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COMPUTATIONAL SIMULATIONS OF HAZARDOUS SUBSTANCES' DISPERSION IN URBAN AREAS

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ABSTRACT
The possibility that terrorist groups might combine non-fissile material with conventional explosives to manufacture a radiological dispersion device (RDD), commonly called a 'dirty bomb,' has led to the need to evaluate alternative scenarios in order to devise effective strategies to prepare for, or respond to such critical events. Atmospheric dispersion of contaminants after such incidents depends on several factors in a complex manner. Therefore state of the art computational models like the micro scale flow and dispersion model QUIC should be applied for these cases. The Quick Urban & Industrial Complex (QUIC) Dispersion Modeling System is intended for applications where dispersion of airborne contaminants released near buildings must be computed quickly. In this paper wind tunnel measurements of an idealized Central-European city, Michelstadt, were used to evaluate the predictive capabilities of the model for flow and dispersion in urban areas. The reference experiments were conducted in the Meteorological Institute at the University of Hamburg. Finally the QUIC model is applied to a real urban area within the port of Keratsini (near Athens, Greece) for the case of a hypothetical detonation of a radiological dirty bomb. The isotope selected to be utilised in the construction of the bomb was Cobalt-60 (^{60}Co), in liquid form. The focus of this last part of the study is on the detailed depiction of the radioactive agent dispersion and the radiation exposure taking into account the complex street configuration to asses QUIC modelling system performance in a realistic incident of a 'dirty bomb'.

Key words: *model validation; wind tunnel studies; 'dirty bomb'; contaminants dispersion modelling; QUIC model;*

1. INTRODUCTION
The computational tool selected for the study is the Quick Urban & Industrial Complex (QUIC) Dispersion Modelling System, developed by the University of Utah and Los Alamos National Laboratory and it is freely available. The QUIC modelling system is comprised of an empirical / diagnostic 3D wind model, QUIC-URB (Röckle, 1990), a Lagrangian dispersion model, QUIC-PLUME (Brown et al., 2009) and a computational fluid dynamics code, QUIC-CFD (Neophytou et al., 2010). The dispersion of aerosols and gases can be simulated, including deposition, gravitational settling and decay. Buoyant rise for explosive releases and dense gas releases are also treated. Algorithms have been developed to account for droplet evaporation and gas-droplet two-phase plumes. The wind field inside the built-up area is calculated either by the fast (but empirical and therefore less accurate) QUIC-URB or by the slower (but more accurate) QUIC-CFD. After that dispersion is modelled by QUIC-PLUME. Short- or long-duration releases can be taken into account, as well as various types of substances (e.g., gases or particles). Air concentration, dosages and deposition on surfaces are some potential results calculated by QUIC. Wind tunnel experiments of flow and tracer dispersion in a model of a hypothetical Central-European city, called "Michelstadt", have been used to evaluate the predictive capabilities of the model in urban areas. The reference experiments were conducted in the Meteorological Institute at the University of Hamburg. The measurements used for the study concerned the flow pattern and the concentration distribution of an ideal passive gas for the cases of short term and continuous releases in a 1:225 - scale model of the idealized urban geometry.
Finally the QUIC model has been set up to run for the port of Keratsini (near Athens, Greece). The extensive analysis of the most appropriate urban areas in Athens has led to the decision of the QUIC model's implementation in the greater area of Keratsini Port. The selection's criteria taken into consideration were the high daily turnover as well as the existence of plenty locations where a 'dirty

bomb' could be hidden. The 'dirty bomb' has been hypothetically created by combining solution of ^{60}Co in acid (liquid form) with TNT explosives. The isotope ^{60}Co is widely available from industrial, food sterilization and medical applications. Due to its relatively long half-life (5.27 years) it could be acquired and stored over an extended period for later incorporation into such a device. It is a beta and especially gamma emitter with high specific activity and an appreciable range of irradiation making an ideal substance in this type of weapon. A considerable part of the contamination is anticipated to be dispersed as fine particles and contaminate a rather large area. The QUIC modelling system is intended for applications like this, where dispersion of airborne contaminants released near buildings must be computed quickly and accurately. The QUIC fast-response urban dispersion modelling system has the potential to compute the three-dimensional wind, concentration, dosage and deposition patterns, as well as the inhalation pathways of airborne contaminants around clusters of buildings.

2. QUIC MODEL SIMULATIONS

2.1. Domain characteristics and meteorological simulation data

The QUIC model is normally run with a building-resolved grid. For the needs of the Michelstadt project the buildings data have been manually imported in the computational domain of QUIC. The full scale (fs) domain consisted of 60 building rings with flat roof which are irregularly placed. Three different building heights were used, 15, 18 and 24 m. The buildings width was 15 m and two street widths of 18 and 24 m were used. It should be also noted that all simulations have been performed in full scale on the computational domain that is defined by a rectangular area of 1500 m along-wind, 1000 m cross-wind and 200 m height. In addition the city model is approached by a fully developed atmospheric boundary layer flow with roughness height z_o = 1.53 m. The vertical profile of the mean velocity in flow direction is best approximated by a power law with exponent $\alpha = 0.27$, consistent with the roughness height. For the Keratsini port simulation 6431 buildings have been imported in the form of polygons via GIS shape files in the domain which is defined by an area of 2000 m west to east, 2000 m south to north and height of 400 m. The wind speed is a function of height. For both cases the power-law profile has been selected. The value of 6.1 ms^{-1} was attributed for the Michelstadt case to the stream wise reference velocity defined at the reference height of 100 m while the wind direction was considered to be 0^o, along x axis. For the Keratsini case the value of 2 ms^{-1} was defined as the wind velocity at the reference height of 10 m while the wind direction was considered to be 225^o. The aforementioned values of the meteorological parameters have been set in order to establish the worst meteorological conditions in regard with the contaminant's dispersion and the radiation exposure.

2.2. Source Properties and Simulation Parameters

For the simulations needs of the Michelstadt case two source release types were considered, namely the continuous and the finite duration (29 s) types. The selected sources were the ground sources S2, S4 and S5. The flow rate of the pollutant was 0.5 kgs^{-1}.For the 'dirty bomb' incident a source term of 91 g of ^{60}Co isotope equaling 3.7×10^{15} Bq (10^5 Ci) with an instantaneous release by 9 kg of TNT explosives at street level was assumed in order to evaluate the consequences of radiological dispersion under the worst case scenario. The release of kinetic and thermal energy when the 'dirty bomb' explodes causes the initial dispersion (1 Kg of TNT generates 4.2 MJ of heat). Thus it was assumed that ^{60}Co isotope, in the form of vapours, (Harper et al., 2007) was immediately released into atmosphere when detonation occurs. Furthermore 100% of the source term was considered to be airborne (Regens et al., 2007) and 100% of the radioactive particles were considered to be respirable ($\leq$10 μm in diameter) in order to take into account the worst case scenario.

2.3. Sensors' characteristics and validation data

Flow data in terms of time series and derived statistics are published in the CEDVAL-LES online validation database, (www.mi.uni-hamburg.de/CEDVAL-LES-V.6332.0.html, cp. Fischer et al., 2010) together with descriptions of the wind-tunnel setup and all relevant details of the model geometry. At each measuring position the horizontal time averaged velocity components and their variances are available. In the database also time series are provided, as it is dedicated to validation of time dependent simulations. In addition there are in total 104 concentration measurement positions. Measured concentration time series as well as time averaged concentrations are available in the above database.

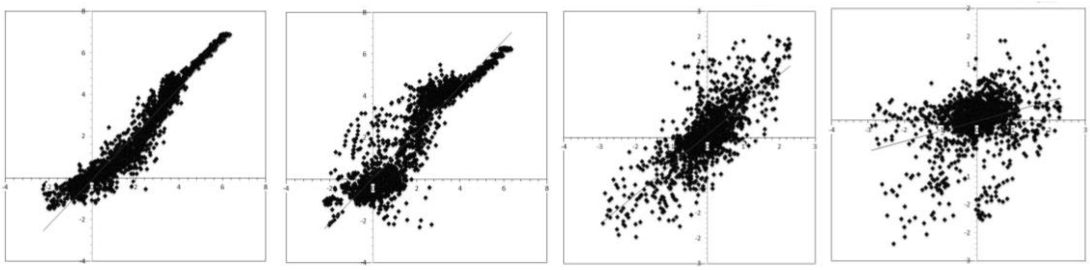
2.4. Simulations

The numerical flow simulations for the Michelstadt case have been performed using the empirical-diagnostic code QUIC-URB and the computational fluid dynamics code QUIC-CFD. For the present study both codes modelled the turbulent flow for neutral atmospheric stability conditions. Afterwards simulations with the QUIC-PLUME code have been performed for both cases. In reality the simulations are consisted of two cases of one-way coupled models: (1) QUIC-URB with QUIC-PLUME model and (2) QUIC-CFD with QUIC-PLUME model. For each available source (S2, S4, S5) and for each type of release (continuous, short-term) both model combinations were applied (i.e., 12 simulations in total). For the 'Dirty Bomb' scenario the coupling of QUIC-URB with QUIC-PLUME modelling system was implemented.

3. RESULTS AND CONCLUSSIONS

3.1. Results

The two horizontal components of the mean wind flow, U the streamwise wind component and V the perpendicular to the mean wind flow component, were compared to the corresponding components of measured wind flow for the Michelstadt case. This comparison was carried out for each model separately and is presented via scatter plots in figure 1.



a. CFD modelled values of U component (Y axis) vs measured values (X axis)	**b.** URB modelled values of U component (Y axis) vs measured values (X axis)	**c.** CFD modelled values of V component (Y axis) vs measured values (X axis)	**d.** URB modelled values of V component (Y axis) vs measured values (X axis)

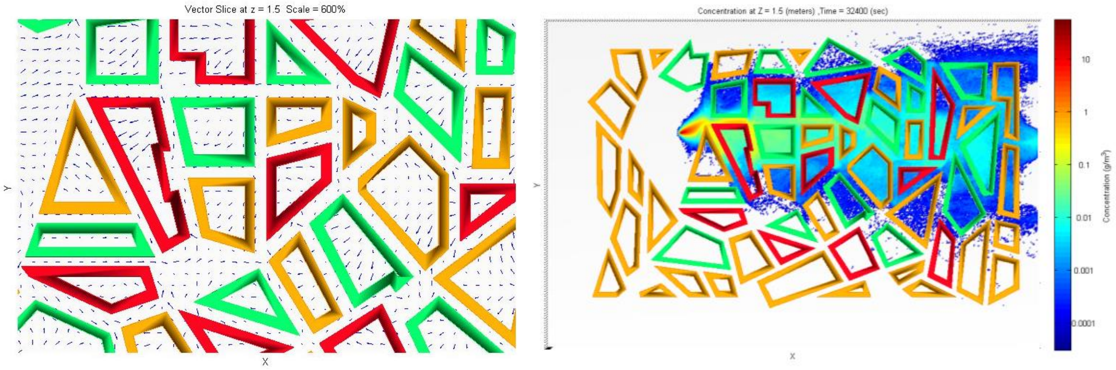
Figure 1. Comparison of the horizontal components of the wind simulated by CFD and URB codes with the corresponded measured values.

Furthermore the distribution contours of wind field and concentration at several horizontal levels have also been plotted for each coupling system and source scenario. The wind field pattern near the surface extracted by QUIC-CFD model (Figure 2.a.) and the horizontal distribution of concentration, simulated with QUIC-PLUME model, for continuous releases from S2 source (Figure 2.b.) have been selected for demonstrations reasons. The influence of the different code used for each case on the numerical concentration results was mainly investigated by comparison with experimental data. The statistical analysis of simulated concentration's values in ppm for each model and for each source versus the respective measurements is illustrated in table 1 for the case of continuous releases. The statistical indices that have been used are the correlation coefficient, bias, fractional bias, geometric mean bias, geometric variance, normalized mean square error, factor of exceedance and factor of two.

Table 1. Statistical analysis of modelled concentration's values in ppm for the case of S2, S4 and S5 source's continuous releases

Statistical_Index	CFD-S2	URB- S2	CFD-S4	URB-S4	CFD-S5	URB-S5
BIAS	14.805	16.049	37.358	9.237	25.461	-8.292
NMSE	4.184	4.173	30.560	5.075	17.220	6.075
FOEX	-1.852%	9.259%	-10.000%	-14.000%	-4.545%	-27.273%
PCC	0.948	0.755	0.098	0.608	0.854	0.040
MG	1.235	2.300	1.083	0.788	0.501	1.113
VG	3.850	5.367	10.222	15.543	11.011	23.501
FAC2	57.407%	22.222%	44.000%	28.000%	45.455%	9.091%
FB	0.669	0.705	0.889	0.330	0.660	-0.382

The dispersion results for puff releases were compared with the ensemble average measured values (Table 2). The selected parameters are the maximum concentration (pc avg) in ppmV, the dosage in ppmVs and the time of occurrence of peak concentration (pt avg) in sec. The aforementioned parameters have been computed for time intervals of 15 s.

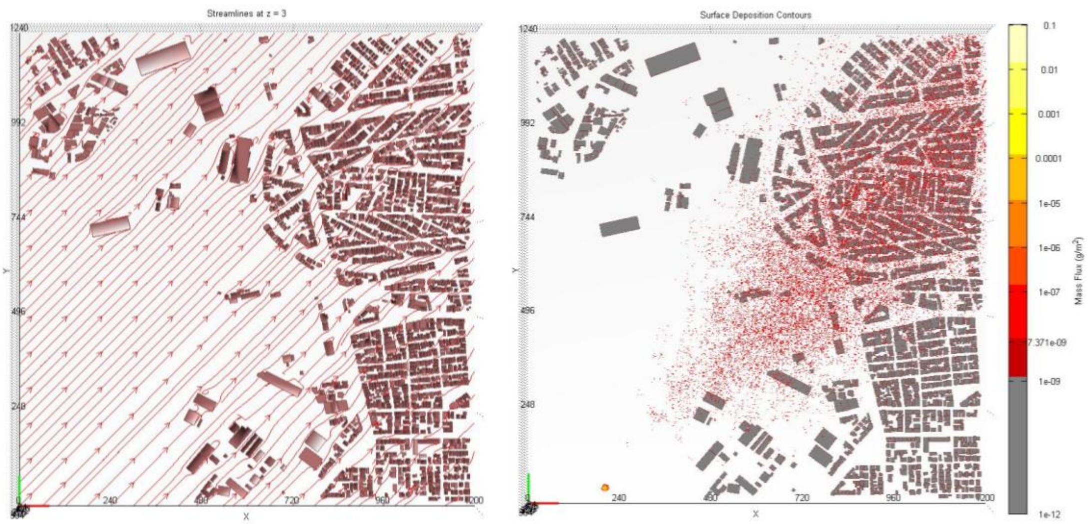


(a) **(b)**

Figure 2. 2D Illustrations for Michelstadt case. **a.** Wind field in ms^{-1} at street canyons (1.5m) in the small domain extracted by QUIC-CFD model. **b.** Horizontal distribution of concentration in gm^{-3}, simulated with QUIC-PLUME model, for continuous releases from S2 source at the height of 1.5 m.

Table 2. Comparison of critical modelled parameters for the case of S2, S4 and S5 source's puff releases with the corresponded values measured at 8 different locations (sensors).

	AVERAGE_MEASURED			CFD SIMULATED			URB SIMULATED		
SENSOR	**pc avg**	**Dosage**	**pt avg**	**pc avg**	**dosage**	**pt avg**	**pc avg**	**Dosage**	**pt avg**
S2P7	35.85	2797.84	117.15	53.50	3668.60	120	46.31	2675.92	105
S2P19	18.35	2042.57	110.27	1.14	298.55	435	4.96	492.61	180
S2P22	14.11	1734.04	148.75	25.25	2665.13	195	2.44	415.83	210
S4P5	24.68	3522.31	161.44	8.20	1976.23	180	18.65	2343.09	120
S4P9	24.17	3825.23	174.92	6.63	1332.98	225	31.30	4295.67	180
S5P2	10.79	1946.93	204.05	12.94	1694.86	240	1.97	361.30	135
S5P9	22.45	3240.81	190.14	0.63	67.03	195	0.00	0.00	0
S5P10	29.64	3136.09	137.43	0.36	47.38	150	1.03	136.95	180



(a) **(b)**

Figure 3. Depiction of the wind flow pattern near the surface at Keratsini port with streamlines produced by QUIC-URB simulations (a) and illustration with URB-PLUME simulations of ^{60}Co isotope's surface deposition (b).

For the case of ‘Dirty Bomb’ incident the QUIC-URB simulation for the wind flow streamlines is illustrated in Figure 3.a. From the 3D simulations of QUIC-Plume model it appears that the plume produced by the detonation of the RDD reaches a height of 400 m and leaves the modelling domain after only 1000 s. The surface deposition of the contaminant in gm^{-2} after 1200 s is illustrated in figure 3.b. For public areas one contamination limit is 0.3 $Bqcm^{-2}$ (8.1 $pCicm^{-2}$) averaged over an area not to exceed 100 cm^2 for all Class A radionuclides like ^{60}Co. The value 8.1 $pCicm^{-2}$ corresponds to the radioactivity of $7.371x10^{-9}$ g ^{60}Co scattered at a surface of 1 m^2. This specific value in gm^{-2} is used in figure 3.b. as threshold value (red coloured).

3.2. Conclusions

As can be seen from figure 1 the simulated values of U and V wind components calculated by the QUIC-CFD model show a better agreement with the measurements compared to the QUIC-URB simulation results. That leads to the conclusion that the wind flow extracted by the QUIC-CFD code is more realistic than the one extracted by the QUI-URB code. The figure 2.a. shows that the wind flow is significantly modified by the street canyons’ characteristics especially within the canyons. The figure 2.b. shows that the concentration distribution pattern at the height of 1.5 m is mainly depended on the building characteristics as well as on the source location. Moreover when the source is located at an atrium (S2) the wind flow can easily disperse the pollutant in the urban canopy. For the case of ideal gas continuous releases, the statistical analysis (Table 1) showed that concentration measurements were better correlated with the simulation results of QUIC-CFD than QUIC-URB code especially for the cases of source S2 and S5. Both models performed a slight overestimation of measurements for the cases of source S2 an S4. On the other hand a moderate underestimation of S5 measured values was resulted from QUIC-URB simulations. For the case of ideal gas puff releases the statistical analysis (Table 2) showed that both models underestimate the measured dosage and the peak averaged concentration (pc avg) in most of the cases. The overall estimation is that both model results show a satisfactory agreement with the measured values in most cases. The much shorter computational times required by QUIC-URB compared to those of QUIC-CFD (minutes compared to hours) indicates that the combination of QUIC-URB with QUIC-PLUME is an appropriate selection of the purposes of the current project.

For the RDD project it is obvious from the figure 3.b. that the contamination limit has been exceeded in all the red marked area. The modelling results also revealed that there is a relatively small circular area with centre the location of the ‘dirty bomb’ where the limit is greatly exceeded (orange coloured) as it was expected. Furthermore for the hypothetical conditions considered for the simulations it is evident that the contamination area (red coloured area) expands from a distance of 200 m downwind the source to the edge of the domain. In this area, significant exposure could occur from groundshine. Moreover the analysis demonstrates that the actual plume trajectory due to its rapid dynamical movement, downwind the source and across the domain reaching at a significant altitude, has the potential to affect also the public health beyond the modelling domain.

4. REFERENCES

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