COMPUTATIONAL SIMULATIONS OF HAZARDOUS SUBSTANCES’ DISPERSION IN URBAN AREAS

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• The purposes of radiological terrorists events are to inflict panic on the public and to create casualties, disruption of the economy and potentially desertion of the contaminated area.
• Highly populated urban areas would potentially be the primary target for an RDD attack to maximize the impact.
• The possibility that terrorist groups might use an RDD, has led to the need to develop strategies to be prepared for, or respond to such critical events.

Radiological Dispersion Device (RDD) or ‘dirty bomb’.
• A ‘dirty bomb’ is the combination of a conventional explosive device with radioactive materials widely available from industrial, food sterilization and medical applications.
• The contaminants are radioactive isotopes. A considerable part of the contamination is anticipated to be dispersed as fine particles and contaminate a rather large area.
AIM OF THE STUDY

• The focus of this study is on the detailed depiction of contaminants dispersion and ground deposition for the case of a hypothetical detonation of a dirty bomb within the port of Keratsini.

• The worst case scenario for the meteorological data and initial amount of the radioactive material was considered.

Several state of the art fast and accurate micro scale flow and dispersion computational models have been developed in order to be applied for cases such the above. Why?

• Fast models are essential for studies where an answer is needed quickly.

• Atmospheric dispersion of contaminants after such incidents depends on several factors in a complex manner.

• Dispersion of airborne contaminants released especially near buildings must be computed accurately and quickly for reasons of optimization of the RDD emergency-response planning.
The Quick Urban & Industrial Complex (QUIC) Dispersion Modeling System has been selected for the aforementioned application. The model has been developed by the University of Utah and Los Alamos National Laboratory and is freely available.

The modelling system uses empirical algorithms (QUIC-URB model) and mass conservation to estimate the wind velocities around buildings quickly and accurately (Röckle, 1990).

Transport and dispersion for different types of airborne contaminants can be computed by the QUIC-PLUME Lagrangian dispersion model on building to neighborhood scales in tens of seconds to tens of minutes (Brown et al., 2009).
MODEL DESCRIPTION

- The QUIC modelling system is comprised of a 3D wind model, QUIC-URB; a Lagrangian transport and dispersion model, QUIC-PLUME; and a graphical user interface, QUIC-GUI.
- The QUIC-PLUME Lagrangian random-walk dispersion model tracks the movement of particles as they disperse through the air, computing concentration and deposition fields around buildings.
- The QUIC-PLUME model utilizes the mean wind fields computed by the 3D empirical-diagnostic QUIC-URB model and produces the turbulent dispersion of the airborne contaminant.
- A simple computational fluid dynamics code called QUIC-CFD has been added to QUIC as a wind solver option.
- In order to make the QUIC-CFD code faster than traditional CFD codes, a simple one-equation turbulence model has been used.
MODEL VALIDATION

Wind Tunnel Setup

• Wind tunnel measurements of an idealized Central-European city, called ‘Michelstadt’, have been used to evaluate the simplified codes used in QUIC model.
• The reference experiments were conducted in the boundary layer wind tunnel facility of the Meteorological Institute at the University of Hamburg.
• An open-return boundary-layer wind tunnel with a closed test section of 18 m length and 4 m width has been used.
  ➢ Scale 1:225.
  ➢ Simulation tests in full scale.
  ➢ 60 building rings.
  ➢ Three different building heights (15, 18 and 24 m).
  ➢ Fully developed atmospheric boundary layer.
  ➢ Roughness height $z_o = 1.53$ m.
MODEL VALIDATION

Wind Flow Database – Simulation Domain

- Validation database: time series of flow data and relevant statistics. The wind flow measurements (2158 measurement positions) were carried out with a 2D Laser Doppler Anemometer (LDA).
- Reference velocity = 6.1 m/s defined at the reference height of 100 m. Wind direction = 0°, along x axis (from West to East).
- Computational domain: 1500 m length, 1000 m width, 200 m height.

- Large domain (450 m × 787.5 m) - 559 points, 40 vertical profiles and 18 horizontal levels (2 - 111 m)
- Small domain (300 m × 300 m) - 1599 points at elevations of 2 m, 9 m, 18 m, 27 m and 30 m.
MODEL VALIDATION

Wind Flow Simulations - Results

- The QUIC-URB and QUIC-CFD codes modelled the turbulent flow within the simulation domain separately and solve their equations for mass and momentum of a fully turbulent and isothermal flow.
- The vertical profile of the mean velocity is best approximated by a power law with exponent $\alpha = 0.27$.

**Figure 1.a.** Horizontal streamlines at 7.5 m extracted by QUIC-CFD model

**Figure 1.b.** Horizontal streamlines at 7.5 m extracted by QUIC-URB model.
Figure 2. Wind field in the small domain at the levels of 1.5m and 28.5m extracted by the QUIC-CFD (a and c) and QUIC-URB (b and d) codes.
MODEL VALIDATION

Wind Flow Simulations - Results

Figure 3. Comparison of the horizontal components of the wind simulated by CFD and URB codes with the corresponded measured values via scatter plots.

The scatter plots show:

- The simulated values of U component produced by the QUIC-CFD model show a very good agreement with the respective measured values in compare to the poor agreement of QUIC-URB model.
- The V wind component exhibits the same behavior although not so intensively.
As can be seen from the figures 1 and 2:
- The wind flow is significantly modified by the street canyons’ characteristics especially within the canyons.
- Above the urban canopy the mean wind flow has gradually become parallel to x axis.
- The difference between the distribution patterns of the wind flow extracted by the two models is more than evident.
- The greatest agreement with the measurements by both models is achieved at heights approximately above 28 m where the wind flow has become parallel to x axis.

As can be seen from the figure 3 (scatter plots):
- The wind field features were very well reproduced by the simulations especially of the QUIC-CFD model.
- The overall wind flow pattern is very well illustrated by the QUIC-CFD rather than the QUIC-URB model.
MODEL VALIDATION
Concentrations Database – Sources Setup

• Validation database: Measured concentration time series as well as time averaged concentrations of released Ethane in the domain.
• The concentration measurement positions are classified in two groups: one group of sensors with respect to sources of continuous release and another of short term release.
• Concentrations were measured in the urban area with a fast Flame Ionisation Detector (FID).
• 104 concentration measurement positions are available.
• The locations of the ground sources used in model simulations are depicted with black dots.
**MODEL VALIDATION**

**Sources Setup**

<table>
<thead>
<tr>
<th>Source</th>
<th>Continuous releases</th>
<th>Short term releases</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pollutant</td>
<td>ethane – M = 28.97 g/mol (Idealized tracer gas)</td>
<td></td>
</tr>
<tr>
<td>Density</td>
<td>1.2043 kg/m³</td>
<td></td>
</tr>
<tr>
<td>Duration</td>
<td>-</td>
<td>29 s</td>
</tr>
<tr>
<td>Flow rate</td>
<td>0.5 kg/s</td>
<td>-</td>
</tr>
<tr>
<td>Total mass</td>
<td>-</td>
<td>10 kg</td>
</tr>
<tr>
<td>Geometry</td>
<td>cylinder with diameter 0.8 m and height 1 m.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sensors for S2</th>
<th>Continuous releases</th>
<th>Short term releases</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>57 in one Horizontal plane at 7.5m and 3 vertical profiles</td>
<td>3 in one Horizontal plane at 7.5m (S2P7-S2P19-S2P22)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sensors for S4</th>
<th>Continuous releases</th>
<th>Short term releases</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>25 in one Horizontal plane at 7.5m</td>
<td>2 in one Horizontal plane at 7.5m (S4P5-S4P9)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sensors for S5</th>
<th>Continuous releases</th>
<th>Short term releases</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>22 in one Horizontal plane at 7.5m</td>
<td>3 in one Horizontal plane at 7.5m (S5P2-S5P9-S5P10)</td>
</tr>
</tbody>
</table>
MODEL VALIDATION

Simulations Setup – Results for Ideal Gas Continuous Releases

<table>
<thead>
<tr>
<th>Simulation set up</th>
<th>Continuous releases</th>
<th>Short term releases</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time step (s)</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>Duration (s)</td>
<td>36000</td>
<td>1200</td>
</tr>
<tr>
<td>Number of particles</td>
<td>1080000</td>
<td>1009026</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Statistical Index</th>
<th>CFD-S2</th>
<th>URB-S2</th>
<th>CFD-S4</th>
<th>URB-S4</th>
<th>CFD-S5</th>
<th>URB-S5</th>
</tr>
</thead>
<tbody>
<tr>
<td>NMSE</td>
<td>4.184</td>
<td>4.173</td>
<td>30.560</td>
<td>5.075</td>
<td>17.220</td>
<td>6.075</td>
</tr>
<tr>
<td>FOEX</td>
<td>-1.852%</td>
<td>9.259%</td>
<td>-10.000%</td>
<td>-14.000%</td>
<td>-4.545%</td>
<td>-27.273%</td>
</tr>
<tr>
<td>PCC</td>
<td>0.948</td>
<td>0.755</td>
<td>0.098</td>
<td>0.608</td>
<td>0.854</td>
<td>0.040</td>
</tr>
<tr>
<td>MG</td>
<td>1.235</td>
<td>2.300</td>
<td>1.083</td>
<td>0.788</td>
<td>0.501</td>
<td>1.113</td>
</tr>
<tr>
<td>VG</td>
<td>3.850</td>
<td>5.367</td>
<td>10.222</td>
<td>15.543</td>
<td>11.011</td>
<td>23.501</td>
</tr>
<tr>
<td>FAC2</td>
<td>57.407%</td>
<td>22.222%</td>
<td>44.000%</td>
<td>28.000%</td>
<td>45.455%</td>
<td>9.091%</td>
</tr>
<tr>
<td>FB</td>
<td>0.669</td>
<td>0.705</td>
<td>0.889</td>
<td>0.330</td>
<td>0.660</td>
<td>-0.382</td>
</tr>
</tbody>
</table>

- It is evident that both models perform a moderate overestimation of measured values for the cases of source S2 an S4 and moderate underestimation of S5.
MODEL VALIDATION
Results for Ideal Gas Continuous Releases

Figure 4. Comparison of concentration’s vertical distribution for S2 source, extracted from the two models’ simulations separately with measurements at 3 different points.

- In most of the cases an increasing (from the ground to the height of 30 m) tendency of overestimation by both models of measured values is evident.
- The QUIC-URB model seems to keep at underestimating the measured values at heights above 30 m with the exception of S2P11.
MODEL VALIDATION
Results for Ideal Gas Continuous Releases

CONTOURS OF CONCENTRATION’S HORIZONTAL DISTRIBUTION AT THE HEIGHT OF 1.5m
MODEL VALIDATION
Results for Ideal Gas Continuous Releases

Figure 5. Simulations with QUIC-CFD model are illustrated on (a), (c) and (e) pictures for S2, S4 and S5 sources respectively. Simulations with QUIC-URB model are illustrated on (b), (d) and (f) pictures for S2, S4 and S5 sources respectively.

- Wherever the source is located at an atrium (S2) the wind flow can disperse the pollutant in the urban canopy more easily than if the source’s location (S4, S5) was at the leeward side of a street canyon.
- The figures show a very good agreement between the two models in predicting the distribution pattern of an ideal gas concentration near the ground
MODEL VALIDATION
Conclusions for the case of Ideal Gas Continuous Releases

• From Table 1 it is obvious that the concentration measurements are better correlated with the simulation results of QUIC-CFD than QUIC-URB code.
• Figure 4 shows in most of the cases an increasing in relation to the height tendency of overestimation by both models of measured values from the ground to the height of 30 m.
• The QUIC-CFD model shows an essential agreement with the measured values at heights above 30 m.
• Both models are frequently perform a slight overestimation of measurements.
• Figure 5 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.
• Overall the QUIC-CFD model’s results are in better agreement with measured values than the QUIC-URB model results.
MODEL VALIDATION
Simulations - Results for Ideal Gas Short Term Releases

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).

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

- The dispersion results are directly compared with the average measured values
- **pc avg**: the maximum average value of concentration in ppmV computed for time intervals of 15 s
- **pt avg**: the corresponding time in s, for the aforementioned value.
MODEL VALIDATION
Simulations - Results for Ideal Gas Short Term Releases

CONTOURS OF DOSAGE’S HORIZONTAL DISTRIBUTION AT THE HEIGHT OF 7.5m
Figure 6. Simulations with QUIC-CFD model are illustrated on (a), (c) and (e) pictures for S2, S4 and S5 sources respectively. Simulations with QUIC-URB model are illustrated on (b), (d) and (f) pictures for S2, S4 and S5 sources respectively.

- The crucial factors that define the parameters of dispersion are the direction of the mean wind flow and the specific characteristics of the urban canopy.
- As can be seen in figure 6, the greatest dosage values occurred close to the source for all cases.
MODEL VALIDATION

Conclusions for Ideal Gas Short Term Releases

- The statistical analysis (Table 2) for the dispersion concluded that both models underestimate the measured dosage and the peak 15s averaged concentration (pc avg) in most of the cases.
- The overall conclusion is that the QUIC-CFD model exhibits a slightly better agreement with the measurements than the QUIC-URB model.

Main Findings

- The wind flow pattern is very well illustrated by the QUIC-CFD rather than the QUIC-URB model.
- Both model results show a very good agreement with the measured values in most cases.
- The dispersion’s results provided by QUIC-URB code were frequently worse than the results provided with the QUIC-CFD code.
- 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.
MODEL PERFORMANCE IN A ‘DIRTY BOMB’ INCIDENT
Simulation Domain – Source Properties

- The combination of QUIC-URB with QUIC-PLUME 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 focus of the study is on the detailed depiction of the radioactive agent dispersion taking into account the complexity of the street.
- 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.
- 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).
- The isotope selected to be utilised in the construction of the bomb was Cobalt-60 (\(^{60}\)Co), in liquid form.
- Cobalt-60 is a beta and especially gamma emitter with high specific activity making an ideal substance in this type of weapon.
MODEL PERFORMANCE IN A ‘DIRTY BOMB’ INCIDENT

Simulation Domain

Horizontal Dimensions: 2 km x 2 km

Coordinates of the Southwest corner in GRS80 (Geodetic Reference System 1980):
X = 464367.0 m, Y = 4199777.0 m

The map data was provided by the National Statistical Agency of Greece for the reference year of 2001
MODEL PERFORMANCE IN A ‘DIRTY BOMB’ INCIDENT

Computational Domain – Simulation Parameters

- Wind velocity = 2 m/s at the reference height of 10 m.
- Wind direction = 225° (towards the densely populated area).
- The wind speed is a function of height. The power-law profile ($\alpha=0.27$) has been selected.
- Height of the Domain = 500 m

<table>
<thead>
<tr>
<th>PARAMETERS</th>
<th>VALUE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Particles</td>
<td>$2\times10^5$</td>
</tr>
<tr>
<td>Time Step (s)</td>
<td>1</td>
</tr>
<tr>
<td>Duration (s)</td>
<td>1200</td>
</tr>
<tr>
<td>Conc. Average Time (s)</td>
<td>100</td>
</tr>
</tbody>
</table>

Figure 7. Input domain (green sector) of the QUIC model’s implementation in the urban area of Keratsini Port.
### Source Properties - Simulation Parameters

<table>
<thead>
<tr>
<th>Half Life (years)</th>
<th>Radiation Type</th>
<th>Mass Corresponding to $3.7 \times 10^{13}$ Bq Release (g)</th>
<th>Physico-Chemical Form of Source</th>
<th>Amount Used in Dirty Bomb (Ci)</th>
<th>Mass Used in Dirty Bomb (g)</th>
<th>High Explosive Used–TNT (kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.27</td>
<td>beta and gamma</td>
<td>0.91</td>
<td>Metal – soluble in acid (Liquid)</td>
<td>100000</td>
<td>91</td>
<td>9</td>
</tr>
</tbody>
</table>

- It is assumed that $^{60}$Co isotope, in the form of vapours, has been immediately released into atmosphere when detonation occurs (due to thermal energy).
- 100% of the source term was considered to be airborne (and 100% of the radioactive particles were assumed to be inhalable ($\leq 10 \mu m$ in diameter) in order to take into account the worst case scenario.
- The value 13.8 L/min was used for the breathing rate (EPA’s guidelines).
Figure 8. Depiction of the wind flow pattern at the height of 3 m (a) and 15 m (b) at Keratsini port with streamlines produced by QUIC-URB simulations.
Figure 9. Illustration of the temporal evolution of the contaminant’s plume produced by 3D simulations of the QUIC-Plume model at Keratsini port (in g/m³).
Figure 10. Illustration of the temporal evolution of the contaminant’s plume produced by 3D simulations of the QUIC-Plume model at Keratsini port (in g/m³).
MODEL PERFORMANCE IN A ‘DIRTY BOMB’ INCIDENT
Simulations - Results

Figure 11. Illustration of the temporal evolution of the contaminant’s plume produced by 3D simulations of the QUIC-Plume model at Keratsini port (in g/m$^3$).
MODEL PERFORMANCE IN A ‘DIRTY BOMB’ INCIDENT
Simulations - Results

Figure 12. Illustration of the temporal evolution of the contaminant’s plume produced by 3D simulations of the QUIC-Plume model at Keratsini port (in g/m$^3$).
Figure 13. Illustration of the temporal evolution of the contaminant’s plume produced by 3D simulations of the QUIC-Plume model at Keratsini port (in g/m³).
Figure 14. Contour of the dosage’s horizontal distribution of the contaminant at the height of 1.3 m (time = 1000 s) produced by the QUIC-Plume model at Keratsini port.
Figure 15. Illustration of the contaminant’s surface deposition in gm$^{-2}$ after 1200 s produced by the QUIC-Plume model at Keratsini port.
Figure 16. Horizontal distribution of the contaminant’s total internal dose at the height of 1.3 m (time = 1000 s) produced by the QUIC-Plume model at Keratsini port.
MODEL PERFORMANCE IN A ‘DIRTY BOMB’ INCIDENT

Discussion - Conclusions

• From the 3D simulations of QUIC-Plume model (Figures 9-13) it appears that the contaminant’s plume produced by the detonation of the RDD reaches a height of 450 m and leaves the modelling domain after only 1000s.

• Safety Office, University of Waterloo, Ontario, Canada. Regulatory limits of contamination for public areas:
  • 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 7.371\(\times\)10\(^{-9}\) g \(^{60}\)Co scattered at a surface of 1 m\(^2\).
  • The value 7.371\(\times\)10\(^{-9}\) in gm\(^{-2}\) is used as an approximated threshold value (red colour) in the distribution of contaminant’s surface deposition (Figure 15).
Overall Conclusions

• From the figure 15 it has been roughly estimated that the limit of contamination has been exceeded in all the orange marked area.
• It is evident that the contamination area (red-orange coloured area) expands downwind the source to the edge of the domain.
• In the above area, significant exposure could occurred from groundshine as well as substantial radioactive absorption received from contaminant’s inhalation (Figure 16).
• 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.