable temperature boundaries are introduced, with a slight increase in the temperatures of the roads surfaces, the surrounding ground and east and south facades of the buildings, over time. The river acts as a heat container, with constant temperature over time.

Figure 3. shows temporal evolution of the relative concentration and temperature at different boundaries.

Figure 3: Right: Sinusoidal time variation of relative concentration of different traffic-level roads with initial value corresponding to 1/3 of the maximum value, which in turn occurs at 08:00h. Left: Linear time variation of temperature of particular objects, with initial value of -0.8°C for all, except the river which has constant temperature of 0°C.

As mentioned above, another feature of the Case 2 was the precursor simulation in a domain of 1.3×1.2×0.2km upwind from the main domain, shown in Fig. 4. This simulation was carried out to generate the inlet profile for the main microscale city domain. The precursor domain also had the orography included and time-dependent ground thermal and concentration sources, but lacked buildings for simplicity. Its primary role was to develop somewhat realistic concentration distribution profiles and even with no buildings included, it was a better choice than a generic inlet profile that would be completely unaware of the time-dependent evolution of concentration. The duration and the time-step of the precursor simulation were both equal to those found in the main domain so the outlet from the precursor domain was directly fed into the city-centre domain at the end of each time-step.
3. Results and discussion

3.1 Diurnal evolution of flow and pollutant transport in the mesoscale domain

A selection of profiles of the potential temperature, for temperature inversion at 300m (strong stratification), are shown in Fig. 5 for three characteristic phase times, (08.00, 14.00 and 02.00 hr). The close-to-uniform profiles in the mixed layer above the ground resemble qualitatively to what can be observed in the generic penetrative convection over a wall heated from below. Figure also shows the evolution and growth of the mixed layer and the erosion of the initial stable stratification from the beginning of the diurnal cycle until the temperature reaches its maximum that balances the peak ground heat flux. A higher ground temperature causes faster air heat-up, generating strong buoyancy that drives convective updraft plumes, which in turn cause very intensive heat transfer and mixing. This drives the evolution of the whole profile. Thermal plumes are very active, as shown by Fig. 5.

Figure 6 shows the temperature fields at two characteristic phase instants and local deviations from the linear inversion layer profile. The orography, combined with thermal sources, plays the key role in the deformation of the temperature profile because the hilly ground is also heated by various activities (domestic heating, traffic) and indirect solar radiation. Moreover, the topmost points of the mountain penetrate the inversion layer physically and the temperature profile is further deformed through thermal action.
Fig. 5: Left - The diurnal time-evolution of the vertical profiles of the potential temperature at characteristic location MEF (initial temperature inversion layer is at 300m); right - thermal plumes occurring during the temperature maximum, colored by the vertical velocity component $W$.

Fig. 6: Temperature field in characteristic vertical planes at different phase instants. Left – the first day heating peak, (14:00h); right - the first day cooling peak (02:00h).
Fig. 7: Diurnal time-evolution of the turbulent kinetic energy at characteristic locations for strong stratification: the Town Hall (left) and the MEF (right monitoring locations).

The effect of the terrain orography is clearly visible in the fields and profiles of the turbulent kinetic energy. The difference in the time-evolutions of the modelled turbulent kinetic energy is seen on the vertical profiles at the two characteristic monitoring locations, the Town Hall and MEF, during the first-day maximum of the ground temperature gradient. Both monitoring points are on the same altitude, but the local effects of orography differently affect the modelled turbulent kinetic energy on these two locations. First, the role of sloped terrain has to be understood properly. Since all ground is heated, there will be a layer of hotter air in the near-ground region. Where the terrain is sloped, the buoyancy naturally drives the hotter air up the slope, causing local anabatic “winds” at low heights. The monitoring location Town Hall is surrounded by hills which, as described, act as “sloped chimneys”, driving the air along their heated sides, which in turn causes “winds” around the ground at Town Hall monitoring location. As a consequence, the shear production of TKE is strong at this location, so a greater near-ground TKE maximum can be observed in Fig. 7.

The aforementioned inference can be also seen in Fig. 8, where the two characteristic locations are compared. On the Flat location (Fig. 8, upper-left), the heat island is active with the maximum intensity (+2°C relative to the initial temperature). Even small terrain peaks appear to be “attractive” locations for the “TKE mushrooms”. Based on the contours at the time instant when the temperature is minimum, it can be seen that there are higher values of TKE only around sloped terrain. Both (Fig. 8, left) show that the terrain plays very important role in the TKE production patterns. The situation is somewhat different for the Hill slice where strong inversion above certain height inhibits air movement, diminishing the production of TKE through the aforementioned “chimney” effect. On the other hand, lower zones, emerged inside the mixing layer, retain more successfully the TKE until the next heating cycle. It is expected that a comprehensive accounting for the ground roughness, primarily vegetation canopy (threes, bushes), would most probably indicate somewhat lesser effect of heated slopes due to the higher mixing due to canopy roughness. Based on the contours of cooling peak, one can see that there are higher values of TKE, but only in zones...
where the local gradient of terrain slopes are higher and for this situation the main contributor to turbulence is the shear production.

Some characteristic distributions of the vertical velocity and relative concentration for two initial stratifications are shown in Fig. 9. It can be seen that the model predicts correct pollution enhancement at a stronger stratification. Also, the convective rolls and their difference among the two cases are shown in (Fig. 9, left). A still better insight into the pollutant dispersion is given in Fig. 10 where the time-snapshots of relative concentration evolution for the two stratifications are presented. It is important to note that the difference between the two can be seen above the zone with the highest emissions. Comparing the stratifications, it is visible that pollutants are entrapped at somewhat lower height in the case of stronger stratification. Entrapment at somewhat lower height was expected, but probably due to the fact that the 300m inversion is very close to the ground, some pollution manages to escape with the help of orography and thermal plumes.
Figure 9: Contours of the vertical velocity ($W$) (left) and relative concentration (right) in characteristic vertical planes at the first day heating peak (14:00h) for two stratifications; above - weak stratification; below - strong stratification

Fig. 10: Contours of relative concentration at characteristic location at the first day heating peak: left - weak stratification : right - strong stratification at the first day heating peak
3.2 Effects of highrise building on pollutant in the city centre at neutral stratification

We begin this section with some results of the preliminary simulation of Case 1 for the city center domain of 1.75×0.75×0.2km accounting for realistic large buildings and high-rise towers. The domain was discretized by a non-uniform buildings-resolving mesh (down to 3.5m) of 614×322×52 ≈ 10.3 M control volumes. As expected, higher cell concentrations are located around and downstream the emission sources and zones with high buildings density, where air velocity is expected to be low trapping the pollutants and making it possible for the contaminants to aggregate. The relative concentration levels in characteristic planes for the city-center micro-domain for neutral stratification and a mild western wind is shown in Fig. 11.

The isosurfaces of concentration show one important finding: the buildings along and downstream from the main traffic arteries can be completely emerged in clouds of pollutants, with concentrations reaching alarmingly high levels. This can have many practical repercussions, e.g. one of the buildings hit is a busy health-care institution with daily visit of a large number of patients.

The stream-tracers and contours of the streamwise velocity at different heights indicate a complex multi-wake vertical flow pattern that has a large impact on the local levels of pollution at considered approaching wind conditions, Fig. 12. Using these simulations as tools for prediction could potentially help to design better urban landscape, where less pollution would be entrapped.
Fig. 12: Characteristic wind patterns in proximity of the most distinct high-rise buildings, with contours of the streamwise velocity at z=2m (left) and z=10m (right) planes.

Fig. 13: Streamlines affected by heated ground and buildings facades at 08:00h. The orange, dark blue, purple, black and red streamlines show substantial deviation in flow direction, with sharp uprising after the parliament building (hit by blue and orange tracers). All of the streamlines show visible mixing after the buildings. The concentration levels are also indicated by semi-translucent fog.

This above discussed simplified “sub-case” of microscale situation, served only as a basis for comparison with the more comprehensive simulations (Case 2) which account for thermal effects – heating and cooling of the ground and buildings outside walls. The flow regime is a mixed convection with an incoming air at 0.5 m/s from the east. This scenario is more realistic, but also more interesting and more challenging as it requires a more advanced turbulence modelling to account for buoyancy effects. Just for an illustration, in Fig. 13 one can observe how radically the flow field is affected after a short period of time by heat sources which are actually only a fraction of a degree warmer than the surroundings.
Another way to visually show this is by using isocontours of concentration, colored by temperature. Figure 14, left, shows exactly that, where it is confirmed that ascend of air is related to higher temperatures. As the air hits the building, it slows down and with low velocity, it stays in the thermally-susceptible region for longer period of time, thus becoming affected by buoyant forces. Interesting ideas for the solution of very high pollutant concentrations during the winter, such as the use of “thermal towers”, objects that would force the still air up into the higher atmosphere zones above the inversion layer, could be tested prior to their realization using a similar simulation to that conducted in the current work.

Turbulence kinetic energy isosurfaces show the locations of enhanced turbulent transport. It can be observed (Fig. 14, right) that due to thermal effects, not only is turbulence increased on the lee sides of the buildings, but also the air parcels behind the buildings, above their height.

Fig. 14: Left - Isosurface of relative concentration \( C/C_0 = 0.5\% \) colored by temperature. Just slightly higher temperature is needed to cause a substantial change in the velocity of the slow-speed incoming wind; Right - Isosurface of turbulence kinetic energy, colored by streamwise vertical velocity \( W \). It is clear that high-rise buildings and building arrays are dominant TKE production locations.

Combinations of all the aforementioned effects, and others, cause complex time-development of the concentration that can hardly be determined using simpler one-dimensional approaches. The best way to visualize this development is to use animation. Here, a sequence of images is shown in Fig. 15, where one can see just how the pollution develops.
4. Conclusions

Dispersion of passive pollutants from street traffic in the city of Sarajevo over a diurnal cycle during critical windless winter periods capped by inversion was simulated using the time-dependent RANS (T-RANS) approach. The simulations were performed using a three-equation algebraic-flux turbulence model (AFM) with enhanced wall functions (SAWF) that account for buoyancy effects. It is shown that this approach and the model applied replicate well the thermal convection over periodically heated and cooled horizontal or sloped ground, which stays out of reach for the standard and commonly used eddy-diffusivity models (SGDH and GGDH). The combined buoyancy effects under variable stable and unstable stratification and the terrain orography create complex thermal structures which govern the pollutant dispersion and concentration.

The method was subsequently applied to a segment of the city centre with urban canopy characterised by a number of high-rise buildings surrounded by major traffic arteries, for a quite realistic scenario of pollutant emissions and temperature variation of traffic lines, buildings, river and the surrounding ground. The simulations returned qualitatively feasible results indicating local critical zones of high pollutant concentrations.

We can conclude that the presented approach can be used as a potential tool for predicting immission at the city scale under various meteorological and emission scenarios, and thus for regulating traffic and pollutant sources in critical conditions.

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References