# NEW CAPABILITIES OF CERES® CBRN-E DECISION SUPPORT TOOL IN THE FIELDS OF EXPLOSION MODELLING AND SOURCE TERM ESTIMATION

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**Abstract**: Developed at CEA since 2008, CERES® CBRN-E is a computational tool designed for crisis management in case of accidental, malevolent or terrorist releases of hazardous radiological, chemical or biological materials. More precisely, CERES® computes atmospheric dispersion in complex environments including buildings (industrial sites or urban areas), assesses the health consequences of the toxic releases on the population and first responders, and delivers operational results (e.g. danger zones, intervention zones...) in less than 15 minutes to rescue teams and decision makers. CERES® is a flexible modular platform, thus capable to integrate both simplified and advanced models adapted to the description of the scenario (leakage from storage, evaporation from a pool, fire…), the AT&D of the hazardous material and the CBRN impact evaluation. This paper aims at discussing two recent developments in CERES®. The first one relates to high-Mach source terms simulation in case of an explosion preceding the toxic dispersion. The near-field unstationary source terms generated by energetic reactions are included in CERES® using either analytical relations (gathered in the so-called $D^2R^2$ modules) derived from multiphase pre-computations or a direct coupling between the pre-established transient results of the HI2LO code (a CFD model able to deal with the transition from high to low-Mach number flows) and CERES®. These models provide the source term geometry and the noxious material granulometry and spatial distribution after the explosion, taking into account the presence of the buildings in the simulation domain. The second development consists in the implementation in CERES® of a simple method for source term estimation using in-field sensors measurements. In a first step, retro-plumes are propagated individually from each of the detectors. In a second step, the possible locations of the source and associated releases rate are determined by retro-plumes overlapping. For both developments, the paper gives more details about the methodology and the validation of the new modules based on experimental data.

***Key words:*** *CERES® CBRN-E, modelling and decision support, explosion modelling, high-Mach to low-Mach flow, source term estimation.*

## INTRODUCTION

CERES® CBRN-E is an operational computational tool devoted to hazmat atmospheric dispersion modelling and impact assessment, gathering several source term models, various dispersion approaches (from Gaussian puff to advanced 4D flow and dispersion computations) and health consequence modules adapted respectively to R-N, C or B noxious agents (Armand *et al*., 2013). CERES® is able to compute atmospheric dispersion in complex environments including buildings (industrial sites or urban areas), assess the health consequences of the toxic releases on the population and first responders, and deliver operational results (e.g. danger zones, intervention zones...) in less than 15 minutes to rescue teams and decision maker. This paper aims at discussing two recent developments in CERES®. The first one relates to high-Mach source terms simulation in case of an explosion preceding the toxic dispersion. The second development consists in the implementation in CERES® of a simple method for source term estimation using in-field detectors measurements.

## HIGH-MACH SOURCE TERMS

Transport and dispersion codes usually run under the assumption of uncompressible flows. This can be translated into maximum local Mach number requirements. The local Mach number of a flow is defined as $u_s/a_s$, $u_s$ being the particle velocity and $a_s$ the local sound speed. Rankine-Hugoniot formulas applied to blast waves (Dewey, 2006) provide a relation between the local Mach number of the flow and density ratios. This relation applied to air (gamma = 1.4) shows that a local Mach number of 0.1 (particle velocity of 35 m/s) corresponds to a density increase of 11%, which could be set as a reasonable limit for the uncompressible flow assumption. Other authors use a threshold value of 0.3 (local Mach number, the particle velocity being 109 m/s) which is arguable since it corresponds to a 36% density increase.

On the contrary, many source terms begin with high Mach flows. This is obviously the case both for source terms involving high explosives (for instance air strikes on chemical facility targets, warheads with chemical or biological payloads, dirty bombs...) and also for many accidental releases from pressurized containers. It is thus not mathematically and physically correct to connect such source terms to uncompressible codes.

In order to compute correct source terms from high-speed events, two possibilities are explored at CEA. The first one requires the preliminary modelling of fast, transient source terms in order to provide the characteristics of the dispersion cloud at the end of the transient phase as an input to the transport code. Examples of this first method are stratified clouds following explosive releases, such as the one already implemented in the explosion module (Armand *et al.*, 2008) of CERES® CBRN-E or the one used in the HOTSPOT health physics code (Homann, 2010), also described in Deaves and Hebden (2004). The second possibility is the direct time-coupling of a code dedicated to high-speed and transitional flows to the code dedicated to low-Mach transport and dispersion.

**Analytical modelling of high-speed source terms**

CERES® embeds analytical or numerical versions of high-speed source terms considered as initial inputs for further simulation. These source terms are encompassed under the name"$D^2R^2$", a French acronym for "Rapid Releases Dynamical Dispersion". The next paragraph is devoted to the modelling of Chemical or Biological Improvised Explosive Device (B-IED and C-IED). On-going work focuses on the dispersion of powders in order to tackle radiological IEDs as well. The $D^2R^2$ analytical model of BC-IEDs is based on small-scale dispersion experiments, multiphase modelling and deep analysis of the various phenomena involved in such systems.

Explosive dissemination of liquids is a mechanism encountered not only in BC-IEDs and weapons, but also as a preliminary step for Fuel-Air Explosives (FAE) and even as an interesting solution for fast extinction of forest fires. Declassified US reports gave insights into such mechanisms, even though only crude modelling of the events was proposed. A distinction is to be made between pictures of the dissemination cloud (showing the external boundaries of the cloud, including finger-like instabilities) and X-ray pictures, revealing the internal structure of the cloud. Modelling of finger instabilities is not accessible through simple models.

Dissemination experiments of various powders and liquids from a 1 litre device have been performed at CEA Gramat. Side-views of water and sand dispersion (with different time intervals) are given in Figure 1, showing that similar features are obtained for both liquids and powders. Front view pictures taken from high-speed videos are presented in Figure 2. They show the donut-shaped cloud as well as radial finger instabilities. The aim of the $D^2R^2$ model for BC-IEDs is to predict the internal structure of the stabilised cloud (two last rows of pictures).

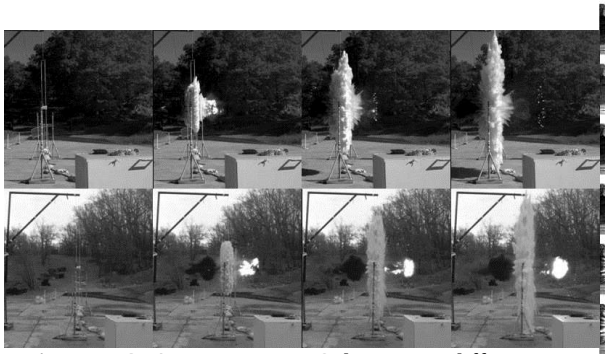

**Figure 1.** CEA experiments – Side views at different time. Top: water, bottom: sand.

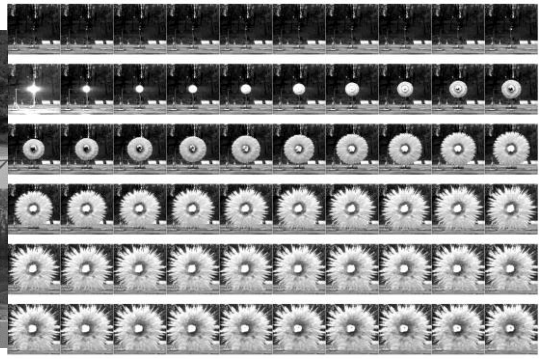

**Figure 2.** CEA experiments – Front views at different times from high-speed videos.

The analytical $D^2R^2$ BC-IED model includes several steps, namely: the acceleration of the liquid surrounding the High Explosive (HE) booster, a criterion for liquid primary break-up, the secondary break-up of initial liquid masses into droplets due to the velocity difference between liquid and gas phases, and droplets deceleration up to the final size of the cloud. For almost each step of the model, analytical expressions have been checked against the results of accurate multiphase simulations. The final outputs of the model are internal and external cloud radii, volume fraction and droplet sizes. Phase change between liquid and vapour is not considered for the moment in the analytical model. A comparison of predicted versus experimental radii for a CEA water dispersion experiment is given in Figure 3. The dotted line is the plot of the so-called "Holland formula", an empirical model of cloud expansion fitted to the initial stage of the experiment.

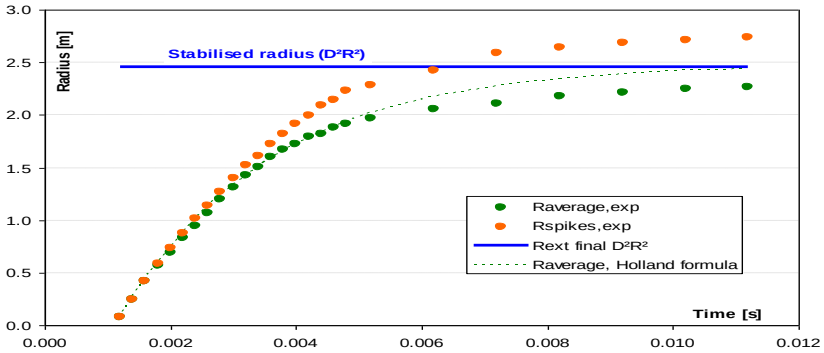


**Figure 3.** Experimental average and maximum radii for water compared with $D^2R^2$ prediction and Holland formula.

**Numerical modelling of high-speed source terms**

Pre-computed analytical or numerical source terms models are interesting solutions if there is no interaction between the modelled process and the surrounding media. For instance, the BC-IED $D^2R^2$ model requires that no interaction with obstacles (including the ground) takes place within the computed stabilized radius. When this assumption does not hold true anymore, it is necessary to perform 3D simulations of high-speed and transitional-speed flows before giving hand to the transport / dispersion code.

CEA Gramat uses a multiphase platform called CHYMERE, developed especially by the RS2N company in order to perform complex simulations of weapon effects and transient dispersion. This platform includes four 3D parallel codes coupled either in space and / or time and covers 10 orders of magnitude in timescales (from $10^{-7}$ s to $10^{2}$ s) and 7 orders of magnitude in lengthscales (from $10^{-4}$ to $10^{2}$ m). This presentation is limited to the last code, called HI2LO for "High-speed to Low-speed transition". Details on HI2LO can be found in Le Métayer *et al.* (2011) and applications have been presented in Hank *et al.* (2012). HI2LO presents specific characteristics compared to more classical CFD codes, among which the ability to import either topographies (DEM: Digital Elevation Maps) from Internet sources and urban geometries from GIS (Geographic Information System) data and especially from the widely used ESRI "shapefile" format.

CERES® CBRN-E also imports urban geometries from GIS data, namely building "layers" available in the IGN BD TOPO (IGN, 2011), and post-processes these data into the internal CERES® urban format. In order to insure compatibility between HI2LO and CERES® it is mandatory to use the same urban geometries as inputs for the HI2LO code. A specific pre-processor has thus been developed to convert shapefile data into 3D extruded obstacles. An example of pre-processing is shown in Figure 4.

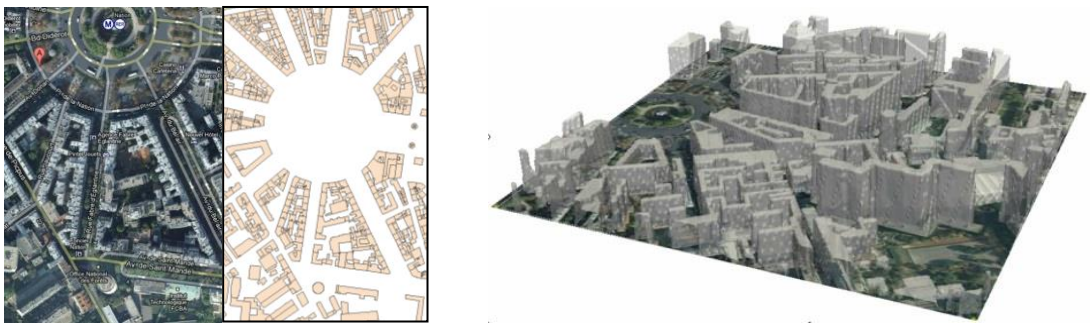

**Figure 4.** From left to right: Google Maps® view, BD TOPO shapefile, and HI2LO geometry after processing.

A HI2LO simulation of large scale explosive dissemination has been performed on this geometry. The outer cloud boundary has been plotted in Figure 5at the moment when the maximum local Mach number of the flow decreased under the threshold value of 0.1. It is evident from the picture that both ground and buildings interact strongly with the high-Mach flow. It would thus not much appropriate to model the input state of the transport / dispersion model by a simple cloud shape. The full 3D data can be exported from HI2LO to CERES® in order to continue the simulation for longer timescales.

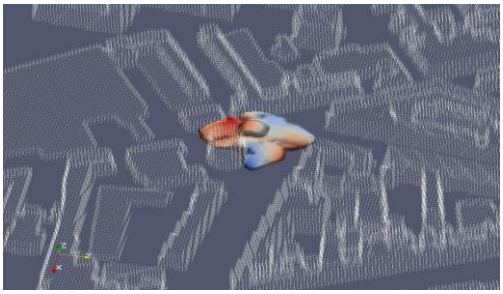

**Figure 5.** Outer boundary of the dispersion cloud for a urban scenario (gas pressure colour-scale).

## SOURCE TERM ESTIMATION

A simple method for identifying the location of radiological, biological or chemical emissions from a set of detectors measurements has been implemented in CERES® CBRN-E. The main objective of this module is to provide maps that represent the probable location of a source, thus possibly an estimation of the source term. Up to now, retro-plume method is only available with the Gaussian plume model included in CERES® to perform atmospheric dispersion calculation for a short-duration release.

Algorithm is based on an inversion technique to retrieve the source. From a set of measurements, retro-plumes are obtained by inverting the meteorological situations in order to calculate the adjoint function $C^*$. Each retro-plume comes from one sensor and is propagated individually for a unit release rate. The release rates actually needed to obtain the concentration measured on the sensor are then calculated on the grid and for several time intervals using the relation:

$$Q = \left(q/C^*\right) C_m$$

where Q is the release rate ($u.s^{-1}$) leading to the concentration level measured by the sensor; q is the unit release rate (1 $u.s^{-1}$), $C^*$ is the adjoint function ($u.m^{-3}$), and $C_m$ the measured concentration ($u.m^{-3}$). Depending on the noxious species, "u" can be expressed as a mass (kg), an activity (Bq) or a number of agents. This relation is applicable only to "non-reactive" species (i.e. not evolving with time). In case of a radioactive release, it can be used for long half-life radionuclides such as americium-241 ($^{241}$Am) which is taken as an example in the rest of the section (half-life of americium-241 is $T_{½}$ = 432 y). Thus, as explained in Achim *et al*. (2006 & 2010), the possible source locations and the associated release rates leading to the whole set of sensors measurements can be identified using the retro-plumes overlapping.

In CERES®, the user defines the positions of the sensors, and the start time, duration, and amplitude of the measurements. At least two measurements are necessary. Once the meteorological situation has been defined, retro-plumes for a unit quantity are computed, and then overlapped. In order to test and validate the algorithm implemented in CERES®, academic cases were used. For example, a 30 second release of $10^7$ Bq of americium-241 was supposed to occur during a neutral meteorological situation. The wind comes from West (270°) and its speed is 3 $m.s^{-1}$. The coordinates of the release are x = 0 m and y = 0 m.

- First, a direct atmospheric dispersion simulation was performed and gave activity concentrations on sensors $R_1$ ($x_1$ = 500 m; $y_1$ = 0 m), $R_2$ ($x_2$ = 800 m; $y_2$ = 0 m), $R_3$ ($x_3$ = 900 m; $y_3$ = -100 m) and $R_4$ ($x_4$ = 500 m; $y_4$ = 0 m). Figure 6 shows the americium-241 activity concentrations detected by the four sensors. As expected, according to the sensors locations relative to the source location, a shift in time is observed for the concentrations in the air.
- Secondly, CERES® was utilized to calculate the retro-plumes from the sensors, and then the probable location of the release by using the method mentioned above.

CERES® graphical interface presents the overlapping map at different times defined by the users. The results given by the retro-plume module for the academic case previously introduced are shown in the Figure 7. $R_1$, $R_2$, $R_3$ and $R_4$ are the receptors. The blue zone defines the probable location of the release 3 minutes before the measurement on sensor $R_1$. It is associated with a release rate between $3.10^5$ and $4.10^5$ $Bq.s^{-1}$, which is very close to $10^7$ Bq if release duration of 30 seconds is considered. Moreover, the "true" release location is included in the area defined by CERES® as the probable release location.

In the near future, the retro-propagation algorithm will be improved in order to take into account longer releases, "reactive" (evolving with time) releases and complex meteorological situations. Moreover it will

be coupled with the other atmospheric dispersion models available in CERES® CBRN-E: the urbanized Gaussian model (taking account of the street canyons) SIRANERISK and the LPDM (Lagrangian Particle Dispersion Model) Micro-SPRAY with the objective to perform source term estimation in urban areas.

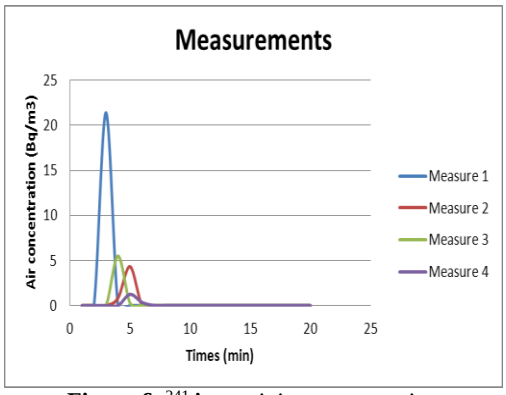


**Figure 6.** $^{241}$Am activity concentration measurements (in Bq.m$^{-3}$) on the 4 sensors.

**Figure 7**. Results given by CERES® retro-plume module for an academic case. R1, R2, R3 and R4 are the sensors. The blue zone defines the probable location of the release which would lead to a release rate between $3.10^5$ and $4.10^5$ Bq.s$^{-1}$.

## CONCLUSION

The study of fast high-Mach source terms cannot be handled in transport / dispersion models by direct simulation or simple inputs. Two methods have been developed at CEA to model these phenomena. The first one consists in a pre-computation (via analytical or simple numerical models) of the transient source term up to its stabilization time. This method is embedded into CERES® CBRN-E as a new source term module (D²R²). The second solution for more complex cases is a time-coupling between the high-Mach HI2LO and the low-Mach CERES® CBRN-E models based on the same 3D urban geometry available through GIS data. On-going work is the development of new models in D²R² for explosive dissemination in light multi-room facilities.

On the other hand, a simple method to estimate location and rate of a short release from measurements has been included in CERES® CBRN-E. Retro-plumes are propagated by inverting the meteorological situation in order to calculate the concentration adjoint function. By overlapping the computed maps of the release rates, CERES® CBRN-E is able to retrieve the zone of the probable release, and the potential release rate. Future work will be to adapt the method to CBRN agents significantly evolving with time during their atmospheric transport (e.g. by radioactive decay or by chemical reactions) and to extend the method to other atmospheric dispersion models included in CERES® CBRN-E in order to take into account the built environments (industrial sites or urban districts).

## REFERENCES


Achim, P., *et al.*, 2006 & 2010: Internal technical reports, CEA.

Armand, P., C. Olry, A. Albergel, and C. Duchenne, 2008: *3D simulation of the dispersion in the urban environment in case of an explosion using TESATEX pre-processor and Micro-SWIFT-SPRAY modelling system*. Harmo'12, October 6-9, 2008, Cavtat, Croatia.

Armand, P., L. Patryl, G. Lamaison, L. Soulhac, L. Deguillaume, and N. Chaumerliac, 2013: *CERES® CBRN – A unified modelling and decision support system to assess the dispersal and health impact of hazardous releases in urban or open-field environments*. Harmo'15, May 6-9, 2013, Madrid, Spain.

Deaves, D.M., and C.R. Hebden, 2004: Aspects of dispersion following an explosive release, ADMLC/2004/3 report.

Dewey, J.M., 2006: The Rankine-Hugoniot equations: their extensions and inversions related to blast waves, *Proceedings of the 19th Symposium on Military Aspects of Blast and Shock*, DRDC Suffield, Canada.

Hank, S., O. Le Métayer, R. Saurel and E. Lapébie, 2012: HI2LO: A 3D unsteady code for the numerical simulation of shock wave propagation and dispersion phenomena in large scale heterogeneous media, 43rd European Safety, Reliability and Data Acquisition Seminar, Rouen, France.

Homann, S.G., 2010: HOTSPOT 2.07.1, *https://narac.llnl.gov/HotSpot/HotSpot.html*, NARAC, Lawrence Livermore National Laboratory.

IGN, 2011: BD TOPO®, http://professionnels.ign.fr/bdtopo.

Le Métayer, O., A. Massol, N. Favrie, and S. Hank, 2011: A discrete model for compressible flows in heterogeneous media, *Journal of Computational Physics 230 (2011) 2470–2495*.