3D SIMULATION OF THE DISPERSION IN THE URBAN ENVIRONMENT IN CASE OF AN EXPLOSION USING TESATEX PRE-PROCESSOR AND MICRO-SWIFT-SPRAY MODELLING SYSTEM

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Abstract: TESATEX was developed to evaluate the source term generated by an open-air explosion with or without obstacles. It lies on deeply modified SARRIM and HOTSPOT models. TESATEX can take account of the wind field influenced by buildings. It was operated with Micro-SPRAY but could be run with any other dispersion model. Experimental validation of TESATEX and Micro-SPRAY was successfully carried out using ‘Double Tracks’ in-field test measurements. Applications of TESATEX – Micro-SWIFT-SPRAY modelling system are shown in the paper. Explosions of Radiological Dispersal Devices (RDD) or ‘dirty bombs’ have been simulated in Oklahoma City (downtown) and Paris (Concorde square district). The radiological pollutants dispersion is strongly influenced by the streets network and the initial cloud configuration. Dispersion results have been post-processed to assess the radiological impact of the considered hypothetical events.

Key words: TESATEX, explosion, stabilized cloud, experimental validation, Micro-SWIFT-SPRAY, RDD, urban environment.

1. INTRODUCTION AND OBJECTIVES

Unexpected explosions occurring in case of an industrial accident or a terrorist attack (probably perpetrated in town) can bring out the sudden atmospheric release of noxious materials, as different as radionuclides or chemicals. The resulting pollutant cloud cannot be considered as coming from a point source located on the ground or at a given height. It has complex geometry and particles distribution and must be modelled in a way to adequately assess the dispersion and potential health impact of the release. On the other hand, the source term modelling should be simple enough to be consistent with operational numerical tools fit for emergency response.

Along with these requirements, the TESATEX module has been designed to evaluate the initial distribution of the pollutants in the cloud generated by an explosion. TESATEX is intended to be used as a pre-processor coupled with 3D Gaussian puff or Lagrangian dispersion codes. In this work, the computations were done with the Micro-SWIFT-SPRAY (MSS) suite dedicated to the urban atmospheric environment (ARIA Technologies, 2005). Micro-SWIFT is a mass consistent diagnostic 3D wind model in which the effects due to the buildings are represented by empirical flow zones. Micro-SPRAY is a 3D Lagrangian particle dispersion model taking account of the rebounds on buildings as well as local turbulence. MSS offers an alternative to CFD quick response capability to simulate the flow field and dispersion processes at the lower urban scale.

Basically, TESATEX is an evolution of SARRIM (Stratified Atmosphere Release of Rockets Impact Model) which was developed by ARIA Technologies and the CNES (French spatial Agency) to evaluate the environmental impact of launchers trials or accidents on a terrain without obstacles (Cencetti et al., 2007). Nevertheless, the modelling in SARRIM was modified to deal with less energetic explosions than launchers explosions and events happening in constructed areas where the buildings influence the cloud shape.

TESATEX also uses the empirical mass distribution in the initial cloud as predicted by HOTSPOT Gaussian model (Homann, 1994). HOTSPOT has been developed since 1985 at Lawrence Livermore National Laboratory and is still used by the US Department of Energy (DOE) notably. The TESATEX module combining SARRIM and HOTSPOT sounds a good compromise between accuracy in physical description and quick computing requirement. It has the major advantage to make the initial cloud evaluation not depending on any dispersion code.

This paper presents (1) the main physical principles implemented in TESATEX, (2) the validation of TESATEX in the case of open field trials on a flat terrain (Operation ‘Roller Coaster’, Nevada, US), and (3) various applications of TESATEX to hypothetical explosion and dispersion cases in Paris (France) and Oklahoma City (US).

2. PHYSICAL MODELLING

TESATEX is a pre-processor dealing with the source term released in the atmosphere from the explosion time to the cloud stabilisation time. The explosion effect is to release mechanical and thermal energy causing materials ejection. As surrounding air is carried along, the cloud reaches its stabilized state. From this moment, the cloud development does no more depend on the energy provided by the explosion. The subsequent dispersion of the cloud is simulated by the dispersion code linked to TESATEX (in this work, Micro-SWIFT-SPRAY).

Cloud stabilisation

In TESATEX the stabilized cloud is represented by a sphere on top of a cylinder with dimensions pending on the height reached by the cloud. The stabilisation height depends on the atmospheric stability, which is determined by the temperature profile (given by a meteorological mast, a rawinsonde or a weather prediction code). This profile sets a vertical grid of the atmosphere.
In stable conditions, the cloud stabilisation height \( z_{stab} \) is computed by solving iteratively Equation 1 while \( z_{stab} > z_k \) where \( z_k \) is the altitude of the \( k \)-level in the profile.

\[
z_{stab} = \left[ \frac{8 F_1}{\gamma_x \gamma_y \gamma_z s_k} \right]^{1/4}
\]

with \( F_1 = \frac{3 g H M_{exp}}{4 \pi c_p T \rho_{sur}} \) and \( s_k = \frac{g}{T} \left( \frac{\Delta \phi}{\Delta z} \right)_k \).

In Equation 1, \( F_1 \) designates the buoyancy term (in \( \text{m}^4\text{s}^{-2} \)), \( g \) the gravity acceleration (in \( \text{m/s}^2 \)), \( H \) the energy released by 1 g of TNT explosion (in \( \text{Jg}^{-1} \)), \( M_{exp} \) the TNT equivalent explosive mass (in \( \text{g} \)), \( c_p \) the air specific heat (in \( \text{Jg}^{-1}\text{K}^{-1} \)), \( T \) the ambient air temperature (in \( \text{K} \)), \( \rho_{sur} \) the air density near the ground (in \( \text{g} \text{m}^{-3} \)), \( \gamma_x \), \( \gamma_y \) and \( \gamma_z \) are coefficients of air entrainment in the cloud, \( s_k \) is the stability parameter (in \( \text{s}^{-1} \)), and \( \Delta \phi/\Delta z \) the virtual potential temperature gradient from the ground to the \( k \)-level (in \( \text{Km}^{-1} \)).

In unstable conditions, the cloud stabilisation height is computed using a threshold value for the potential temperature gradient in order to maximise the impact.

The stabilized cloud dimensions and so-called initial vertical matter distribution are presented in Figure 1. The sphere volume and cylinder volume are adjusted to respect the mass ratios.

**Cloud displacement**

At this stage, the cloud shown in Figure 1 is not influenced by the wind blowing in the time period between explosion and stabilisation. To take the wind effect into account, the cloud is cut out in layers defined by the meteorological vertical grid. In each layer, the wind velocity and wind direction are known by observations or 3D model output. The layers are moved using the local wind conditions according to the following algorithm.

For each \( K \)-layer between \( z_{k-1} \) and \( z_k \) located under the stabilisation height \( z_{stab} \) the cloud arrival time \( t_k \) at the \( k \)-level is calculated with relation (2).

\[
t_k = \frac{1}{\sqrt{s}} \cdot \text{Arc}\cos \left[ 1 - \left( \frac{8 \gamma_x \gamma_y \gamma_z s_k z_k^4}{4 F_1} \right) \right]
\]

The \( K \)-layer displacement \( (\Delta x_K, \Delta y_K) \) is computed between the explosion time \( t_0 \) and \( t_k \) then between \( t_k \) and \( t_{stab} \).

Step 1 – Till \( t_k \), the displacement \( (\Delta x_{t_0-1_k}, \Delta y_{t_0-1_k}) \) takes account of the lower layer displacement (by iteration).

\[
\begin{align*}
\Delta x_{t_0-1_k} &= \Delta x_{t_0-2_k} - (t_k - t_{k-1}) \cdot \text{VIT}^K \cdot \sin \text{DIR}^K \\
\Delta y_{t_0-1_k} &= \Delta y_{t_0-2_k} - (t_k - t_{k-1}) \cdot \text{VIT}^K \cdot \cos \text{DIR}^K
\end{align*}
\]

with \( \Delta x_{t_0-1} = -t_1 \cdot \text{VIT}^1 \cdot \sin \text{DIR}^1 \)

\( \Delta y_{t_0-1} = -t_1 \cdot \text{VIT}^1 \cdot \sin \text{DIR}^1 \)

\( \text{VIT}^K \) and \( \text{DIR}^K \) designate respectively the local velocity and direction of the wind in the \( K \)-layer.

Step 2 – The total displacement till \( t_{stab} \) of each \( K \)-layer is given by relation (3).

\[
\begin{align*}
\Delta x_K &= \Delta x_{t_0-1_k} - (t_{stab} - t_k) \cdot \text{VIT}^K \cdot \sin \text{DIR}^K \\
\Delta y_K &= \Delta y_{t_0-1_k} - (t_{stab} - t_k) \cdot \text{VIT}^K \cdot \cos \text{DIR}^K
\end{align*}
\]

Finally, the displacement of the stabilisation layer \( K_{stab} \) and upper layers verifies relation (4).

\[
\begin{align*}
\Delta x_K &= \Delta x_{t_0-1_{k_{stab}}} - (t_{stab} - t_k) \cdot \text{VIT}^K \cdot \sin \text{DIR}^K \\
\Delta y_K &= \Delta y_{t_0-1_{k_{stab}}} - (t_{stab} - t_k) \cdot \text{VIT}^K \cdot \cos \text{DIR}^K
\end{align*}
\]
This method can be applied either with observations or with 3D computed meteorological fields. In this case, the cloud displacement with the wind is obtained using a 3rd order Runge-Kutta algorithm. The displacement takes into account the topography and the presence of obstacles as the 3D wind field integrates these effects.

3. EXPERIMENTAL VALIDATION

TESATEX coupled with MSS was validated using the experimental data of the ‘Double Tracks’ test which took place in the frame of the ‘Operation Roller Coaster’. This campaign was a series of open field trials operated in 1963, in the Tonopah Range test site located in Nevada (US). The tests were carried out on a flat terrain without obstacles.

‘Double Tracks’ test consisted in the open air detonation of an edifice containing plutonium and 53.5 kg of TNT. The experimental results were normalized to 1 kg of initial mass of plutonium. The specific activity of this military grade plutonium was assumed to be $0.081 \text{ Ci g}^{-1}$ (Homann, 1994). The cloud rise was recorded with photographic devices and theodolites. In the test, the meteorological conditions, the particles distribution in the cloud, the activity concentration in the atmosphere and the activity deposition on the ground were also measured. Figure 2 shows the observed wind and temperature profiles (Church, 1969), and also the polydisperse plutonium aerosol generated by the explosion (Dewart et al., 1982). Note that neither pressure nor relative humidity profiles were measured or available. In TESATEX module, standard atmospheric profiles were substituted for these missing data.

A 3D wind field was computed with Micro-SWIFT using ‘Double Tracks’ meteorological conditions. TESATEX was then run to determine the main characteristics of the cloud produced by the detonation. The stabilisation height and the cloud top height calculated with TESATEX were respectively 199 m and 243 m at a stabilisation time of 118 s. These numerical results are close to the measured data, i.e. a stabilisation height of 210 m at 105 s after the explosion. Figure 3b illustrates the cloud configuration determined by TESATEX when taking into account the wind influence. It compares very well to the observed cloud geometry (see in Fig. 3a).

Micro-SPRAY dispersion computations were carried out using the stabilized cloud issued by TESATEX as the source term. Then, the results obtained along the cloud axis were compared with the ‘Double Tracks’ measurements, and with HOTSPOT numerical results.

Figure 4a shows the integrated aerosol activity concentration in the air. Only the inhalable fraction of the plutonium aerosol is considered, that is to say particles with aerodynamic diameter less than 10 µm. The peak observed at a few
hundreds metres from the explosion point is visible in the TESATEX – Micro-SPRAY results which is not the case with HOTSPOT. In the far field, both modelling systems give similar results near ‘Double Tracks’ measurements.

Figure 4b presents the plutonium activity deposited on the ground (both inhalable and not inhalable particles). At distances less than one kilometre, TESATEX – Micro-SPRAY results are in reasonable agreement with ‘Double Tracks’ measurements while the experimental maximum observed 2 km away from the test location is also predicted by the model. On the contrary, HOTSPOT numerical results are not so close to the in-field observations. Finally, TESATEX and Micro-SPRAY computations agree pretty well with the reference test ‘Double Tracks’ measurements and perform better than HOTSPOT which would be used in case of a nuclear weapon radiological accident.

4. APPLICATION
TESATEX coupled with MSS have been used to simulate hypothetical explosion and dispersion events in Oklahoma City (US) and in Paris (France). The meteorological conditions and explosion locations (in a narrow street, in a broad street or on a large square) were varied to enlighten the differences in cloud shape, atmospheric distribution, dry deposition, and finally, the potential impact of the simulated events. As the vertical distribution and the horizontal transport of the initial cloud take account of the influenced by the buildings wind field, the numerical results seem remarkably realistic.

As an example, Figure 5a presents the radioactive cloud occurring after a Radiological Dispersal Device (RDD) or ‘dirty bomb’ explosion downtown Oklahoma City and Figure 5b indicates the location of each layer setting up the stabilized cloud. Obviously, the displacement of the cloud lower part depends on the channelled flow in the urban canopy while, above the buildings the cloud is advected by the wind.

Figures 6, 7a and 7b relate to the virtual explosion of a RDD in Paris near Concorde square. This device implies 1 kg of TNT and 3 TBq of cobalt-60 ($^{60}$Co). At the time of the event, wind blows from the East. Figure 6 shows the trajectories of the layers which render both the cloud rise and the complicated wind field noticeably influenced by the buildings. Despite the wind direction is transverse to the street in which the explosion happens, the lower part of the cloud travels along the street and reaches Concorde square.
Micro-SPRAY dispersion results were post-processed to evaluate the radiological exposure due to the RDD. Figures 7a and 7b present the total effective dose (by inhalation and external irradiation by the cloud and by deposition) computed with or without TESATEX. In the case TESATEX was not used (b), it was simply considered a point source at the explosion place. The results given in Figures 7a and 7b are very different. With TESATEX, the doses are lower near the source and the contaminated area is larger than without the pre-processor. This is explained by the ascent and the transport of the cloud above the buildings while the pollutant remains in urban canopy in the other case.

Figure 6. Cloud generated by the explosion in Concorde square district in Paris. Layers trajectories till stabilisation time and shape of the stabilized cloud.

Figure 7. Total effective doses evaluated after Micro-SPRAY dispersion simulation with the explosion source term issued by TESATEX (a) or supposed to be punctual (b).

5. CONCLUSIONS
TESATEX was designed as a pre-processor needed to model the source term generated by an open-air explosion in the urban environment. The module uses, in particular, Briggs assumptions to determine the initial cloud geometry (stabilisation height and horizontal dimensions) and HOTSPOT empirical mass distribution in the cloud. Notice that TESATEX takes into account the wind field, possibly influenced by buildings, in the initial cloud development till stabilisation. TESATEX modelling seems a satisfactory compromise between accuracy in physical description and computational speed. It does not depend on the later dispersion code. In the presented computations, it was operated with Micro-SPRAY but could be run with any other model. TESATEX and Micro-SPRAY were validated by simulating the ‘Double Tracks’ test performed by the US and UK in the frame of the ‘Roller Coaster Operation’. The agreement between numerical results and measurements was successful. For this trial, TESATEX gave better results than the widely used HOTSPOT model dedicated to nuclear weapon radiological accidents. Some applications of TESATEX - Micro-SWIFT-SPRAY (MSS) modelling system are proposed through the paper. Virtual explosions of Radiological Dispersal Devices (RDD) have been simulated in Oklahoma City (downtown) and Paris (Concorde square district). The radiological contaminants dispersion is strongly influenced both by the streets network and the initial cloud configuration. Taking adequately buildings effects into account leads to more realistic results not only concerning the pollutant distribution, but also in terms of health impact assessment, and possibly counter-measures to carry out. In the future, further applications of TESATEX – MSS could concern the impact assessment of accidental events, malevolent actions or terrorist attacks in industrial built sites or in the urban environment.

REFERENCES
ARIA Technologies, 2005: Notes de principe et notes d’utilisation des modules Micro-SWIFT et Micro-SPRAY.