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

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## **Introduction – General description of CERES®**

CERES® CBRN-E is an operational decision-support computational tool devoted to hazmat atmospheric dispersion modelling and impact assessment, gathering:

- Several source term models
- Various dispersion approaches (Gaussian, "urbanized" Gaussian, Lagrangian)
- Health impact modules adapted to R, C or B noxious agents

CERES® is able to compute atmospheric dispersion in complex environments including buildings (industrial sites or urban areas), assess the health consequences of releases on population and first responders, and deliver operational results (e.g. danger zones, intervention zones...) in less than 15 minutes to rescue teams and decision makers

This presentation aims at discussing two recent developments in CERES® CBRN-E

- High-Mach source terms simulation in case of an explosion
- Implementation in CERES® of a simple method for Source Term Estimation

- AT&D codes usually run under the assumption of uncompressible flows which implies criteria on Mach number (Ma =  $u_s / a_s$  with  $u_s$  particle velocity and  $a_s$  local sound speed) *Relation between local Ma and density ratios is given by Rankine-Hugoniot formulas* 
  - Local Ma of 0.1 ( $u_s = 35 \text{ m.s}^{-1}$ ) corresponds to a density increase of 11%
  - Local Ma of 0.3 ( $u_s = 109 \text{ m.s}^{-1}$ ) corresponds to a density increase of 36%
- On the contrary, source terms involving high explosives (for instance air strikes on chemical facility targets, warheads with chemical or biological payloads, dirty bombs...) and many accidental releases from pressurized containers begin with high Mach flows
  To compute source terms from high-speed events, two possibilities are explored at CEA
  - Preliminary modelling of fast source terms to provide the cloud characteristics at the end of the transient phase as an input to the transport code (e.g. stratified clouds following explosions like in HOTSPOT – Homann, 2010)
  - Direct time-coupling of a code dedicated to high-speed and transitional flows to the code dedicated to low-Mach transport and dispersion

CERES® CBRN-E embeds in D<sup>2</sup>R<sup>2</sup> (Dynamical Dispersion of Rapid Releases) module analytical and numerical models of high-speed source terms considered as initial inputs

- D<sup>2</sup>R<sup>2</sup> analytical model of Chemical or Biological Improvised Explosive Device (BC-IED) is based on small-scale dispersion experiments, multiphase modelling and deep analysis of the various phenomena involved in such systems (from declassified US reports)
- D<sup>2</sup>R<sup>2</sup> analytical model aims at predicting the internal structure of the stabilised cloud (modelling of finger instabilities is not accessible through simple models)
- D<sup>2</sup>R<sup>2</sup> analytical model includes several steps checked against multiphase simulations:
  - Acceleration of the liquid surrounding the High Explosive (HE) booster
  - Criterion for liquid primary break-up
  - Secondary break-up of initial liquid masses into droplets
  - Droplets deceleration up to the final size of the cloud
- Final outputs are internal and external cloud radii, volume fraction and droplet sizes (liquid / vapour phase change is not considered for the moment in the analytical model)
  - On-going work focuses on the dispersion of powders to tackle radiological IEDs as well

# Cea Liquids and powders dissemination experiments (1)

#### CEA experiments (1 L container device / 125 g HE disperser) – High-speed video results



Water (top) and sand (bottom) dispersion – Side view (time intervals are not the same) Similar features are obtained for both liquids and powders

# C22 Liquids and powders dissemination experiments (2)

#### CEA experiments (1 L container device / 125 g HE disperser) – High-speed video results



Sand dispersion (1,510 kg) – Front view at different times ( $R_{max} \approx 2,4 \text{ m}$ ) Donut-shaped cloud as well as radial finger instabilities are clearly visible on the pictures

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# Cell Liquids and powders dissemination experiments (4)



#### CEA water dispersion experiment (cylindrical 1 L device)

and maximum radii with D<sup>2</sup>R<sup>2</sup> prediction and Holland formula (dotted line), an empirical model of cloud expansion fitted to the initial stage of the experiment

Comparison of experimental average



Comparison for a spherical device (picture from a declassified US report)

## Numerical modelling of high speed source terms

- Pre-computed source terms models like those in BC-IED D<sup>2</sup>R<sup>2</sup> are interesting solutions if there is no interaction between the modelled process and the surrounding media
- If interaction with obstacles (or ground) takes place within the computed stabilized radius, it is necessary to perform 3D simulations of high-speed and transitional-speed flows
- CEA Gramat uses a multiphase platform called CHYMERE, developed by the RS2N company to carry out complex simulations of weapon effects and transient dispersion
  - Four 3D parallel codes coupled either in space and / or in time
  - 10 orders of magnitude in time scales (from  $10^{-7}$  s to  $10^2$  s)
  - 7 orders of magnitude in length scales (from  $10^{-4}$  to  $10^{2}$  m)

HI2LO (High speed to Low speed transition) is the fourth code of CHYMERE platform

- Details on HI2LO in Le Métayer et al. (2011) and applications in Hank et al. (2012)
- Import of topographies (DEM) from internet & urban geometries from GIS (ESRI "shp")
- Computation of blast propagation and particle / gas dissemination at high Mach
- Time coupling with CERES® which takes the full 3D output of HI2LO (for instance at M = 0.1) as an input for longer time scales simulations

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### Large scale explosive dissemination in a city (1)

#### An example of HI2LO shapefile importation





Google Maps® view and IGN BD TOPO® building data (IGN, 2011)

HI2LO 3D geometry after processing

N.B. A pre-processor converts shapefile data into 3D extruded obstacles (same urban geometries in HI2LO and CERES®)

## Large scale explosive dissemination in a city (2)

HI2LO outer boundary of the product cloud (gas pressure colour-scale) from a spherical explosion at the end of the high-speed phase showing ground and buildings influence on the flow





HI2LO mass fractions at 0.8 s Top: detonation products Bottom: particles

## Source term estimation in CERES® CBRN-E (1)

- Simple method for identifying CBRN emissions from a set of detectors measurements
- Aim of the module is to provide maps of the source probable location and an estimate of the source term (at this time, limited to Gaussian model and short-duration releases)
- The algorithm is based on the "adjoint method" to retrieve the source
  - Each detection is a retro-source from which a retro-plume is propagated individually for a unit release rate in the inverted meteorological field
  - The release rate actually needed to obtain the concentration measured on the sensor is calculated on the grid and for several time intervals using the relation  $Q = (q / C^*) C_m$ where Q is the release rate (u.s<sup>-1</sup>) leading to the measurement, q the unit release rate (1 u.s<sup>-1</sup>), C<sup>\*</sup> is the adjoint function (u.m<sup>-3</sup>) and C<sub>m</sub> the measured concentration (u.m<sup>-3</sup>)
  - *N.B.* #1 "u" can be expressed as a mass (kg), an activity (Bq) or a number of agents
  - *N.B.* #2 This relation is applicable only to "non-reactive" species
  - Thus, the possible source locations and the associated release rates leading to all the set of sensors measurements can be identified using the retro-plumes overlapping

### Source term estimation in CERES® CBRN-E (2)

Sensors positions and detections start, duration, and amplitude are defined by the user; once given the meteorological situation, retro-plumes are computed and overlapped
 The algorithm implemented in CERES® has been validated using academic cases
 *E.g.* 30 s release of 10<sup>7</sup> Bq of <sup>241</sup>Am (half-life T<sub>1/2</sub> = 432 y) at x = 0 m and y = 0 m; wind of 3 m.s<sup>-1</sup> coming from West (270°) in a neutral meteorological situation
 First, a direct atmospheric dispersion simulation gives activity concentrations on sensors (as expected, according to the sensors locations relative to the source location, a shift in time of the <sup>241</sup>Am activity concentrations in the air is observed)



<sup>241</sup>Am activity concentration measurements (in Bq.m<sup>-3</sup>) on the sensors

 $R_1 (x_1 = 500 \text{ m}; y_1 = 0 \text{ m}), R_2 (x_2 = 800 \text{ m}; y_2 = 0 \text{ m}),$  $R_3 (x_3 = 900 \text{ m}; y_3 = -100 \text{ m}) \text{ and } R_4 (x_4 = 500 \text{ m}; y_4 = 0 \text{ m})$ 

## Source term estimation in CERES® CBRN-E (3)

Secondly, <u>CERES® calculates the retro-plumes from the sensors and their overlapping</u> which is shown in the graphical interface at the times defined by the users



Results given by CERES® retro-plume module (R1, R2, R3 and R4 are the sensors)

The blue zone defines the probable location of the release 3 min before the measurement on  $R_1$ 

The release rate is between  $3.10^5$  and  $4.10^5$  Bq.s<sup>-1</sup> very close to  $10^7$  Bq for a release duration of 30 s

The "true" release location is included in the area given by CERES® as the probable release location

The retro-propagation algorithm will be improved in order to take into account longer releases, releases evolving with time and complex meteorological situations;
 it will be coupled with the other atmospheric dispersion models available in CERES®,
 SIRANERISK (urbanized Gaussian model) and Micro-SPRAY (LPDM) with the objective to perform source term estimation in urban areas

### Source term estimation in CERES® CBRN-E (4)

#### Individual retro-plumes expressed as necessary release rates and their intersection



t<sub>0</sub> + 1 mn

t<sub>0</sub> + 2 mn





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#### **Source term estimation in CERES® CBRN-E (5)**

#### Number of retro-plumes which overlap (maximum = 4)



t<sub>0</sub> + 3 mn

t<sub>0</sub> + 4 mn

t<sub>0</sub> + 5 mn





- Two methods have been developed at CEA to model fast high-Mach source terms which cannot be handled in AT&D models by direct simulation or simple inputs
  - Pre-computation (via analytical or simple numerical models) of the transient source term up to its stabilization time embedded into CERES® CBRN-E as a new module (D<sup>2</sup>R<sup>2</sup>)
  - For more complex cases, time-coupling between the high-Mach HI2LO and the low-Mach
    CERES® CBRN-E models based on the same 3D urban geometry (GIS data)
  - On-going development of models for explosive dissemination in light multi-room facilities
- A simple method to estimate the characteristics of a source term from measurements has been included in CERES® CBRN-E
  - Retro-plumes are propagated 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 evolving with time during AT&D and to extend the method to the built environments (industrial sites or urban districts)



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# Thank you Questions?

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# C22 Liquids and powders dissemination experiments (3)

#### CEA experiments (1 L container device / 125 g HE disperser) – High-speed video results



Illustration of the uncertainty in determining external cloud radius due to "finger" instabilities

## Liquids and powders early times dispersion (1)

#### Multiphase modelling with CHYMERE platform (four 3D codes developed by RS2N for CEA Gramat)

- High speed flow in / out of mechanical and thermal equilibrium
- Powder compaction, liquid cavitation, droplet break-up, drag forces, heat and mass transfer...



Front and side view comparisons for water dispersion at early times (before instability growth)

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## Liquids and powders early times dispersion (2)

Analysis of cloud structure – Inner cloud structure (toroid shape)



Simulation results (2D axisym.) at two different times Left: map of apparent density Right: map of pressure gradient

3D rotational extrusion of apparent density contours showing the internal cloud structure (the small axial shift is caused by one-side initiation)

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