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SIMULATION OF EXPLOSIVE EVENTS IN THE URBAN ENVIRONMENT COUPLING A FAST DYNAMICS CFD MODEL WITH LOW MACH NUMBER DISPERSION SOLVERS IN CERES® CBRN-E

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Abstract: CBRN-E threats are a major concern of the public authorities, relayed by the people and sadly rekindled by recent events, notably in Paris, France. In case of hazardous atmospheric releases, preceded or not by an explosion, first responders in particular, and all decision makers in general, wish to gain as quick as possible the most accurate and reliable representation of the situation in order to foster the crisis management and return to normalcy. This is precisely the role that a modelling and decision-support computational tool could play in the emergency preparedness and response process. Consistently, this is also the objective of CERES® which is entirely developed by the Atomic and alternative Energies Commission (CEA) in France. In this framework, our paper is intended (1) to recall the main principles and characteristics of CERES® placing an emphasis on the ability to carry out explosion and dispersion simulations in the same tool, then (2) to comment on recent advances of experimental and modelling activities in the field of the detonations, and finally (3) to describe the coupling between explosion and dispersion modules with the announcement of computations related to realistic scenarios in large urban domains to be presented in the conference.

Key words: *Explosion, dispersion, low Mach, high Mach, D2R2, HI2LO, CERES® CBRN-E.*

INTRODUCTION

CBRN-E threats may have various expressions including possibly deleterious atmospheric releases and / or explosions originating from industrial accidents or terror events. In such cases, a rapid assessment of the situation is of high-stake for both rescue teams and stakeholders (facilities operators, local or national authorities…). It can even constitute a strong element of differentiation between the emergency handling strategies to efficiently control the situation and return to normal, a fact exemplified through examples of CBRN-E emergency exercises in Armand *et al.* (2013) (a), (2014), and (2015).

Since 2005, CEA has been mandated to coordinate and run the inter-ministerial R&D program dedicated to CBRN-E threats in France. Modelling and simulation contribute to the cross feeding of topics included in this program such as prevention, detection, alert, intervention, and / or mitigation. In this framework, CERES® CBRN-E (shortened as CERES® in the paper) is a recent operational modelling and decision-support system which is being developed in collaboration between services of the Atomic and alternative Energies Commission (CEA) in France. The software has been specifically designed to evaluate the short term and the long term health consequences of chemicals, radionuclides or biological pathogenic agents, accidentally or maliciously emitted into the air. CERES® is committed to provide numerical results in a limited amount of time (less than 15 minutes in most cases), thus to be applicable in an emergency.

The present paper is divided in three main parts, including (1) a quick recall of the principal development guidelines and features of CERES®, (2) an insight on experiments and models related to the detonations, recently achieved in connection with the software, and (3) the presentation of the coupled explosion and dispersion modelling system with near future applications to simulations in very large urban domains As a matter of fact, CERES® modelling edge is to tackle explosions, dispersions or the combination of both.

CERES® MODELLING SYSTEM IN CASE OF CBRN-E EVENTS

The specifications of CERES® software are to be a modelling and decision-support tool able to deal with several types of threats and scenarios and give the possibility to run flow and dispersion models adapted to complex built-up (industrial and urban) environments (Armand *et al*., 2013 (b)). Moreover, the 2D / 3D simulation results have to be produced within a fairly short time consistent with the “hot phase” of an emergency. Finally, the results must be provided as a mapping of danger zones (health consequences) or counter-measures zones (sheltering-in-place or evacuation) to be directly useable by the civilian security.

The major features of CERES® are reported hereafter.

- The software deals with 3D dispersion at local and regional scale in both natural and complex built-up environments (industrial sites or urban areas).
- It handles various categories of threat agents (radionuclides, chemicals or biological pathogens); thus, it has endpoint health impact models specifically devoted to these kinds of releases.
- It is equipped with a large panel of scenarios (leakage from a tank or a pipe, evaporation from a pool, fire, explosion...) and associated simplified or more advanced “source term” models.
- Depending on the skill and computational resources of the user, it gives the choice between three dispersion models: Gaussian puff, sophisticated urbanized Gaussian and, more farsighted and R&D oriented, a Lagrangian Particle Dispersion Model (LPDM) using a 3D flow field.
- It can use a range of meteorological data: measurements at one or more stations, vertical profiles, and / or meso-scale numerical weather forecasting.

CERES® encompasses not only physical models, but also numerous data bases with the terrain elevation, land-use, building data, physicochemical properties of stable or radioactive elements, transfer coefficients in the soil and the biota, radiological dose conversion coefficients, toxicological reference values, etc.

Along with the transport and dispersion, the fate of the gases or particles released in the air is considered according to their nature (radioactive decay chains, chemical reactions, or bio-agents degradation).

CERES® input data are recorded and CERES® output results are disseminated through a tried and tested ergonomic graphical user interface. All kinds of maps are exportable to Graphical Information Systems (GIS), like e.g. ArcGIS®, as a support to the intervention and decision-making processes.

All models implemented in CERES® have been rigorously validated using experimental wind tunnel or in-field data (see validation cases in a mock-up and full-scale city centre in Duchenne *et al.*, 2016).

On-going developments include source term estimation and data assimilation. As the computational time is reduced, CERES® simulations can be performed repeatedly using all the present available information. In an emergency, the first aim is to quickly provide atmospheric dispersion and health impact assessment, afterward to improve gradually the initial evaluation using more and more complete and reliable data.

Finally, the software motto is to be modular and flexible as versions can be instantly generated with the one and only software components the user is interested in. As modules are plug-ins, it is easy to derive a version for instance devoted to the chemical risk with the *ad hoc* data bases, source term, dispersion and chemical dose models.

While CERES® is aimed at the CEA own safety needs and missions, its interest for more users has been also clearly identified. Thus, CERES® has been licensed for more than five years to the French nuclear and non-nuclear industry and distributed to civilian security services for experimentation and feedback.

HIGH-MACH SOURCE TERMS

While most of the atmospheric transport and dispersion models use the assumption of incompressibility, a special attention has to be paid to highly transient source terms like those generated by energetic events. As a matter of fact, uncompressible flows are limited to flows with a local Mach number less than 0.1. (The Mach number, Ma, is defined as u_s/a_s, u_s being the particle velocity and a_s the sound speed. Ma = 0.1 corresponds to a particle velocity of 35 m.s^{-1} or a density increase of 11%, thus a reasonable limit for the uncompressible flow hypothesis. See Patryl *et al.* (2014) for more details.)

However, there are several source terms beginning with high Mach flows, for instance in the accidental releases from pressurized containers or in the events involving high explosives (dirty bombs, Biological / Chemical – Improvised Explosive Devices), etc. As it would not be mathematically and physically correct to connect such source terms to uncompressible models, ways to overcome this issue have been studied and graduated simplified or full CFD strategies have been implemented in CERES®:

- First of all, source terms with no interaction with obstacles may be described analytically up to the extent where the flow is nearly at rest. For instance, this is the case for Improvised Explosive Devices using the D2R2 model (see more below) or for stratified clouds models after explosive releases such as TESATEX in CERES® (Armand *et al.*, 2008) or HOTSPOT (Homann, 2010).
- Another method for more complex events is to describe the mass, impulse, and energy flow rates through a given surface. For instance, this is the case of an indoor detonation and dissemination in a single- or multi-room building followed by an outdoor flow through windows and doors. As the resulting flow may be a high-Mach one, it is computed as a boundary condition by the 3D compressible solver HI2LO (Hank *et al.*, 2012). Then, HI2LO results may be further computed by the LPDM dispersion solver in CERES® with a time coupling of the two models.
- In the most complex cases, it might be necessary to use 3D multiphase computations from the beginning. Once again, the results can be remapped in HI2LO and, step by step, when reaching a low-Mach state, also remapped in CERES® and its low-Mach dispersion solvers.

The following paragraphs give some more details about the experimental validation and application of the D2R2 and HI2LO models.

Analytical model for Improvised Explosive Devices

Several explosive dissemination experiments have been conducted at CEA with liquids and powders. The reference setup is a cylindrical plastic shell (external diameter of around 10 cm) with an inner cylinder of high explosive of variable diameter. This setup allows the mass ratio between the explosive and the inert material to vary. For experiments with water, the M_{inert} / M_{TNT} ratio ranged from 1.6 to 12.8.

From the analysis of experiments, two regimes can be identified as illustrated in Figure 1. The first one is a highly structured regime with the formation of characteristic “finger” instabilities. After a transitional break-up process, the second one forms cloudy shapes soon followed by the end of the expansion.

The D2R2 (Rapid Releases Dynamical Dispersion) model describes these two regimes correctly as shown for example in Figure 2. One can notice that the predicted external cloud radius compares quite well with the experimental values for three different M_{inert} / M_{TNT} ratios. D2R2 has been successfully applied to the CEA experiments and also to literature results such as Apparao et al. (2013) or Zabelka et al. (1969).

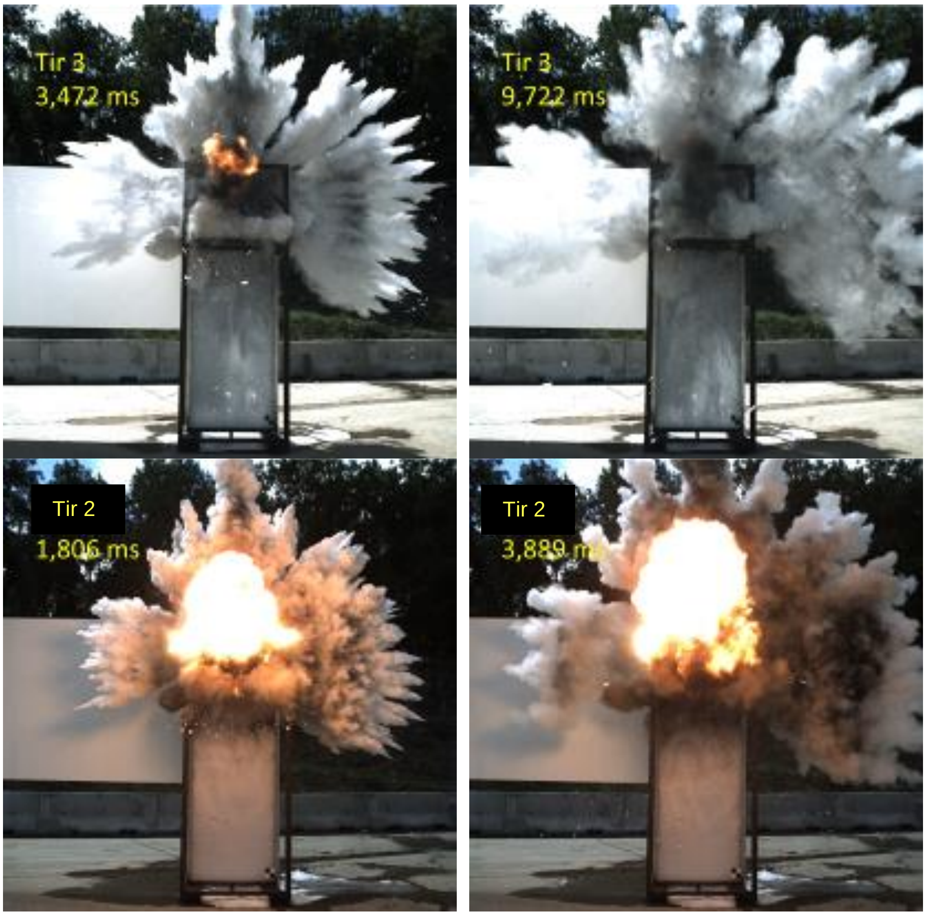

Figure 1. Change of morphology for two mass ratios (from top to bottom: 4.8 and 1.6).
Left: fingers structures – Right: cloudy shapes.

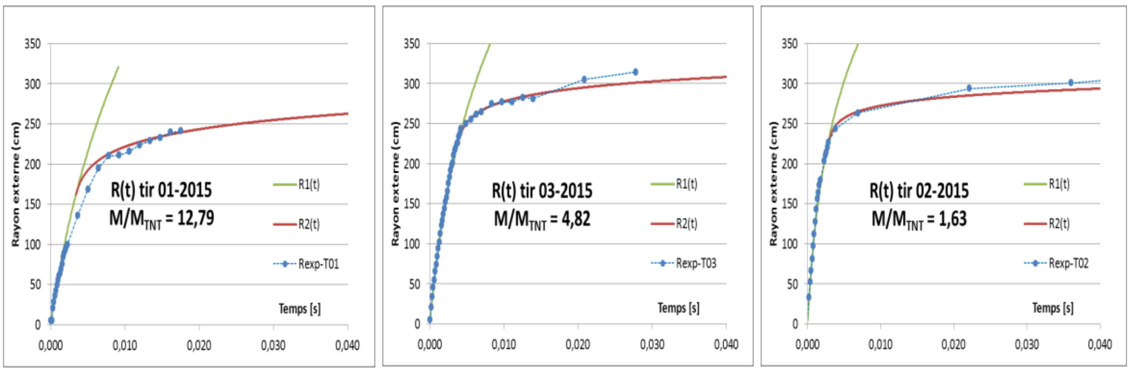

Figure 2. D2R2 results compared to CEA experiments (time evolution of the external radius).
Blue: experiments – Green: D2R2 first regime – Red: D2R2 second regime.

Source term as a boundary condition in a high-Mach 3D solver

HI2LO is the CEA reference model for 3D high-Mach to low-Mach transition computations. Albeit not a fully multiphase model, HI2LO is able to remap results obtained with the other models of the multiphase CHYMERE suite developed for CEA by the RS2N company (www.rs2n.eu).

HI2LO is able to use complex boundary conditions as well as in-cell obstacles which may also serve as a source for boundary conditions. For instance, one can declare a subsonic, sonic or supersonic injection in a computational cell as if the cell was connected to a pressurized tank. Many other options are available, and it is also the way chosen to branch some of the analytical source term models (which may also spread on more than one cell).

Figure 3 shows the result of a HI2LO simulation involving such an "internal" source term. A reservoir boundary condition (internal pressure 3.67 bar and temperature 991 K) is defined inside a computational cell and the release is allowed to take place during 0.02 second. The domain size is 3.2 m x 0.8 m x 0.8 m and the release is located at (3.1 m, 0.4 m, 0.4 m) and is directed towards "–X". Strong turbulent mixing with ambient air is accounted for through a simple model. At the end of the simulation, the local Mach number is everywhere lower than 0.06, so the uncompressible approximation is valid.

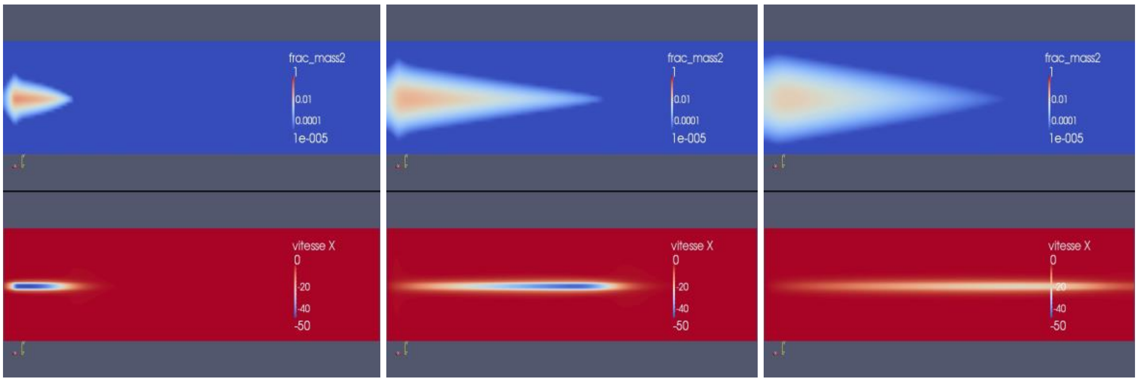

Figure 3. Pollutant mass fraction (top) and axial velocity (bottom).
Times from left to right: 5 ms, 25 ms and 45 ms (X axis flipped for clarity).

COUPLING EXPLOSION AND DIPERSION IN A REAL URBAN DISTRICT

As mentioned before, graduated strategies have been developed to take account of either open air or more or less confined explosions and, possibly, the coupled dispersion of noxious species. Models consisting in analytical relations like D2R2 are integrated in CERES® while the CFD model called HI2LO is coupled to the Lagrangian dispersion solver in CERES®.

HI2LO and CERES® share the ability to import topographies (DEM: Digital Elevation Maps) and urban geometries from GIS (Geographic Information System) data, especially from the widely used "shapefile" format. To make HI2LO and CERES® compatible, the same urban geometries are used in both models and a pre-processor has been developed to convert shapefile into 3D extruded obstacles (see Figure 4).

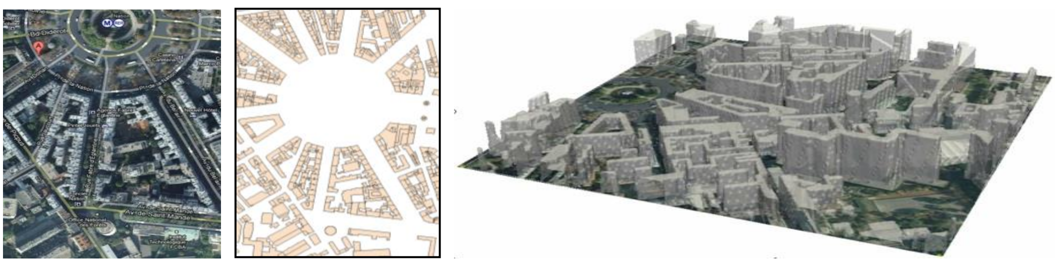

Figure 4. From left to right: Google Maps® view, BD TOPO shapefile, and HI2LO geometry after processing.

HI2LO simulations of explosive disseminations have been performed in this geometry and other ones. In such complex environments, the high-Mach flow strongly interacts with the ground as the buildings. The plume outer boundary and internal distribution of the species may be obtained when the maximum Mach number of the flow is under the threshold value of 0.1. It gives the appropriate input state for the LPDM model in CERES® where the HI2LO data are imported to continue the simulation for longer timescales. Such computations in some Paris districts are under way and will be presented during the conference.

CONCLUSION

Explosions may happen as a consequence of accidents or terror events with dramatic consequences on the human health and the infrastructure. Moreover, explosions may generate the dissemination of hazardous species in more or less confined species, from open air spaces to semi-confined built-up industrial sites or urban districts, or even initially confined buildings or underground networks. Explosion modelling is thus a complicated task for many reasons and, in the same time, intuited to be very useful in an emergency.

CERES® is the fast-response modelling and decision-support computational tool developed by the CEA. It is equipped with both explosion and dispersion models adopting a graduated range of strategies to deal with more or less complicated environments and threat scenarios. One ambitious approach which may be necessary in the case of industrial sites or urban districts is the direct time-coupling between the transient results of the HI2LO (high- to low-) Mach number CFD model with the Lagrangian dispersion solver in CERES® taking account of both the explosion characteristics and the obstacles influence. This approach will be soon applied to districts in Paris in order to simulate the flow and the dispersion pattern and assess the overpressure and the toxicity consequences in case of hypothetical explosive noxious releases.

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