CERES^{TM} CBRN – A UNIFIED MODELLING AND DECISION SUPPORT SYSTEM TO ASSESS THE DISPERSAL AND HEALTH IMPACT OF HAZARDOUS RELEASES IN URBAN OR OPEN-FIELD ENVIRONMENTS

Patrick Armand[1], Luc Patryl[1], Guillevic Lamaison[2], Lionel Soulhac[2], Laurent Deguillaume[3], Nadine Chaumerliac[3], and Marguerite Monfort[1]

[1]CEA, DAM, DIF, F-91297 Arpajon, France
[2]ECL, LMFA, F-69134 Ecully, France
[3]CNRS / UBP, LaMP, F-63171 Aubière, France

Abstract: CERES^{TM} CBRN is a new operational computational platform devoted to multi-threat hazardous materials atmospheric dispersion modelling and health impact assessment. It addresses emergent CBRN issues for the Civilian Security and it is by design committed to the response in case of emergency (in 15 minutes at the maximum). CERES gathers source term models, flexible dispersion approaches (from Gaussian puff to advanced 4D flow and dispersion computations), and human health consequences modules adapted to R-N, C or B noxious agents. CERES is a recent development, still in progress, by CEA (French Atomic and alternative Energies Commission) and research partners of the French CNRS. The paper aims at presenting and commenting on two recent major advances in CERES: the integration of the urban dispersion solver SIRANERISK (ECL / LMFA), and the coupling of MITHRA Gaussian model with M2C2 or KPP / SAPRC-99 atmospheric chemistry modules (UBP / LaMP). More particularly, the article illustrates the good results obtained for realistic applications of both developments in a few minutes on a standard multi-core laptop rendering CERES a promising decision support tool for crisis preparation and management.

Keywords: CERES^{TM}, CBRN releases, atmospheric dispersion, impact assessment, modelling & decision support.

INTRODUCTION

CERES^{TM} CBRN (simply named "CERES" all along this paper) refers to a new operational 4D modelling and decision support system which has been developed since 2008 by CEA in the framework of academic collaborations. Basically, it is devoted to assess atmospheric dispersion, environmental impact and human health consequences of potentially deleterious (accidental or chronic) releases in the air. CERES has dual applications as it can be utilized both for safety studies (established for regulatory purpose) and for crisis preparedness or handling in case of an emergency. When applied for crisis management implying noxious atmospheric emissions, CERES platform is committed to deliver operational results (like danger zones or intervention zones) in a few minutes whatever the situation, should it be an accident, a malevolent action or a terrorist attack, so that the modelling system is by design oriented towards the emergency response. In the following sections, this paper aims at giving the fundamental properties of CERES, then focuses on urbanized Gaussian modelling and coupled chemistry and Gaussian dispersion modelling.

MAIN FEATURES OF CERES MODELLING SYSTEM

The major characteristic of CERES is flexibility as illustrated by its main features described here below.

1 – CERES platform can cope with situations as various as regular emissions from industrial facilities in routine operations, moderate or serious accidents affecting industrial (nuclear or non nuclear) plants or occurring during hazardous materials transports, and even, malicious activities resulting in toxic releases.

2 – CERES can handle all categories of threat agents like radionuclides, chemicals or biological agents. It means that it is not only a computational tool, but it includes large data bases with the main characteristics of the hazardous gases or particles potentially released in the atmosphere.

For example, physical and chemical properties of stable or radioactive elements (including half-lives and daughter products), simplified or detailed chemical mechanisms, transfer coefficients of elements through the soil and biota for long-term environment and human health impact assessment...

3 – CERES has been conceived as a flexible platform gathering modules dedicated sequentially to source term description and modelling, meteorological data processing, atmospheric dispersion simulation at the local or regional scale, and environmental or health impact evaluation.

4 – CERES simulations can be performed repeatedly using, at each step, the whole available information. The results are spread through a tried and tested ergonomic graphical user interface and can be visualized in CERES own Geographic Information System (GIS) or exported in formats adapted to other GIS.

In an emergency, CERES first aim is to quickly provide atmospheric dispersion and exposure assessment. The following steps consist in successive improvements of the initial evaluation using more realistic and

complex input data. Consequently, gradual levels in dispersion models are accessible depending on the requested accuracy and available time to deliver results. As a matter of fact, CERES^{TM} incorporates a first intent Gaussian puff model, an advanced urbanized Gaussian model (*see section below*), and, at a later stage, a Lagrangian Particle Dispersion Model (LPDM) using diagnostic or prognostic 3D models of the wind field. The fate of C, B, or R-N emissions during transport and dispersion in the air is considered by taking account of respectively the interaction of the atmospheric background and released chemicals (*see section below*), the bio-agents degradation linked to the meteorological situation or the radioactive decay chains. If applicable, dry and wet deposition of CBRN agents on the ground and vegetation is evaluated. Finally, as the atmospheric and surface deposited concentrations are an important step, but often not the final goal of a computation, a series of models is provided for the assessment of radiological exposures, chemical doses or postponed health effects of pathogenic agents.

At each step of the simulation, crisis or expert modes may be used. The "crisis mode" allows evaluating a case very rapidly with a simple meteorological definition: one direction and one velocity of the wind and the atmospheric stability are the only necessary data to run the case. Impact points are set automatically in the wind axis. In the "expert mode", it is possible to utilize meteorological evolution or 3D wind fields. Impact points can be set everywhere graphically or manually with geographic coordinates or chosen in a database. Moreover the 3D implemented viewer provides cartographies as support to decision processes.

From here, the paper concentrates on two recent developments in the fields of (i) dispersion in the urban environment and (ii) chemical reactivity in the atmosphere. Both are based on CERES^{TM} coupling with respectively SIRANERISK and M2C2 or KPP / SAPRC-99. The methods and validation of the modelling system are discussed, and CERES^{TM} use is exemplified for accidental and intentional releases.

CHEMISTRY AND TRANSPORT MODELLING IN CERES^{TM} CBRN

Aim of chemistry and transport coupling

As it is quite complicated to take account of the chemical reactivity, most of the simple computational tools based on Gaussian modelling simply ignore the interaction, if any, of the atmospheric background chemistry with the released gaseous or particulate species. However, this approach may lead to erroneous impact assessment as it may either overestimate the consequences if the chemicals disappear when being transported in the air, or underestimate them if the species produced by the reactions in the atmosphere have a worst impact on the human health than the chemicals initially released. Thus, in order to take into account the chemical reactivity, a coupling has been implemented between MITHRA, the Gaussian puff dispersion model in CERES, and M2C2 or KPP / SAPRC-99 atmospheric chemistry modules.

Chemistry modules

1 – M2C2, the acronym of "Model of Multiphase Cloud Chemistry", has been developed at CNRS / UBP (Clermont-Ferrand, France) by the LaMP (*Laboratoire associé de Météorologie Physique*). It results from the coupling between a multiphase explicit chemistry model for gases and aqueous phase (Deguillaume *et al*., 2005) and a cloud microphysics two-moment model (Chaumerliac *et al*., 1990). The chemical module includes several detailed mechanisms, among which for HO_x, NO_y, sulfur, methane and COV, chlorine and ammonia in gaseous phase. The module can also consider a variable photolysis which is calculated by the radiative transfer model TUV developed by Madronich and Flocke (1999).

2 – More recently, an alternative approach has been incorporated in CERES platform to take into account chemical reactions. Thus, it is now possible to use KPP pre-processing module (Sandu and Sander, 2006) which has been specially developed for 3D chemistry and transport models (CTM), such as WRF-CHEM. KPP module is based on the chemical mechanisms in SAPRC-99 which have been complemented by the LaMP with new chemical reactions for NH_3, HCN and N_2O_5 species. Other important improvements have been made available like the computation of photolysis rates (with TUV 4.6 radiative transfer modelling), and the emission and deposition rates of chemical compounds. Moreover, a variable release in terms of intensity and duration can also be considered.

Dispersion and chemistry interactions

Among various methods to implement the calculation of atmospheric transport and dispersion / chemistry interactions in CERES, the one chosen keeps a moderate computation time to provide results very quickly in case of emergency and is explained here below.

Although other models are present in the platform, atmospheric dispersion in CERES is often evaluated with a Gaussian puff model, dubbed MITHRA. This model assumes that a continuously emitted plume or an instantaneous cloud of pollutant can be simulated by the release of a series of puffs which are carried

in a time and space varying wind field. The puffs are assumed to have Gaussian concentration profiles in the vertical and horizontal planes. For given meteorological conditions and for a puff with small initial dimensions (compared to those at the observation time t), the instantaneous volumetric concentration C of a gaseous or particulate species at the point of coordinates (x, y, z) is calculated by equation (1) with Q the released quantity, D a depletion factor corresponding to dry and wet deposition and to the chemical or radioactive decay, u the wind velocity and σ_x^2, σ_y^2, σ_z^2 the horizontal, lateral, vertical standard deviations.

$$C(x,y,z,t) = \left(\frac{1}{\sqrt{2\pi}}\right)^3 \frac{Q\,D}{\sigma_x\,\sigma_y\,\sigma_z} \exp\left[-\frac{(x-u\,t)^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2} - \frac{(z-h)^2}{2\sigma_z^2}\right] \quad (1)$$

During atmospheric dispersion, each puff is followed in space and time. The chemical species quantities and standard deviations are recorded for each puff at each time step. The chemistry / transport interaction thus consists in modifying the species quantity according to its chemistry reactivity using the equation (2) where Q_{puff} is the quantity of the chemical species in the puff before the chemical correction and $Q_{puff\,C}$ is its quantity corrected by the concentration gradient dC / dt during the internal time step Δt.

$$Q_{puff\,C} = \left(Q_{puff} + \frac{dC}{dt} \times \frac{\left(\sqrt{2\pi}\right)^3 \sigma_x\,\sigma_y\,\sigma_z}{2}\,\Delta t\right) \quad (2)$$

dC / dt is given by M2C2 or KPP with SAPRC-99 and computed either "on line" at each step time of the dispersion model, or before the dispersion calculation and placed in a "look-up" table. The second way is recommended for its greater computational efficiency, as the coupling is expected to be used in crisis situations. It means that before any dispersion evaluation, several simulations have to be carried out using the chemistry module along with the source term characteristics (species and released quantity). Look-up tables must be completed with as many species concentrations C and gradient values dC / dt for the most possible release conditions. Once the tables are constituted, according to the concentration at the plume centre, and for a given time step, dC / dt is screened in the tables and applied to correct the puff quantity.
This method involves three hypotheses: 1) each puff is independent from the other ones, 2) there is no chemical correction during the release, 3) inside the puff the reactivity follows the same Gaussian law that the "passive" dispersion. The third point has been checked by calculating with M2C2 the reactivity at the puff centre, then applying a normal law to rebuild the Gaussian puff. In most cases, results are successful when compared to M2C2 calculations for each concentration inside the Gaussian puff. However, the puff reconstruction may be quite an approximation when the species reactivity is too strong or when there is a release threshold that leads to several regimes of chemical reactivity. Although M2C2 was satisfactory, it had to be adapted to allow high concentration chemical releases. Thus, it has been decided to use also the KPP solver which has proven to be numerically robust and able to deal with stiff chemical reactions.

Validation of MITHRA / M2C2 coupling – Application to an accidental release of ammoniac

The joint use of MITHRA and M2C2 has been tested and validated in simple situations considering a flat terrain (thus ignoring local topography and buildings effect – *see the next section for this topic*), constant meteorological conditions (although it's possible to define time varying meteorology in CERES), and the release of usual Toxic Industrial Chemicals. One of the accidental cases corresponds to the release of 100 kg gaseous ammoniac NH_3 at 12 am during 30 min. The wind blows from the North at a speed of 3 $m.s^{-1}$; the atmosphere is unstable. NH3 emission is triggered 36 hours after the beginning of M2C2 simulation to obtain a stable chemical environment. An unpolluted, called "remote", chemical background is applied.

Figure 1 presents the maximum NH_3 concentration (in $mg.m^{-3}$) in the time sequence. It appears clearly that if dispersion is not corrected by the chemical reactivity (Figure 1 on the left side), the maximum concentration value of 0.1 $mg.m^{-3}$ is observed well beyond 5 km. When chemical reactivity is taken into account, NH_3 max atmospheric concentration significantly decreases (Figure 1 on the right side), and, at 5 km, NH_3 maximum concentration is less than 0.1 $mg.m^{-3}$. This is an expected result as NH_3 undergoes photolysis and oxidation by hydroxyl radical (OH), both reaching a maximum at noon.

In a next future, these simulations will be done with KPP solver / SAPRC-99 chemical mechanisms.

Figure 1. NH_3 maximum concentration (in $mg.m^{-3}$) without (left) and with (right) chemical reactivity.

Interim conclusion

MITHRA Gaussian puff dispersion model and M2C2 or KPP with SAPRC99 chemical modules may now be used together in CERES for better assessing concentration in the air and health consequences in case of toxic releases. Coupling is carried out by modifying the quantity of species in each puff according to the previous puff concentration and time step. Consistently with crisis handling, it is wise to pre-compute puff corrections for relevant scenarios of chemical releases in various environments and to store them in "look-up" tables as this method does not involve time consuming simulations in an emergency, but only efficient search of factors in the look-up tables. Validation test-cases demonstrate that chemical reactivity may notably influence the dispersion in a number of scenarios. Moreover, using M2C2 with CERES, it is possible to take account of the species produced by the chemical reactions which may be more hazardous for human health than the initially released species. Developments based on KPP are in progress as the evaluation of the chemical reactivity in the release or the implementation of the aqueous phase in KPP (as it is done in M2C2), accompanied by sensitivity studies implying various types of releases and chemicals.

URBAN SIMPLIFIED DISPERSION MODELLING IN CERES^{TM} CBRN

Interest of an advanced Gaussian model for urban environment

Following the sarin gas attack in Tokyo underground in 1995, most of the hypothesized CBRN scenarios with atmospheric releases have been supposed to occur in urban districts of large cities. Malicious actions also represent a real threat for built industrial sites, especially those holding large quantities of hazardous materials. On one side, try to simulate atmospheric dispersion in so complex environments with a simple Gaussian model not only gives unrealistic results, but does not guarantee the conservative assessment of a noxious release health consequences. On the other side, due to limited computational resources or limited experience of or access to more complicated models or by lack of time, operating a CFD or a "simplified" CFD tool is not always achievable. Thus, an intermediate model combining the simplicity of the Gaussian approach with a description (even partial and not perfect) of the buildings and streets network sounds like an interesting solution and justifies the implementation of SIRANERISK in CERES platform.

Description and validation of SIRANERISK model

SIRANERISK (Lamaison et al., 2011) has been developed at CNRS / ECL (*Ecole Centrale de Lyon*) by the LMFA (*Laboratoire de Mécanique des Fluides et d'Acoustique)* jointly with CEA in order to predict the unsteady dispersion of pollutants in and over the streets of dense European cities. It is the combination of a Gaussian puff model in the atmosphere over the street level and a specific mass-consistent model accounting for flow and dispersion of pollutants inside the urban canopy. The concentration in the streets canyons is obtained by solving a transport equation with air fluxes evaluated by semi-empirical formulae derived from a range of wind tunnel experiments. SIRANERISK takes into account the main geometric complexity of an urban area, neglecting the effects of small topological elements (details of the buildings, trees...). Urban topography is constituted by a network of parallelepipeds representing each street. Each of these boxes contains a volume of contaminated air which can be exchanged with the next boxes through the intersections of the street arrays or with the atmosphere over the urban canopy, so that the air fluxes and the mass budget of any pollutant can be computed in each street canyon. SIRANERISK requires the map of the considered urban area presented as a network of interconnected streets defined by their length, width and height. The model validation has been performed by two ways as SIRANERISK numerical results have been compared with wind tunnel experiments (for continuous and short releases on a rough surface and inside an idealized urban canopy), and with the results of a LPDM developed at ECL. Good agreement has been obtained especially for the mean arrival time and longitudinal spread of the plume.

An example of application to a fictitious malevolent release in Lyons city (France)

Figure 2 shows the schematic 2D network of the streets in the centre of Lyons city. The computation domain is about 4 km x 4 km and contains 3,180 streets and 1,902 intersections nodes. In the studied hypothetical scenario, a dirty bomb blows up on a week day, at 8 am, near a major railway and underground station, resulting in the quick release of a radioactive aerosol.

Figure 2. Streets network of Lyons (France) town centre as represented in SIRANERIK.

In the calculation, the wind is uniform above the urban canopy (reference velocity of 3 $m.s^{-1}$), but varies with time around the South-West direction (120° to 150°). The atmospheric stability class is B in Pasquill formalism (very unstable). Figure 3 presents the radioactive particles instantaneous activity concentration in the streets network of Lyons city centre at four successive instants (1, 2, 4, and 8 min after the initial explosion). As clearly visible in the figure, the basic Gaussian dispersion pattern is strongly modified by the channelling in the streets canyons. For a simulated period of 50 minutes, computation time is around 10 minutes. It is thus possible to integrate the activity concentration and to evaluate with the radiological impact module in CERES the exposures by the different pathways (inhalation and irradiation) as the Total Effective Dose Equivalent (TEDE) (not shown here).

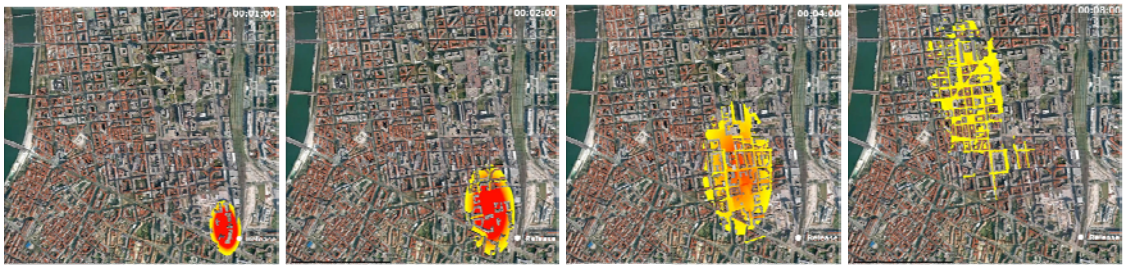

Figure 3. Instantaneous activity concentration of a radionuclide, 1, 2, 4, and 8 minutes after the fictitious explosion of a dirty bomb near *La Part-Dieu* railway station in Lyons (France).

Interim conclusion

The CERES platform now integrates SIRANERISK, a dispersion solver specifically adapted to the urban environment. In SIRANERISK, the atmosphere above the street level is dealt with a Gaussian puff model while a transport equation is resolved inside the streets network with transfers between the two air layers. This is a significant progress as simple Gaussian modelling is definitely not able to cope with the densely built and intricate environment of large cities whose description have been introduced once and for all in CERES data bases (Paris, Lyons and Marseilles streets networks are now available). Finally, it must be pointed out that computing a quite precise pollutant distribution inside the streets also permits to correctly assess the health impact of the released species.

GENERAL CONCLUSION

The CERES^{TM} CBRN platform is an innovative computational tool addressing both emergent and more usual issues such as accidental or malevolent releases of hazardous materials in the atmosphere. CERES is a recent development, still in progress, by CEA (French Atomic and alternative Energies Commission) and research partners of the French CNRS. In this respect, two recent major improvements of CERES are discussed in this paper: the integration of the urban dispersion solver SIRANERISK (ECL / LMFA), and the coupling of MITHRA Gaussian puff model with M2C2 or KPP / SAPRC-99 atmospheric chemistry modules (UBP / LaMP). The article brings together the main principles, implementation, basic validation, and first realistic applications of both models which give satisfactory and promising results. In all cases, computation times are moderate, up to 10-15 minutes on a standard multi-core laptop, even utilizing quite advanced modelling, thus satisfying one main request of the authorities facing an emergency. This makes CERES^{TM} CBRN a modelling and decision support tool fully consistent with crisis management and a unified multi-threat and multi-risk platform offering adapted dispersion models, together with population and first-responders health impact assessment.

REFERENCES

Chaumerliac, N., E. Richard, and R. Rosset, 1990: Meso-scale modelling of acidity production in orographic clouds and rain. Atmos. Environ. Vol. 24 A, pp. 1573-1584.

Deguillaume, L., M. Leriche, and N. Chaumerliac, 2005: Impact of radical versus non-radical pathway in the Fenton chemistry on the iron redox cycle in clouds. *Chemosphere*, 60-5, pp. 718-724.

Lamaison, G., L. Soulhac, and P. Armand, P, 2011: Presentation of SIRANERISK-2.0 – A decision-support oriented computational tool adapted to the dispersion of deleterious RBC agent in the urban atmospheric environment – Examples of application. *14th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes.* Kos Island, Greece, 2-6 October 2011.

Madronich, S., and S. Flocke, 1999: the role of solar radiation in atmospheric chemistry. In Handbook of Environmental Chemistry. Edited by P. Boule, Springer-Verlag, New-York, pp. 1-26.

Sandu, A., and R. Sander, 2006: Technical Note – Simulating chemical systems in Fortran 90 and Matlab with the kinetic preprocessor KPP-2.1. *Atmos. Chem. and Phys*. Vol. 6, pp. 187-195.