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SIMULATION WITH MICRO-SPRAY AND POST-PROCESSOR SPRAYSHINE OF THE IRRADIATION DUE TO A RADIOACTIVE PLUME AND ITS DEPOSITION ON ALL ACCESSIBLE SURFACES IN THE URBAN ENVIRONMENT

Patrick Armand¹, Christophe Olry², Olivier Oldrini³, Jérôme Carrère², Christophe Duchenne¹ and Armand Albergel²

¹CEA, DAM, DIF, F-91297 Arpajon, France ²ARIA Technologies, F-92100 Boulogne-Billancourt, France ³MOKILI, F-75014 Paris, France

Abstract: Radiological impact assessment implies to estimate the dose rate due to the plume and deposition irradiation. The gamma exposure is influenced by the space and time distribution of the radionuclides which may be tricky in the case of non-flat terrain, complex meteorological conditions and, moreover, built environments (industrial sites or urban zones). With a significant relief and buildings, it is also necessary to account for the possible interception of the gamma rays by the obstacles. Finally, to be useful even in a crisis situation (accidental or terrorist releases), the results must be delivered in times as short as possible, at least consistent with the emergency handling. All of this was incitement to develop the so-called "SPRAYSHINE" post-processor which is run after the Lagrangian particle model Micro-SPRAY and inserted in a local scale operational modelling chain of the dispersion and impact of radionuclides in urbanized areas. The post-processor results from the improvement of the existing CLOUDSHINE complemented by DEPOSITIONSHINE which computes the irradiation by the radionuclides deposited on all accessible surfaces (not only ground, but also façades, roofs and ceilings of buildings) also taking into account the shading by the obstacles. Finally, a parallel version of SPRAYSHINE has been developed consistently with Parallel-Micro-SWIFT-SPRAY (PMSS) aiming at (i) noticeably reducing the computational times and (ii) coping with huge computation domains covering with multiple tiles a large city like Paris, New-York or London. PMSS and SPRAYSHINE have been tested and exhibit convincing performances, notably in terms of speedup, even if progress is still necessary to optimize the gamma ray tracing in the case of extended calculation areas.

Key words: Radioactive releases, impact assessment, irradiation, exposure rate, industrial sites, urban environment, micro-scale, Parallel-Micro-SWIFT-SPRAY, 3D Lagrangian dispersion, post-processor, SPRAYSHINE, modelling and decision-support system.

INTRODUCTION

Radioactive materials may be released in the air, intentionally or not, in as various circumstances as normal operation of industrial facilities like Nuclear Power Plants, or in case of an accident or a malevolent action like a terrorist attack using a "dirty bomb". Among the radiological internal and external exposure pathways, the immediate ones are the inhalation and the irradiation by the plume when it disperses following the release and by the radioactive deposition on all accessible surfaces (ground, façades and roofs of buildings...) which remains once the plume has gone away.

Thus, it is crucial to assess as quickly and as precisely as possible the radionuclides exposure rate and the possible health consequences on the workers, population and /or rescue teams. This is not obvious as the radiation exposure is an effect from a distance (a person staying in a zone without radioactive materials can receive a non-zero dose) and, on the other side, there is a protective effect by the shading of the obstacles located between radioactive particles and people potentially subjected to radiation. The dose rate estimation also becomes challenging in complex atmospheric environments characterized by topography and numerous buildings on industrial sites or in urban areas.

Past years, it was generally considered a uniform atmospheric or surface activity concentration distribution to roughly estimate the plume or surface irradiation rate. The plume was supposed to extend semi-infinitely in all directions over a flat terrain. For each radionuclide, a coefficient was calculated in advance taking into account the gamma rays flux in the idealized geometry, a unit activity concentration, and factors to convert the activity flux into irradiation dose. Then, the dose rate at a given point was estimated using the local aerial or surface activity concentration.

Such a gross assumption ignoring the actual airborne and deposited radioactivity distribution is no more acceptable, especially considering that 3D models now permit to calculate the radionuclides dispersion even between buildings. Following Raza and Avila (2001), Armand *et al.* (2005) proposed to compute the distribution of Lagrangian discrete particles with Micro-SPRAY and the dose field due to gamma radiations emitted by a plume with the CLOUDSHINE post-processor. At successive instants, the algorithm sums the contribution to radiation exposure by gamma rays of the particles in Micro-SPRAY output file accounting for the shading by the topography and all the obstacles. But it does not consider the contribution of the particles deposited on the accessible surfaces to the total radiation exposure.

This was our motivation to upgrade CLOUDSHINE with a more general module, dubbed "SPRAYSHINE", capable to compute at points or "receptors" and along horizontal planes (at various heights above the ground) the gamma rays irradiation by the radionuclides in the air (improved version of CLOUDSHINE) or deposited on all "visible" surfaces (DEPOSITIONSHINE). Moreover, the post-processor was developed consistently with the parallel version of Micro-SWIFT-SPRAY (see Oldrini *et al.*, 2011). Thus, SPRAYSHINE is able to deal with particles distributed to multiple processors, also handling sub-domains of an extended calculation domain.

In the remaining of the paper, we describe CLOUDSHINE and DEPOSITIONSHINE (which, by the way, can deal with hollow geometries like arches or tunnels and take into account the radioactive decay of particles) and we give some examples of the validation and use of the modules. Then, we mention and illustrate through various test-cases the SPRAYSHINE parallelization principles before exploring the foreseen perspectives.

DESCRIPTION OF CLOUDSHINE

Equation of the gamma rays flux

The equation describing the gamma radiation photons flux (from ca.10 keV to 10MeV) of a given radionuclide is:

$$\Phi(E) = \iiint \frac{f(E) C(r) B(E, \mu r) \exp(-\mu r)}{4\pi r^2} d^3r$$
 (1)

where Φ (E) (in Bq.m⁻²) is the flux at the energy level E (in MeV), f (E) the disintegration fraction at the energy level E (in %), C (in Bq.m⁻³) the activity concentration of the radionuclide, B (no unit) the build-up factor representing the scattering of the flux, μ (in m⁻¹) the linear attenuation coefficient in the air and r (in m) the radial coordinate whose origin is the point where the flux is estimated. There are many equivalent forms of the build-up factor available in the literature. We take the above formula of Berger where a (E) and b (E) are coefficients depending on the energy level:

$$B(E,\mu r) = 1 + a(E) \mu r \exp(b(E)\mu r)$$
⁽²⁾

Resolution of the equation of the gamma rays flux in a Lagrangian model

In a Lagrangian model, the activity concentration is obtained from the projection of the particles positions on a target meshing and the summation of each particle activities. Thus, the integral (1) has to be transformed into a discrete sum of all the particles surrounding the location where the flux is calculated. Q_i standing for the radioactivity of particle i (in Bq), this yields to:

$$\Phi(E) = \sum_{\text{particles } i} \frac{f(E) B(E, \mu r_i) \exp(-\mu r_i)}{4\pi r_i^2} Q_i$$
(3)

Computation of the gamma exposure rate

The gamma exposure rate D(E) (in Sv.s⁻¹) for the specified energy level E is defined as:

$$D(E) = C_{b}(E) E \mu_{a}(E) \Phi(E)$$
⁽⁴⁾

where μ_a (E) (in m².kg⁻¹) is the mass coefficient of energy absorption in the air, and C_b (E) (in Sv.Gy⁻¹) converts the dose absorbed in the air to the dose absorbed in the body tissues. The coefficients in the formulae (1-4) depend on the gamma rays spectrum of each radionuclide and are interpolated from the tabulated values. Finally, the total exposure rate D (in Sv.s⁻¹) of a given nuclide is computed by adding the exposure rates of its discrete energy levels and reads:

$$\mathbf{D} = \sum_{\text{energy level } j} \mathbf{D}(\mathbf{E}_j) \tag{5}$$

Influence of the relief and buildings

Let us remind that the particles in the shadow of topography or buildings do not contribute to the photon radiation. To do this, CLOUDSHINE determines the equation of the straight line representing the ray between each given particle and each receptor point. There is interception if the height of the ray is less than the relief at one point at least of the meshing. For the buildings, the computation is performed along the ray-triangle interception algorithm of Möller and Trumbore (1997). The screening of the obstacles is optimized by checking that the buildings edges positions are on both sides of the line joining the considered particle and receptor. This noticeably reduces the calculation time.

Handling of the near or distant particles

The photon flux and the dose rate tend to infinity when the distance between the numerical particle and the receptor goes to zero. In CLOUDSHINE, this is prevented by (i) limiting each particle contribution to a fraction of its energy (which is equivalent to introduce a minimal distance) or (ii) by analytically calculating the dose rate in a hemisphere or a sphere of radius R (*ca.* 1 or 2 m) around the receptor where the activity concentration is supposed to be uniform.

On the other side, it is useless to account for particles far from the point where the gamma flux is estimated as their contributions become negligible. Thus, a threshold is defined as the distance beyond that the calculated dose rate is less than $\sim 10^{-19}$ or 10^{-20} Sv.s⁻¹. For a given radionuclide, a series of "cutting" distances are tabulated for increasing activity concentrations. Depending on each particle actual concentration, the maximal distance is then interpolated between the precomputed values. This results in a significant CPU time saving.

DESCRIPTION OF DEPOSITIONSHINE

In order to compute the exposure rate due to the radionuclides present on the ground or on the accessible surfaces of the buildings, the deposited numerical particles are considered as "frozen" (no displacement, nor rebound...) and they are given a status depending where the deposition takes place (on the ground or buildings façades, roofs or ceilings). The radiation evaluation is done distinctly for the airborne particles and the particles on the different kind of surfaces.

Test-case #1: the cube

In this academic situation, a 10 m edge cube is placed in a stationary wind field (5 m.s⁻¹ far from the obstacle) in a neutral atmosphere. A 60 Co release (4.10⁴ Bq in 5 min) is done at some distance of the cube. The particles settle on the cube with a

velocity of 5 m.s⁻¹ whatever the face (this value is numerical rather than physical). Figure 1 shows the wind module and the streamlines at 2 m above the ground level (AGL) and the particles stuck on the cube walls and roof. SPRAYSHINE is then used with receptors located along horizontal planes at heights of 0 m, 10 m, 11 m and 20 m AGL.



Figure 1. Particles deposited on a cube in a rectilinear wind field (far from the obstacle).

Figure 2 illustrates the results at the four mentioned levels when deposition happens only on the roof. At 0 m (a), the dose rate is zero as can be expected. At 20 m (d), the "iso-doses" are concentric circles with the maximum located just above the roof. At 10 m (b) or 11 m (c), the "iso-doses" are more like squares as the dose rate is evaluated on or very near the roof.



Figure 2. Gamma dose rates in planes at 0 m (a), 10 m (b), 11 m (c) and 20 m (d) AGL due to ⁶⁰Co particles deposited on the cube roof.

Figure 3 illustrates the results at the four mentioned levels when deposition happens only on the cube walls. The plume coming from the East, the number of deposited particles and the dose rate are greater on the cube eastern part than on the western part. The receptors located just in front of each cube wall only see the particles present on this face while the South-East (North-West, etc.) receptors see the particles on both South and East faces (North and West, etc.). That explains higher dose rates in the North-East and South-East quarters than in the East, North or South areas and higher dose rates in the North-West and South-West quarters than in the Western region.



Figure 3. Gamma dose rates in planes at 0 m (a), 10 m (b), 11 m (c) and 20 m (d) AGL due to ⁶⁰Co particles deposited on the cube walls.

Finally, it is verified that the shape and value of the exposure rate in case of deposition on all faces of the cube is the addition of the respective contributions of the roof and of the walls.

Test-case #2: the tunnel

This situation corresponds to a 60 Co release (5.10⁵ Bq in 1 hr) from a point source inside and in the middle of a 100 m long tunnel (with 16 m x 5 m inner and 22 m x 7 m outer width and height). Out of the tunnel, the wind module is equal to 2.3 m.s⁻¹ (at 10 m). The numerical particles settling on the tunnel roof and internal walls is important due to a high value of the deposition value of 1 m.s⁻¹. From Figure 4 which shows the particles positions and the gamma dose rate at 2 m AGL at four successive instants, it is worth noticing that the irradiation is null out of the tunnel and that the highest dose is computed near the source where the maximum deposition occurs.



Figure 4. ⁶⁰Co irradiation shape and value inside a tunnel at four successive times. (t₁ to t₄)

PARALLEL VERSION OF SPRAYSHINE

The dual objective of SPRAYSHINE parallelization is to drastically reduce the computational time by splitting the particles among numerous cores and to cope with huge simulation domains (which a standard configuration would not handle with) by dividing the domain into "tiles" distributed to a shared memory and many processors (using MPI instructions).

In the case of a simple domain (only one tile), the irradiating particles are simply distributed to the available cores at each time of the computation. If SPRAYSHINE simulation domain consists of multiple sub-domains, a particle in a given tile may contribute to the exposure rate in the other tiles. It means that, in principle, the possible interception of the gamma rays by the topography or the obstacles should be determined for each tile crossed through. This would result in a not acceptable computation time. As the radiation vanishes with the distance and the tiles are chosen large enough, the radiation in a tile is assumed to depend on the particles present in this tile and the eight neighboring ones. Subsequently, the relief and obstacles description are extended only to this area and the information exchange is significantly limited. Depending of the time, SPRAYSHINE is active on different tiles and able to create a varying neighborhood chronology. The necessary cores in a computation must be at least the number of SPRAYSHINE active tiles. If there are many cores available allocated to the same tile, the particles are distributed between them.

E.g. Consider a 100 tiles Micro-SWIFT computation, 50 tiles active during the Micro-SPRAY dispersion simulation and SPRAYSHINE launched with a pool of 200 cores. Two cores should be attributed to each SPRAYSHINE tile. Indeed, after neighborhood checking, four cores are given to each tile which optimizes the computational procedure.

Efficiency of the parallelization on one-tile

One of the test-cases of SPRAYSHINE parallel version operating on a single non-subdivided domain has concerned an urban district in the city of Lyons (France). The main features of the case are indicated in Table 1. The calculations have been done on a 47.7 Tflops Bull Itanium cluster comprising 932 nodes of 8 nodes (1.6 GHz), running from 1 to 400 cores. The computational time and speedup are presented on Figure 5 (a and b). Up to 10 cores, the gain is quite-linear. Between 10 and 100 cores, the slope of the curve tends to decrease however maintaining a high performance. Between 100 and 400 cores, the gain oscillates around its maximum value before it goes down.

Table 1. Main characteristics of the parallel SPRAYSHINE run in Lyons (France).								
Total number of nodes in the horizontal grid	65,511 (= 261 x 251)							
Number of receptors (after clearing of the nodes inside the buildings)	38,492							
Number of obstacles (after grouping them together)	2,583							
Number of computed irradiating particles	Time frame #1	Time frame #2	Time frame #3					
	6,431	7,883	7,883					



Figure 5. Computational time (a) and speedup (b) according to the number of operated cores in Lyons (France) simulation.

Application of the parallelization on multiple tiles

The first major test-case is a simulation in the business district "La Défense" situated in the North-West part of Paris. A hypothetical short release of ⁶⁰Co particles (1 GBq in 1 min) is done from a point source in the main "La Défense" avenue lined with high buildings. The settling velocity on the ground as on the buildings façades and roofs and on the ceiling of the "Big Arch" is taken equal to 0.1 m.s^{-1} . The principal other features of the calculation are mentioned in Table 2.

Table 2. Wall characteristics of the parallel SI KATSTING full fill alls – La Defense.									
Total number of nodes in the horizontal grid	105,651 (= 351 x 301)								
Number of obstacles (after grouping them together)	6,486								
Number of time frames	30								
Meteorological data (in neutral atmosphere, along with observations recording)	Time	12:00	12:05	12:12	12:20	12:22	12:30		
	Wind module (in m.s ⁻¹)	2.00	1.69	1.69	1.69	2.81	2.25		
	Wind direction (in °)	120	125	80	120	160	170		

Table 2. Main characteristics of the parallel SPRAYSHINE run in Paris - La Défense

Following the flow and dispersion computation with Parallel-Micro-SWIFT-SPRAY (PMSS), the gamma dose rate is evaluated by SPRAYSHINE distinguishing the irradiation by the plume and the surface deposition. The simulation domain is divided into nine tiles distributed to nine cores. The duration of this big size calculation in a Windows 7 - 64 bits environment is less than one hour.

Figure 6 (resp. 7) shows the topography outline, the airborne and deposited particles positions and the exposure rate due to the cloud (resp. the deposition on all surfaces) in a horizontal plane at 20 m AGL at successive instants. These images illustrate the shading by the obstacles and the non-zero dose rate "inside" the Big Arch hollow obstacle (*i.e.* between the ground and the ceiling of the arch).



Figure 7. DEPOSITIONSHINE computation in "La Défense" district at four instants (t1 to t4) with receptors at 20 m AGL.

CONCLUSION AND PERSPECTIVES

The precise evaluation of 3D gamma exposure is an essential point of the impact assessment in case of normal and, moreover, accidental or malevolent releases of radioactive materials. As the irradiation is a distant effect influenced by the shading of the topography and obstacles, especially the buildings on an industrial site or in an urban district, it is advisable to utilize modelling systems adapted to the built environment in order to determine the micro-scale flow and numerical particles dispersion. For some years, Micro-SWIFT-SPRAY has been developed with intent to become a compromise solution between the "full CFD" preciseness and computational times consistent with a crisis situation.

In 2005, Armand *et al.* presented the CLOUDSHINE post-processor working with the Lagrangian particle dispersion model Micro-SPRAY and dedicated to the computation of plumes dose rate. At this time, the modelling system was validated for a uniform distribution of a radionuclide (133 Xe) over a flat terrain where the post-processor results were directly comparable with values of the semi-infinite irradiation dose coefficients tabulated in the literature.

Recently, CLOUDSHINE has been significantly improved and supplemented with the DEPOSITIONSHINE module devoted to the exposure rate evaluation of radionuclides deposited on all accessible surfaces (ground and buildings façades, roofs or ceilings) also taking account of the shading by the obstacles. The post-processor "SPRAYSHINE" includes the ability to handle with hollow geometries (arches, tunnels...) and to estimate the gamma radiation at any heights above the ground with also a new algorithm for the interception between the gamma rays and the obstacles.

Furthermore, a parallel version of SPRAYSHINE is now available consistently with Parallel-Micro-SWIFT-SPRAY development. This version has been tested and proven to be efficient as speedup is concerned, on domains consisting of one or multiple tiles. This makes SPRAYSHINE performing together on a mono-processor laptop or on a super-computer dedicated to a high-resolution post-processing over a whole city. Nevertheless, progress must still be made in terms of ray tracing in order to reduce computational time for a huge simulation domain covering e.g. all Paris.

A micro-scale modelling system designed to predict the dispersion of radionuclides and post-process the gamma dose exposure at high resolution with moderate computational times opens perspectives to assess the impact of releases in the vicinity of industrial buildings or in the urban context. As a matter of fact, it offers a complete and very relevant answer in case of an emergency. Moreover, as the gamma exposure rate is directly measured in the field, the system should be relevant to improve the inverse algorithm used to determine a source term from available measurements.

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