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Decision support system ESTE for nuclear and radiological emergencies: Atmospheric dispersion models

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Abstract: The systems ESTE are running in nuclear crisis centers at various levels of emergency preparedness and response in Slovakia, the Czech Republic, Austria, Bulgaria, and Iran (at NPP monitored by International Atomic Energy Agency, IAEA). ESTE is a decision support system, running 24/7, and serves the crisis staff to propose actions to protect inhabitants against radiation in case of a nuclear accident. ESTE is also applicable as decision support system in case of a malicious act with radioactive dispersal device in an urban or industrial environment. Dispersion models implemented in ESTE are Lagrangean particle model (LPM) and Puff trajectory model (PTM). Described are models approaches as implemented in ESTE. PTM is applied in ESTE for the dispersion calculation near the point of release, up to 100 km from the point of nuclear accident. LPM for general atmospheric transport is applied for short-range, meso-scale and large-scale dispersion, up to dispersion on the global scale. Additionally, a specific micro-scale implementation of LPM is applied for urban scale dispersion modelling too. Dispersion models of ESTE are joined with radiological consequences models to calculate a complete spectrum of radiological parameters - effective doses, committed doses and dose rates by various irradiation pathways and by various radionuclides. Finally, radiation protective measures, like sheltering, iodine prophylaxis, or evacuation, evaluated on the base of predicted radiological impacts are proposed. Dispersion and radiological models of the state-of-the-art ESTE systems are described. Results of specific analyses, like number of particles applied, initial spatial distribution of the source, height of the bottom reference layer, are presented and discussed.

Keywords: nuclear accidents; decision support; protective measures, LPM, PTM, CBRN.

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1. Introduction

The key elements of decision support systems (DSS) for emergency preparedness and response in case of nuclear and radiological emergencies are assessment of the level of threat to the population due to the predicted or already released radioactivity to the environment, and recommendations of actions to secure the health of the inhabitants in the first place. For these aims, the DSS perform radiological impact calculation, consisting of calculation of atmospheric transport and dispersion of the radioactive material and consequently of dose prognosis evaluation. The dose calculation results in the recommended actions which are primarily sheltering, iodine prophylaxis and evacuation, secondarily e.g. actions in agriculture.

These are the basic features of the nuclear decision support system ESTE, whose approaches and solutions to the atmospheric dispersion and to radiological dose evaluation, are described and compared. Besides these features, the system ESTE is a complex decision support system for nuclear emergencies, and it also provides analysis and evaluation of various input data, like technological and radiation measurements, and assessment of source term based on such analysis, (detailed

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description for source term estimation see [1]). The most important feature and unique approach of the nuclear DSS ESTE is in connection of modules for assessment of accidental release of harmful radionuclides, with the state-of-the-art dispersion models and with radiological impacts models.

The calculated ensemble of radiological parameters considered in ESTE are dose rates, doses by external irradiation from radionuclides in atmosphere, doses by external irradiation from radionuclides deposited on terrain, doses by inhalation of airborne radionuclides, and doses by ingestion of contaminated foodstuffs.

The system ESTE is used for real time response to accidents at nuclear installations, and that fact determines the features of the implemented transport and dispersion models. The system is running in the nuclear crisis centers of Slovakia, the Czech Republic, Austria, Bulgaria or Iran, either directly on the national level or on the level of nuclear facility still with close connection to national level (in case of Iran, it is the crisis center of the nuclear power plant Bushehr, a facility monitored and inspected by the IAEA).

Demonstrated and discussed are models implemented in the ESTE system - application of Puff trajectory model (PTM) and Lagrangian particle models (LPM). Lagrangian particle model is introduced in two alternative ways - one implementation covers the dispersion calculation on meso- and long-scales, the other covers micro-scale on the level of dispersion in urban environment. The LPM for real-time long-range calculation is based on the methods of parallel computing and utilization of graphical card (CUDA technology). Emphasize is given to description and comparison of the applied atmospheric dispersion models. Demonstrated are results on case studies and on dispersion calculation after Fukushima accident.

The urban-oriented LPM is applicable i) either in case of a malicious act with application of radiological dispersion device (RDD) or dirty bomb in urban environment, or ii) in industrial accidents. In both the system performs evaluation of situation in the very close vicinity of the event.

2. Atmospheric dispersion models in ESTE

2.1. Lagrangean Particle Model, specific set-up assumptions in ESTE

LPM uses a large number of independent particles to describe diffusion of radionuclides in the atmosphere, and it performs a simulation of movement and dispersion of particles inside the wind field. Each particle carries a specific amount of radionuclides from the radioactive cloud. In general, the wind field consists of a mean wind field and a turbulent field. The basic equations for the particle positions are

$$x\,(t+\Delta t) = x(t) + U.\Delta t + u.\Delta t, \quad (1a)$$

$$y\,(t+\Delta t) = y(t) + V.\Delta t + v.\Delta t, \quad (1b)$$

$$z\,(t+\Delta t) = z(t) + W.\Delta t + w.\Delta t, \quad (1c)$$

where (x,y,z) specifies the position of the particle (at the times t and $t + \Delta t$), Δt is the time step, (U,V,W) is the velocity vector of the mean wind field at the given position (x,y,z). (u,v,w) is the turbulent component of velocity vector.

The LPM implemented in ESTE is based on theoretical description of the FLEXPART model [2], within which the turbulent wind field is described. The implementation in ESTE was successfully several times validated in various projects, e.g. a comparison was performed directly with FLEXPART model implemented in TAMOS (The Austrian emergency response modelling system). The implemented LPM applies numerical weather prediction data (NWP data), with possibility to apply various sources of NWP data, for example ECMWF or data of NWS/NOAA.

Specific aspects of LPM of ESTE which have influence on dispersion and radiation impacts calculation are:

Dry deposition – is characterized by deposition velocity v_d (in $m.s^{-1}$), which is specified for various types of airborne material (e.g. gases, aerosols, iodine forms) and ground features (e.g. urban, forest, water). Deposited material in time step Δt is then calculated as:

$$\Delta m = m\ (1 - \exp(-v_d\,\Delta t/h\ )). \tag{2}$$

Here m is the amount of activity born by particles in the lowest reference layer with the height h.

Wet deposition – following the model in [3], is governed in LPM of ESTE (and in the implemented PTM too) by a washout coefficient Λ, which depends on precipitation rate I (in mm/hr):

$$\Lambda = c_{wo}\, I. \tag{3}$$

c_{wo} is coefficient of wet deposition and is set to c_{wo} = 1.3E-04 s^{-1} for elemental iodine, c_{wo} = 1.3E-06 s^{-1} for organic iodine, c_{wo} = 2.6E-05 s^{-1} for all radionuclides in aerosol form. The deposited material in time step Δt is assumed to follow the formula

$$\Delta m = m\ (1 - \exp(-\Lambda\ \Delta t\ )). \tag{4}$$

Here the approach applied in ESTE assumes the washout along the whole height of atmospheric boundary layer (ABL), and the height of the clouds is not taken into account.

Release points - the position of the leakage point affects the impacts in the vicinity of nuclear facility in which the accident took place, but the leakage point in case of a real nuclear disaster can be uncertain and unknown. Generally, the leak of harmful radionuclides can occur in any part of the containment structure in case of containment leakage, in the outlet of plant ventilation stack or in the outlet of containment ventilation system. Moreover, the inner conditions inside the nuclear facility premises, like overpressure, fire and explosions, can affect considerably the leak conditions. The initial spatial distribution of the release points in LPM of ESTE system can be set up as a point source at a given height, a line-shape source, a source in the shape of a cylinder or a hemisphere. In ESTE running in nuclear crises centers, an assumption of a vertical-line-shaped source is applied, with the line center at the height of the realized release pathways. The center might be located at the height of the containment building, or at height of the roof of machinery room, or at the height of outlet of reactor building ventilation stack or outlet of containment annulus ventilation. The performed study of influence of initial spatial distribution of the release points at the beginning of dispersion calculation are presented and discussed in Section 3.2.

Height of the bottom reference layer of air – it is the air layer which is used to evaluate the air concentration over the ground surface, applied in dry deposition calculations as well as in impacts calculations (especially for effective dose by inhalation). As the previous aspect of the simulation setup, also modeled bottom-air-layer height above ground affects the calculated impacts in the vicinity of the nuclear facility in which the accident took place. In LPM of ESTE system, the height of the bottom layer of air is set to 100 m. The results of our study of influence of the height of the bottom reference layer of air are presented and discussed in Section 3.3.

Total number of modeled particles - the accuracy of dispersion calculation and radiological impacts calculation is determined by the total number of modeled particles. A relatively high number of particles is expected for the calculation in order to achieve acceptable level of accuracy. The higher is the number of particles, the longer is the time to carry out the calculations. The time is strictly controlled in decision support systems which are in real operation in nuclear crisis centers, like is ESTE. An acceptable time to carry out the calculations in local scale and mesoscale is about 15 minutes. In case of ESTE, the parameters affecting the duration of impacts calculation, to which the number of particle belongs, are set to fulfill this time limit. Naturally, if the calculations are performed in large or global scale where the modeled phenomenon is on the level of several days or weeks, for example modelling of the atmospheric transport and impacts of Fukushima accident to central Europe, then the time limit for duration of the calculation is less strict, allowing a longer calculation and a higher number of modelled particles. Our study of the influence of the total number of modeled particles are presented and discussed in Section 3.1.

Number of radionuclides in the source term - the nuclear reactor core inventory consist of more than one thousand various isotopes created as a result of nuclear fission. At the same time, many of

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them are short lived isotopes or isotopes with negligible radiological impact. In case of a nuclear disaster about 50 isotopes have potential to be released to the environment in a significant amount and also to cause significant threat to human and to environment. This group is covered by the set of radionuclides (list of these isotopes are in Table 1) assumed at the input, in all modeled processes of LPM in ESTE as well as in radiological models of ESTE.

Table 1. List of isotopes significant for radiological impacts calculations in case of events on a nuclear facility like nuclear power plant and applied in ESTE models.

Kr85m	Sr89	Zr95	Ru105	Te127	I132	Xe133	Cs137	Ce143	Pu241
Kr85	Sr90	Zr97	Ru106	Te129m	I133	Xe135	Cs138	Ce144	
Kr87	Sr91	Nb95	Rh103m	Te129	I134	Xe135m	Ba140	Np239	
Kr88	Y90	Mo99	Rh105	Te131m	I135	Xe138	La140	Pu238	
Rb86	Y91m	Tc99m	Sb127	Te132	Xe131m	Cs134	Pr143	Pu239	
Rb88	Y91	Ru103	Sb129	I131	Xe133m	Cs136	Ce141	Pu240	

The calculation of radiological parameters includes evaluation of the following quantities:

Committed effective dose by inhalation: The instant dose rate DR_{inhal} and the integral dose D_{inhal} are calculated as:

$$DR_{inhal}(n) = C_0(n)\, CF_{inhal}(age,n)\, BR(age), \tag{5}$$

$$D_{inhal}(n) = C_{int}(n)\, CF_{inhal}(age,n)\, BR(age). \tag{6}$$

Here C_0 is actual air concentration, C_{int} is time-integrated concentration in the bottom reference layer and for radionuclide n, BR is breathing rate depending on the age category. CF_{inhal} is conversion factor for the committed effective dose for inhalation depending on the age and nuclide.

External dose by deposition: the instant dose rate is calculated as

$$DR_{depo}(n) = D_0(n)\, CF_{depo}(n), \tag{7}$$

where $D_0(n)$ is deposition of radionuclide n on the terrain. CF_{depo} is conversion factor for external dose via deposition, as function of radionuclide.

External dose by cloudshine: the instant dose rate is calculated as:

$$DR_{cloud}(n) = C_0(n)\, CF_{cloud}(n). \tag{8}$$

Here $C_0(n)$ is air concentration in the bottom reference layer. CF_{cloud} is conversion factor for cloudshine, and dependent on radionuclide. The factors represent approach of semi-infinite cloud of constant concentration, i.e. the point of interest, either radiation monitor or man, is immersed in the activity of air hemisphere with constant concentration.

2.2. Puff Trajectory Model

Puff Trajectory Model (PTM) implemented in ESTE is a puff transport model combined with Gaussian dispersion model in horizontal direction and with a model based on a diffusion equation in vertical direction. The release consists of puffs where each puff carries its particular amount of the released radionuclides, which is the released activity per a specific time period, e.g. in units [Bq/1 hour] or [Bq/10 min]. The trajectories of the puffs are obtained as simple integrated paths for the wind field of numerical weather prediction data:

$$x(t+\Delta t) = x(t) + U.\Delta t,\ y(t+\Delta t) = y(t) + V.\Delta t. \tag{9}$$

Here U, V represent horizontal components of the wind field, x and y characterized position of the puff in the given times t and t + Δt. Both components U and V are dependent on height, and the height is taken as the height of center of mass of the puff.

General model assumptions of PTM, including Gaussian sigma functions, applied in the decision support systems ESTE are described in [1].

In the implemented approach to the equations of vertical diffusion, we assume a division of the atmosphere into 10 equally thick layers. The assumed height of the atmosphere, here meaning air between the ground and the atmospheric boundary layer (ABL), is related to the Pasquill category of stability (see [4]). In cases of very unstable conditions (i.e. category A) and very stable conditions (i.e. category F), which represent two extreme situations, the height of ABL is 1600 m and 200 m above the ground, respectively. The assumed layer approach for vertical diffusion defines only mean, evenly distributed concentration within the given layer. The bottom air layer is the reference layer for calculation of air concentration, applied in calculation of deposition and radiological parameters.

The height of the release together with timing of the release and nuclide composition of the release are the attributes of the source term. The release height specifies one of the calculation layers in which the release point is situated and in which we assume an even distribution of released radioactive material. Releases as a function of time are realized as series of puffs, where each puff carries the specific amount of the leaked activity corresponding to a specific time interval of the release. Time intervals that express the course of the leak in time are 15 minutes to 1 hour. Any number of puffs can be modelled simultaneously from different locations at the same or different heights, or from the same location but at different heights.

The calculated radiological parameters are defined in similar manner as for LPM, with a few exceptions. Committed effective dose by inhalation and external dose by deposition are evaluated using the same approach as described above.

External dose by cloudshine in large distance from the release point is evaluated by approach of semi-infinite cloud of constant concentration. But for distances up to 2-5 km from the release point, the presumption about immersion into hemisphere with air volume activity is not valid. Therefore, for these distances, a specific model approach that enables to account for contribution of airborne activity of nuclides in the puff dispersed in various heights to gamma dose rate at a point 1 m above the ground was created and is applied in ESTE.

2.3. Dispersion in urban or industrial area

For calculation of dispersion of radionuclides and radiological impacts in urban or industrial area, specifically in areas with the size on the level of 1 - 4 km^2 with non-flat surface, a specific implementation of Lagrangean Particle Model is applied in ESTE. Procedure is analogous like in case of mesoscale calculations, see Section 2.1. Two potential examples of situations and events considered as cases for application of radiological impacts calculation in urban area are accidental releases within area of a nuclear power plant or application of radiological dispersal device (dirty bomb) in inhabited urban area (e.g. city centers).

A specific feature of the impact calculation for urban area is the inclusion of building effect of present buildings. Particularly in case of detailed and more-accuracy-required calculation, the applied meteorological data have to reflect position, shape and size of buildings in the impacted area. I.e. the applied wind field follows distribution of streets and building as well as the dispersion coefficient is a field parameter, which reflects distribution of turbulence in the given urban area. Since each urban locality is practically unique, the corresponding urban meteo fields have to be evaluated uniquely if large accuracy is required.

The calculation of urban meteo fields means calculation of a variant of Navier-Stokes equations or some their effective versions where point meteo data from direct meteorological measurements or from predicted meteo data represent a boundary and initial condition for solving the equations. For example, the point meteo data could be a meteo measurement in one point at various heights which due to its position and quality could be considered as representative for boundary condition of the inlet boundaries. In practice, the urban wind-field calculation is a time-consuming process and

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therefore a questionable aspect within emergency response (as it is so for mesoscale distances where the numerical weather prediction data are applied as source of wind field data, prepared beforehand). Therefore, an application of urban meteo field which reflects the actual condition on the impacted site ought to be based on the pre-calculated set of urban meteo fields. In emergency, the applied urban meteo field is chosen as the most adequate to the actually measured condition. Obviously, the ensemble of the pre-calculated fields determines the accuracy of such approach: the larger ensemble is used, the more accurate result is obtained. A guidance for preparation of such a pre-calculated ensemble might be probabilistic distribution of meteo situations for the given site.

In the model of ESTE, the urban meteo field is calculated as solution to the Reynolds-averaged Navier–Stokes equations with the k–ε closure model. The applied numerical approach as well as the description of the boundary conditions are explained in [5].

In ESTE implementation of urban approach for the area of nuclear power plant (for example NPP Mochovce, Slovakia), the pre-calculated ensemble of meteo fields is characterized by 3 parameters:

- Category stability: taking into account unstable weather condition (specified by Monin-Obukhov lenght L = 100 m), neutral weather condition (L = infinity) and stable weather condition (L = -100 m).
- Wind direction: taking into account 36 different wind direction (with uniform step of 10°). The wind direction specifies direction of the wind entering into the meteo field calculation as boundary condition.
- Wind speed: taking into account 40-50 values of wind speed (depending on the stability category), ranging from low wind speed of about 0.2 m/s up to 9 m/s (in case stable weather) and 25 m/s (in case of neutral and unstable). The wind speed means wind rate at the height of 10 m in the specification of boundary condition.

The studied area is discretized on cells with the size 20 m x 20 m. The calculation domain has the size of 2800 m x 1400 m. Example of 3D model of the site is in the Figure 1.

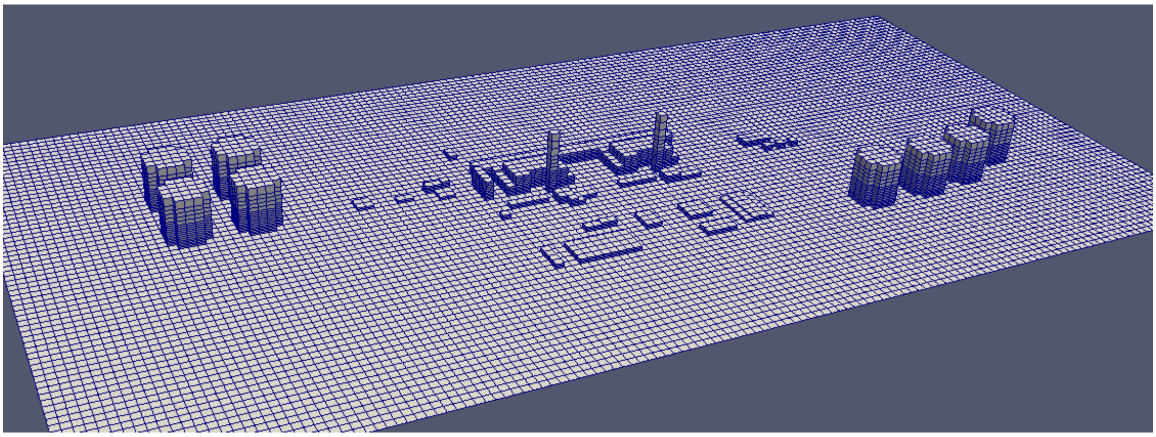

Figure 1: 3D model of the area of the Mochovce nuclear power plant, Slovakia

The Lagrangian particle model (LPM) for urban environment is based on theoretical description of [6,7]. Basic transport equations are (1). The mean wind represents averaged wind over a specific time interval (with a length in the interval of 10 minutes to an hour) in the computational domain, and the mean wind is calculated as solution of the Navier-Stokes equations. The vector (u,v,w) represents the random walk term of the wind, and is calculated as the Thompson's simplest solution [6,7]. In that solution, the random walk term is a function of the Reynolds stress tensor τ which is a meteo field given as the other outcome of the solution of the Navier-Stokes equations on the computational domain.

The outcomes of the dispersion simulation are concentration of airborne radionuclides and deposited material. Dry deposition A_{dd} on a surface is calculated using the similar approach as described above in (2) except inclusion of surface orientation parameter c_{so}:

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$$A_{dd} = C_0\, v_d\, c_{so}. \tag{10}$$

As example, c_{so} for aerosols is equal to 1 if the surface normal is vertical, and it is equal to 0.1 if the surface normal is oriented horizontally (based on [8], [9]). C_0 is the air concentration in the particular cell whose surfaces are considered as the surfaces undergo contamination by deposition. The evaluation of wet deposition takes into account all cells above the particular horizontal surface, but the vertical surfaces are assigned with zero wet deposition.

The radiological parameters are calculated for ground cells, i.e. cells having at least one ground or building surface. Such cells are potential locations for being occupied by persons. In case of committed effective dose by inhalation, the instant dose rate DRinhal and the integral dose Dinhal for a particular cell are calculated using (5) and (6), but with C_0 being the actual air concentration in the given cell and , C_{int} is time-integrated concentration in that cell.

The dose rate in the case of external dose by cloudshine is calculated as a sum of contribution of all cells j to the dose for the particular cell i as follows:

$$DR_{cloud}\,(i) = \sum_j C_0\,(j)\; CF_{cloud}\,(i,j)\; SF(i,j). \tag{11}$$

Here $C_0(j)$ is air concentration in the contributing cell. SF is shielding factor (equal to 1 if there is no building along the straight line between the cell centers of i and j, and equal to 0 if there is a building). CF_{cloud} is conversion factor for cloudshine, as function of nuclide and of distance between cell centers i and j.

Similarly, the dose rate of external dose by deposition is calculated as a sum of contribution of all ground and building surfaces j to the dose for the particular cell as follows:

$$DR_{depo}\,(i) = \sum_j D_0\,(j)\; CF_{depo}\,(i,j)\; SF(i,j). \tag{12}$$

Here $D_0(j)$ is deposit on the contributing cell. SF is shielding factor (equal to 1 if there is no building along the straight line between the cell centers of i and j, and equal to 0 if there is a building). CF_{depo} is conversion factor for external dose via deposition, as function of nuclide and of distance between cell centers i and j. The factors CF_{cloud} and CF_{depo} are prepared as a pre-calculated library (prepared by calculation using MCNP code), for various distances between the cells and various cell sizes.

Example of results for release in case of urban environment is in Figure 2. The simulation is done for release of 1.0E+15 Bq of Cs-137 from the roof of the reactor building. Shown is deposit on all surfaces (buildings and ground), effective dose rate corresponding to this deposit, effective dose rate from cloud during the duration of the release, and committed effective dose by inhalation. Doses and dose rate are calculated for ground cells.

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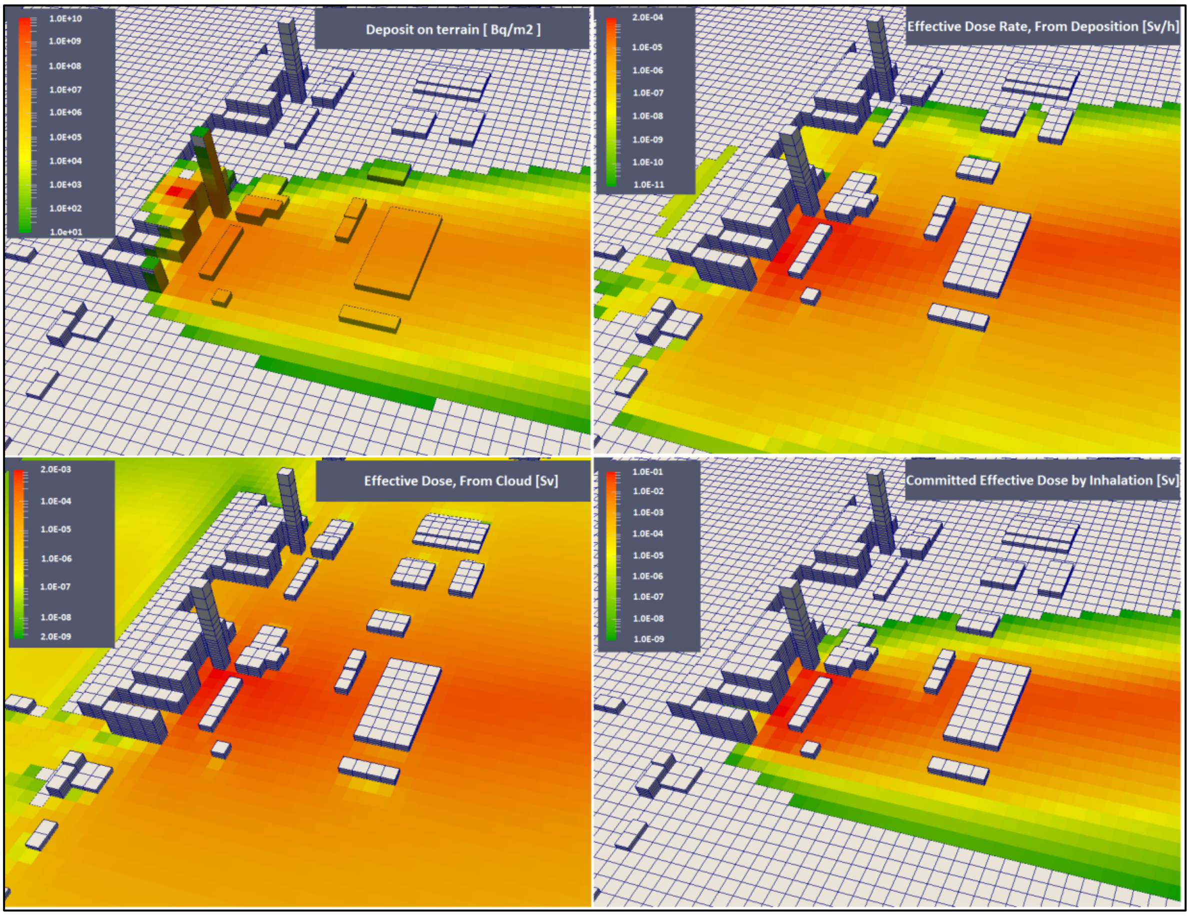

Figure 2. Example of impact calculation for urban environment – Simulated is a release from the reactor building in Mochovce NPP). Deposit on surfaces (top left), effective dose rate from deposition (top right), from cloud (bottom left) and by inhalation (bottom right) are shown.

3. Analysis and discussion of calculation settings for LPM in mesoscale impacts

Description of specific assumptions of LPM set up in ESTE is in Section 2.1. These assumptions could influence the results of the modeled dispersion, and, especially, the calculated radiological impacts. Influence of the total number of modeled particles, influence of initial spatial distribution of the release particles and influence of the height of bottom reference layer of air were analyzed, presented consecutively in Sections 3.1, 3.2 and 3.3.

All the analyses were performed in a case study, in which we assumed a release of 1.0E+15 Bq of Cs-137, started at 10:00 (UTC) of November 09 and lasted 1 hour. The release was assumed at NPP Bohunice, in Slovakia. The height of the release point was set to 80 m above ground. The applied meteorological data were the numerical weather prediction data as predicted by ECMWF for November 09 up to November 16, 2020. Modelled were dispersion in the atmosphere and radiological impacts up to 7 days from the release time.

The analyzed properties were studied in a set of locations which were chosen to lie approximately along the transport of the main activity. The analyses were performed in these 6 locations:

- Point1 - the village Nižná, Slovakia, located in about 4 km from the release location.
- Point2 –the village Prašník, located in about 17 km from the release location.
- Point3 –the village Strání, Czech Republic, located in about 45 km from the release location.
- Point4 –the town Valašské Meziříčí, Czech Republic, located in about 110 km from the release location.
- Point5 – Warsaw, Poland, located in about 480 km from the release location.

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- Point6 – Rovno, Ukraine, located in about 665 km from the release location.

In case of analyzing integrated paths, or trajectories, starting from the defined release point and time in the given field of NWP data and leading in specific heights, the first 5 points are chosen to lie near the trajectory related to the assumed release height (see Figure 3). The appropriateness of the choice of these 5 points were also approved by studying the impacts of dispersion calculation. The choice of the Point6 were justified according the impact calculation – one of the most impacted region in larger distances (see map of impacts in the next sections). The points 5 and 6 are on a similar level of direct distance from the release point (about 500 - 600 km), but the trajectories of radionuclides dispersed to the point 6 were longer than 1 000 km

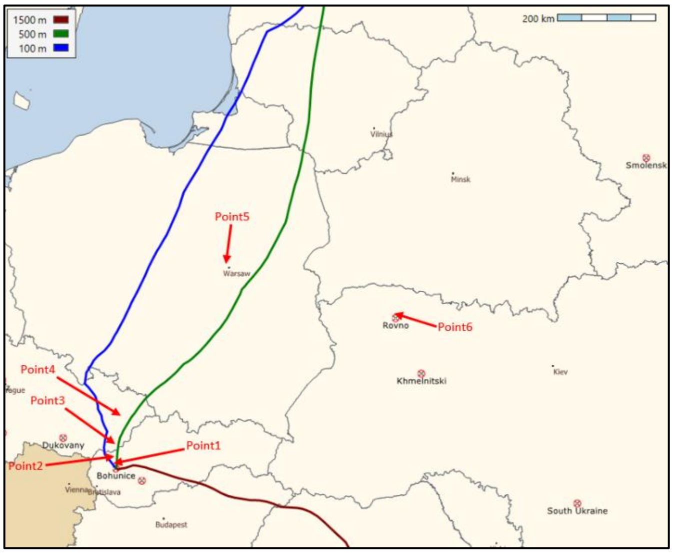
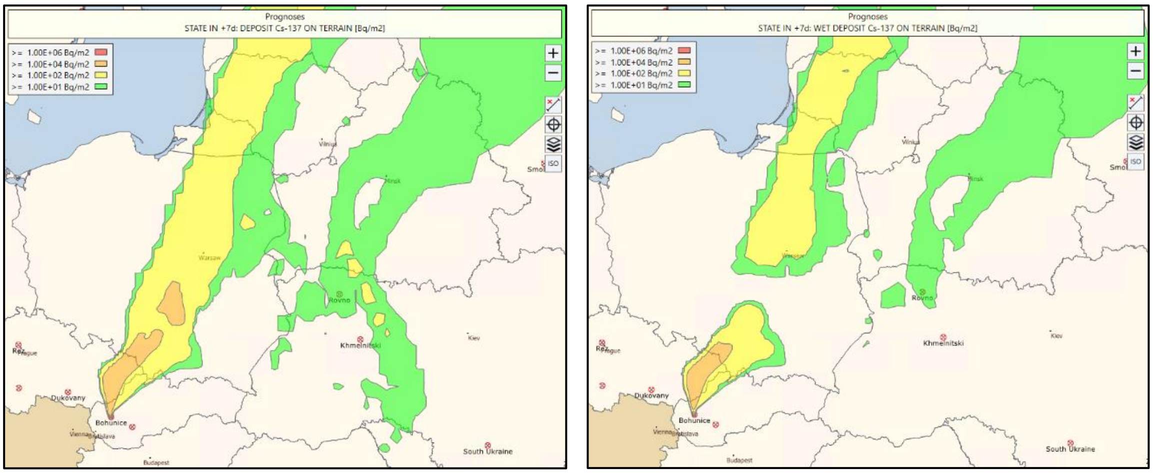


Figure 3. Trajectories, i.e. integrated paths, of the wind field for initial point in Bohunice NPP, at 10:00 UTC, November 09, 2020, for three various height - 100 m (blue line), 500 m (green line), and 1500 m (red line) above terrain. Shown are also locations of the 6 studied points.

3.1. Total number of modeled particles

In case of ESTE designed for nuclear crisis centers, the time limit for availability of calculated radiological impacts of a predicted release is 15 minutes. The number of particles is set to 250 000 in ESTE system to meet the time limit. The results of the analysis of the influence of particle number on the ground deposit for Cs-137 are presented in Table 2. The map of resulted ground deposit of Cs-137 is displayed in Figure 4.



(**a**) (**b**)

Figure 4. Ground deposit of Cs-137 as a result of release of 1E+15 Bq of Cs-137 from Bohunice NPP, at 10:00 UTC, November 09, 2020. (**a**) Total deposit of Cs-137 in +7 days from the time of release; (**b**) Wet deposit of Cs-137 in +7 days from the time of release.

Table 2. Deposit of Cs-137, seven days from the beginning of the release of 1E+15 Bq, in various points as a function of number of particles modelled. (a) Dry deposit, [Bq/m^2], and ratio to dry deposit in case of 1 000 000 particles; (b) Wet deposit, [Bq/m^2], and ratio to wet deposit in case of 1 000 000 particles.

(a)

Number of particles	Point2	Point3	Point4	Point5	Point6
25 000	4.3E+04/0.93	5.7E+04/0.98	7.8E+03/0.95	1.2E+03/1.23	1.6E+00/0.23
100 000	4.8E+04/1.03	5.8E+04/1.00	8.1E+03/0.99	1.0E+03/1.06	7.8E+00/1.15
250 000	4.7E+04/1.01	5.9E+04/1.02	8.1E+03/0.99	9.7E+02/1.02	3.5E+00/0.51
1 000 000	4.6E+04/1.00	5.8E+04/1.00	8.2E+03/1.00	9.5E+02/1.00	6.8E+00/1.00

(b)

Number of particles	Point2	Point3	Point4	Point5	Point6
25 000	8.8E+03/1.03	1.6E+05/1.00	3.2E+04/0.96	6.8E+01/1.08	1.3E+00/0.08
100 000	8.5E+03/0.99	1.5E+05/0.99	3.3E+04/0.99	6.8E+01/1.07	7.7E+00/0.49
250 000	8.6E+03/1.00	1.6E+05/1.00	3.3E+04/0.99	6.4E+01/1.01	1.5E+01/0.94
1 000 000	8.6E+03/1.00	1.6E+05/1.00	3.4E+04/1.00	6.3E+01/1.00	1.6E+01/1.00

Number of particles applied for the study was set to 25 000, 100 000, 250 000, and 1 000 000. All calculations were performed using the parallel computing platform CUDA exploiting graphics purpose unit (GPGPU). The respective times of calculations were 8 minutes, 9 minutes, 11 minutes, and 22 minutes. The LPM dispersion mesh has the resolution of 0.025°×0.025°, i.e. a resolution with size about 2-3km. The presented results are at points 2, 3, 4, 5, 6. From the results in Table 2 (a), (b) it is evident that when distances up to hundreds of km are taken into account, the results of a release simulated by 100 000 and higher number of particles are well converged and lead to little fluctuating results of ground deposit in the test. Large and random fluctuations of ground deposit, and, implicitly, of any other radiological parameter, are evident in case of larger distances.

Conclusion for number of particles applied in LPM of ESTE system is that 250 000 particles for distances at the level of hundreds of kilometers is appropriate and adequate number. At the same time, if dispersion along trajectories at the level of thousand kilometers or more is modelled, then much higher number than 250 000 particles ought to be applied.

3.2. LPM: Initial spatial distribution of released particles

The decision support systems running in nuclear crisis centers, like the system ESTE, have the task to predict and to assess radiation situation in close vicinity of the release. It is a task of higher importance than the mesoscale dispersion since the population in the close vicinity is the most exposed to release. The close vicinity is meant namely the area of nuclear facility and the emergency planning zone, a zone with usually radius of about 15 to 30 km. For calculation of impacts at distances at the level of emergency planning zone, an assumption about the initial spatial distribution of the source plays a non-negligible role. Influence of the initial spatial distribution of the source was analyzed, and results are reported in Table 3.

In the analysis, we assumed the following types of source: a) Point source at 80 m, meaning that the starting height of all particles was set to the height of 80 m above ground; b) Line source with 80 +/- 20 m, meaning that the starting height of particles was uniformly generated between 60 m and 100 m; c) the line source with 125 +/- 20 m means a uniform generation of particles between the heights 105 m and 145 m; and d) the line source with 35 +/- 10 m means a uniform generation of particles between the heights 25 m and 45 m above the ground. All defined sources reflect specific uncertainties in the release height occurring in the dispersion simulations: a) limited knowledge about the right release point – the release could happen through various building structures, walls or roofs; b) limited knowledge about the release conditions – the volume of air from containment undergoes thermal and pressure changes when released to the atmosphere and leading e.g. plume rising.

Table 3. Deposit of Cs-137, seven days from the beginning of the release of 1E+15 Bq, in various points, as a function of initial spatial distribution of the source. Dry deposit, [Bq/m^2], and ratio to dry deposit in case of point source at 80 m.

Spatial distribution of the source	Point1	Point2	Point3	Point4	Point5
point at 80 m	4.4E+05/1.00	1.0E+05/1.00	5.9E+04/1.00	8.1E+03/1.00	9.7E+02/1.00
line with 80 +/-20 m	3.9E+05/0.88	1.0E+05/1.01	5.8E+04/0.98	8.1E+03/1.00	9.6E+02/0.99
line with 125 +/-20 m	3.2E+05/0.73	1.0E+05/1.04	6.1E+04/1.03	8.5E+03/1.05	1.0E+03/1.08
line with 35 +/-10 m	4.3E+05/0.97	1.0E+05/1.00	5.7E+04/0.97	8.1E+03/1.00	9.4E+02/0.97

Since we focused on the closest points in this analysis, the presented results are at the points 1, 2, 3, 4, 5. The conclusion from the results (shown in Table 3) is that the influence of initial spatial distribution of the source of particles to the impacts calculated is significant at distances close to the source of release (e.g. for point 1 lying 4 km from the release point). At distances above 20 km from the source, the initial spatial distribution and height of the source above the ground has small or negligible influence to results.

Naturally, we are dealing with a different situation when the released radionuclides are lifted to a great height, for example due to an explosion. In such case, due to potentially different wind directions at higher heights of the atmosphere, the trajectories of particles lifted to higher heights from the terrain can be completely different from a leak at ground level heights. A demonstration of this phenomenon is in Figure 3. In the decision support system ESTE, the initial spatial distribution of particles is one attribute of the source term. The source term is assessed either by the ESTE system itself or is a part of the information from the damaged nuclear facility.

3.3. LPM: Height of the bottom reference layer of air

The height of the bottom reference layer of air above ground could affect calculated impacts near nuclear facility in which the release took place. In LPM of ESTE system, the height of bottom layer of air is set to 100 m. Influence of the assumed height of the bottom layer of air was studied and the results are reported in Table 4.

Table 4. Deposit of Cs-137, seven days from the beginning of the release of 1E+15 Bq, in various points, as a function of the height of the bottom layer of air. Dry deposit, [Bq/m2], and ratio to dry deposit in case of 100 m layer.

Bottom layer of air	Point1	Point2	Point3	Point4	Point5
100 m layer	4.4E+05/1.00	4.7E+04/1.00	5.9E+04/1.00	8.1E+03/1.00	9.7E+02/1.00
50 m layer	4.1E+05/0.94	4.5E+04/0.97	5.7E+04/0.97	8.1E+03/1.00	8.8E+02/0.91
25 m layer	4.2E+05/0.95	4.6E+04/0.98	5.6E+04/0.95	8.2E+03/1.01	8.5E+02/0.88

The presented results are at points 1, 2, 3, 4, 5. The conclusion from the results in Table 4 is that the influence of the model-applied height of the bottom layer of air above the ground is not significant. Effect of modelled bottom layer height could be significant if the number of particles is low. Such a situation could occur if the total number of applied particles in calculation is low. In our analysis we applied 250 000 particles, i.e. we are not expected to see influence on the results at least in the vicinity of about 100 km from the source. But if we are analyzing points or regions further from the source where the concentration of particles is low, non-negligible influence could be observed on the calculated parameters, see e.g. point 5.

5. Conclusions

System ESTE is a decision support system for nuclear crisis centers, modeling atmospheric transport of radioactive material leaked to the atmosphere as a result of accidents at nuclear facilities. Described are dispersion models of ESTE, which cover modeling of dispersion in mesoscale up to global range as well as dispersion in microscale meaning transport in urban and industrial environment. The implemented models are Lagrangean particle model and Puff trajectory model. The parameters of models are set so that calculations in emergency situation can be performed with high accuracy in relatively short time, within about 15 minutes. Presented and discussed values of parameters like is the number of applied particles in calculation, initial spatial distribution of the source, height of the bottom reference layer, lead to a conclusion that discussed parameter setting in ESTE is acceptable and adequate.

Supplementary Materials: Supplementary to Figure 4 (a) and (b), an evolution of total and wet deposit of Cs-137 over time on the map of Europe is presented in video S1 and video S2.

Lagrangean Particle Model of ESTE was applied for radiological impacts analyses of Fukushima Daichi releases to central Europe. Results of time integral of air concentration (TIC) of I-131 in bottom layer of atmosphere, in time steps of 2 days / 4 days / 6 days / 8 days / 10 days / 12 days / 14 days from the beginning of release are presented in video S3. Blue-colored are Particles dispersed from Fukushima at all levels of atmosphere, not only in bottom layer, are also demonstrated.

The following are available online at www.mdpi.com/xxx/s1,

Video S1: Ground deposit of Cs-137 as a result of release of 1E+15 Bq of Cs-137 from Bohunice NPP, at 10:00 UTC, November 09, 2020. Evolution of total deposit over time on the map of Europe in time steps: 8 h, 16 h, 24 h, 2 days, 3 days, 4 days, 5 days, 6 days, and 7 days from the time of release.

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Video S2: Ground deposit of Cs-137 as a result of release of 1E+15 Bq of Cs-137 from Bohunice NPP, at 10:00 UTC, November 09, 2020. Evolution of wet deposit over time on the map of Europe in time steps: 8 h, 16 h, 24 h, 2 days, 3 days, 4 days, 5 days, 6 days, and 7 days from the time of release.

Video S3: Fukushima Dai-ichi Catastrophe, Radiological Impacts to Central Europe Modelled by LPM of ESTE. Time integral of air concentration (TIC) of I-131 in bottom layer of atmosphere, state after 2 days / 4 days / 6 days / 8 days / 10 days / 12 days / 14 days from the beginning of release. Blue-colored are particles dispersed from Fukushima at all levels of atmosphere – from the terrain up to >5 km above the terrain.

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