

IDŐJÁRÁS

*Quarterly Journal of the Hungarian Meteorological Service
Vol. 114, No. 1–2, January–June 2010, pp. 101–120*

Simulation of accidental release using a coupled transport (TRES) and numerical weather prediction (ALADIN) model

Róbert Mészáros^{1*}, Csilla Vincze¹, and István Lagzi²

¹*Department of Meteorology, Eötvös Loránd University
P.O. Box 32, H-1518 Budapest, Hungary; E-mail: mrobi@nimbus.elte.hu*

²*Department of Chemical and Biological Engineering, Northwestern University
2145 Sheridan Road, Evanston, Illinois 60208, U.S.A.*

** Corresponding author*

(Manuscript received in final form March 18, 2010)

Abstract—A dispersion model-system called TRES (TTransport–EXchange) was developed at the Eötvös Loránd University (Budapest, Hungary) for modeling the transport and deposition processes of air pollutants originated from either continuous or accidental releases. In this study, a multi-layered, Eulerian version of the TRES model is presented that can simulate transport, transformation, and deposition processes of radionuclides or chemically toxic substances over Central Europe. The TRES model was coupled to the ALADIN mesoscale limited area numerical weather prediction model used by the Hungarian Meteorological Service to predict the path of nuclear contamination in the atmosphere. Two case studies – hypothetical accidents at the Paks Nuclear Power Plant (Paks NPP) – are presented to show how the coupled model can capture the dispersion of radionuclides from a single point source. Another effort of this study is to present a new method, a simple spatial semi-adaptive grid algorithm, which could be an effective tool for accelerating simulations. In this method, model calculations are performed only in the grid cells where concentrations in the previous time step are higher than a user defined threshold concentration. Reduction of the computational time depends on this threshold value, but decreases of more than 60% are found without decreasing the accuracy of the results. The efficiency of this method and a comparative analysis of model estimations with and without this method are also presented in this study.

Key-words: dispersion model, numerical weather prediction model, accidental release, semi-adaptive grid

1. Introduction

The potential for an accident in a nuclear power plant requires continuous developments of atmospheric dispersion models and widespread simulations of an accidental release of radionuclides with these models. Since the accident at the nuclear power plant in Chernobyl in 1986, an increasing demand is observable on the part of countries for construction of sophisticated dispersion models. On the basis of accurate model calculations, the decision makers have to make important arrangements, which can save human lives. In the last two decades, several accidental release models for different spatial and time scales have been developed. Some of these models are based completely or in part on the traditional Gaussian formulation. The DERMA (Danish Emergency Response Model of the Atmosphere) model uses a hybrid stochastic particle-puff diffusion description (*Sørensen et al.*, 1998, 2007). In the horizontal, a Gaussian distribution of the concentration is assumed for each puff. For puffs inside the boundary layer, an assumption of complete mixing is applied in the vertical, while for puffs above the boundary layer, a Gaussian distribution is used. The RIMPUFF (Risø Mesoscale PUFF) model (*Mikkelsen et al.*, 1997) was applied for example, in the study of *Gultureanu et al.* (2000). The Hungarian Meteorological Service has also adapted the RIMPUFF model for mesoscale simulations of a plume. The NAME model of the UK MET Office (the British Meteorological Service) and the Norwegian SNAP model apply Lagrangian description which simulates numerous particles that provide facility to take account of the effect of the fluctuation in the meteorological data (*Ryall and Maryon*, 1998; *Saltbones et al.*, 1998; *Bartnicki et al.*, 2003; *Jones et al.*, 2007). The Austrian emergency response modeling system, TAMOS (*Pechinger et al.*, 2001) is based on the Lagrangian particle dispersion model FLEXPART (*Stohl et al.*, 1998, 2005; *Srinivas et al.*, 2006) and the trajectory model FLEXTRA (*Baumann and Stohl*, 1997; *Stohl and Wotawa*, 1997). The Hungarian Meteorological Service has also adapted FLEXRTA/FLEXPART for calculating the long-range transport of particles from a nuclear power plant.

The Lagrangian models have the advantage that they can afford to use high spatial resolution, although they rely on the interpolation of meteorological data. Their potential disadvantages are that in some cases they neglect important physical processes and often experience problems when strongly diverging flows lead to uncertainties in long-range trajectories. In contrast to the Lagrangian approach, the Eulerian models use grid based methods and have the advantage that they may take into account fully 3D descriptions of the meteorological fields rather than single trajectories. An Eulerian dispersion model, MEDIA was joined to the emergency response system of the Hungarian Meteorological Service (*Ferenczi and Ihász*, 2003). However, Eulerian models show difficulty in resolving steep gradients, when fixed meshes are used. This causes particular problems for resolving dispersion from a single point source,

which creates very large gradients close to the point of release. For a coarse Eulerian mesh, the release is immediately averaged into a large area, which smears out the steep gradients and creates a large amount of numerical diffusion (*Lagzi et al.*, 2004). Therefore, in some cases a mixed approach is used. In these models (e.g.: DREAM – Danish Rimpuff and Eulerian Accidental release Model, or MATCH – Multiscale Atmospheric Transport and Chemistry model), close to the source, a Lagrangian description is used, while an Eulerian model calculates the long-range transport (*Langnera et al.*, 1998; *Brandt et al.*, 2000, 2002). The accidental release models are usually coupled with a nuclear decision-support system, e.g., the DERMA model has become interfaced with the Accident Reporting and Guidance Operational System – ARGOS (*Baklanov et al.*, 2006), or RIMPUFF was jointed to RODOS (Realtime Online DecisiOn Support) system (*Ehrhardt et al.*, 1997; *Mikkelsen et al.*, 1997).

The European real time modeling exercise RTMOD was developed to the comparison of long-range transport and dispersion models and support of decision making. It gathers the results of more than 20 models, and it provides not only one-to-one model comparison but ensemble dispersion forecasts (*Bellasio et al.*, 1999; *Galmarini et al.*, 2001, 2004).

Although several different kinds of dispersion models are available, further and continuous developments of simulation techniques are required. Based on the experience of our previous investigations (*Lagzi et al.*, 2001, 2004, 2006; *Lovas et al.*, 2006; *Mészáros et al.*, 2006; *Dombóvári et al.*, 2008), a newly developed Eulerian dispersion model is presented in this study. Model simulations and tests were carried out to estimate the long-range transport of radionuclides from a nuclear power plant (Paks NPP).

Dispersion simulations must have a high degree of accuracy and must be achieved faster than real time to use it for decision making strategy. There are several well defined methods and techniques to decrease the calculation time of the applications. One useful solution is the parallelization of source code and the application of the supercomputers, clusters, and grid systems to solve these tasks (*Dabdub and Seinfeld*, 1996; *Martin et al.*, 1999; *Larson and Nasstrom*, 2002; *Alexandrov et al.*, 2004; *Dimov et al.*, 2004; *Martín et al.*, 2004; *Ostromsky et al.*, 2005; *Singh et al.*, 2006). A new method for parallelization using newly developed video-card in CUDA environment is presented in *Molnár et al.* (2010). On the other hand, there are several numerical models, in which adaptive gridding techniques have been implemented (*Lagzi et al.*, 2004, 2006, 2009; *Zegeling and Kok*, 2004). The numerical algorithm automatically places a finer resolution grid in regions characterized by high spatial numerical errors. Therefore, the fine resolution grid follows the plume of the air pollutants.

In this study, a new semi-adaptive calculation method was introduced to reduce the CPU time for simulating dispersion processes. Using this simple algorithm, faster simulations are achievable due to decreasing of the active cells determined by a user-defined critical (or threshold) concentration. Numerical

simulations are performed only in these active cells, where the concentration of air pollutant in the previous time step exceeded the predefined level. The effectiveness of this method (how fast and precise the model) depends on this critical value. Very large critical concentration may cause uncertainty in the simulation, and very low critical concentration cannot call forth effective acceleration. However, the optimal choice of the critical value decreases the computational time without decreasing the quality of the results.

2. The TREX-Euler model

2.1. Model description

As a part of TREX model-system, developed at the Eötvös Loránd University, Hungary, the TREX-Euler is a multi-layered, Eulerian passive tracer dispersion model to describe transport and deposition of air pollutants over the Central European region. The model was developed in a flexible framework, and therefore, can simulate both single source accidental releases and photochemical air pollution. In this study we only focus on the dispersion of radionuclides from a nuclear power plant. All required meteorological data were obtained from the ALADIN mesoscale numerical weather prediction model (*Horányi et al.*, 1996, 2006). In the TREX-Euler model, horizontal dispersion of radionuclides is described within a regular Eulerian grid framework. The vertical mixing is parameterized using K-theory. Dry and wet deposition and also the transformation of radionuclides by nuclear decay are considered in each grid cell. The simulation of the dispersion is based on the following atmospheric diffusion equation:

$$\frac{\partial \mathbf{c}_i}{\partial t} = -\underline{\mathbf{V}}\nabla \mathbf{c}_i + \nabla \underline{\mathbf{K}}\nabla \mathbf{c}_i - (k_{c_i} + k_{d_i} + k_{w_i})\mathbf{c}_i + \mathbf{E}_i, \quad (1)$$

which describes the advection, diffusion, and source and sinks of the radionuclides. In the equation \mathbf{c}_i is the concentration of the i th radionuclides, $\underline{\mathbf{V}}$ is the three-dimensional velocity vector, $\underline{\mathbf{K}}$ is the tensor of turbulent diffusions coefficient, k_{c_i} is the coefficient of radioactive decay, k_{d_i} and k_{w_i} are the dry and wet deposition coefficients, and \mathbf{E}_i is the emission of radionuclides, respectively.

This partial differential equation has been solved by ‘method of lines’ technique. The two main components of the method of lines are spatial discretization followed by time integration. A second-order central difference stencil and upwind approximation are used for spatial discretization of the turbulent diffusion and advection. The model uses the forward Euler method to solve the obtained original ordinary differential equations. However, this

method is robust only with the appropriately chosen grid spacing (Δx) and time step (Δt). An accidental release model must be precise and fast at the same time. It is difficult to achieve both, because the more accurate and complex the model is the more computational time is required. The accuracy and the CPU time depend on model algorithms and also on the spatial and time resolution. For example, a shorter time step increases the accuracy of solution, at the same time, the computational efficiency decreases. To preserve the stability of the solution, the following conditions must be realized between the Δx spatial resolution and Δt time step for advection and diffusion, respectively:

$$\frac{|\mathbf{V}|\Delta t}{\Delta x} \leq 1, \quad (2)$$

$$\frac{2K\Delta t}{\Delta x^2} \leq 1, \quad (3)$$

where $|\mathbf{V}|$ is the amplitude of wind velocity vector and K is the horizontal turbulent diffusion coefficient. The spatial resolution is same as the resolution of the meteorological data from the ALADIN model, therefore, the model calculation was discretized on an equidistant rectangular grid with resolution of 0.0375×0.025 degrees ($\sim 2.5 \text{ km} \times 2.5 \text{ km}$). For this spatial resolution the time step Δt was set to 10 s, which assures the stability of solution.

In the vertical direction the model contains 32 levels and the resolution increases exponentially with height. Each vertical level was determined with the barometric formula (assuming isothermal layers) in a hypothetical air column, where the surface pressure is equal to 1013.25 hPa. Up to 200 m above the surface, the column was divided into 12 levels with equidistant pressure difference (197 Pa in isothermal layers), up to 3000 m the layers were thicker with higher pressure difference (1514 Pa), and these two resolutions were joined together. Two additional levels were added to the bottom and the top of column to ensure the boundary conditions.

The horizontal turbulent diffusion coefficients (K_x and K_y) were considered with a constant value equal to $10^4 \text{ m}^2 \text{ s}^{-1}$ (Brandt, 1998). In regional scale, in the function of the wind speed, the effect of the advection on dispersion is one or two orders of magnitude higher than the effect of the horizontal turbulent diffusion. Vertical transport was parameterized using the K-theory. The vertical turbulent diffusion coefficient (K_z) at a given level z has spatial and temporal variation:

$$K_z = \frac{ku_* z}{\Phi_T} \left(1 - \frac{z}{H_{mix}}\right)^2, \quad (4)$$

where k is von Kármán's constant taken to be 0.41, u_* is the friction velocity, z is the height above the surface, Φ_T is the similarity function for heat, and H_{mix} is the height of the mixing layer. Similarity functions for stable and unstable stratifications were used after Arya (1988). The value of H_{mix} was obtained from ALADIN model. The friction velocity was calculated by the following equation:

$$u_* = \frac{ku}{\log \frac{z_{ref}}{z_0} - \Psi_m}, \quad (5)$$

where z_{ref} , u , z_0 , and Ψ_m are the reference height, wind velocity at this height, roughness length, and integral form of universal stability correction functions for the momentum, respectively.

Universal function in stable stratification was estimated after Businger *et al.* (1971) in case of $z_{ref}/L \leq 0.5$, and an empirical relationship of Holtslag and de Bruin (1988) was used in other cases, where L is the Monin-Obukhov length. In case of unstable stratification, the stability function was based on Paulson (1970). The stratification of the layer was determined iteratively by the Monin-Obukhov length:

$$L = -\frac{T u_*^3}{\frac{gk}{\rho c_p} H}, \quad (6)$$

where T is the air temperature at 2 m (data from ALADIN model), g is the acceleration of gravity, ρ is the air density, c_p is the specific heat at constant pressure, and H is the sensible heat flux. In this study, this latter term was calculated after Brandt (1998).

The vertical dispersion was calculated with a Lagrangian stochastic, random displacement method. In this method, the particles, which are in a cell, are divided into a number of groups or packages (10 packages in this study) with equal number of particles, and the 'packages' are moving together. The vertical displacement of a package l_n is calculated as follows:

$$l_n = R \sqrt{K_z(n) \Delta t}, \quad (7)$$

where R is a random number with normal distribution and $K_z(n)$ is the vertical turbulent diffusion coefficient at the n st level (z_n). During a time step, a particle package can move only into the adjacent cells (the direction of the movement depends on the sign of the l_n). The i th ($i = 1$ to 10 in this study) package from the level

z_n gets into the level z_{n+1} (upward) if $l_n(i)$ is positive and $l_n(i) > (z_{n+1} - z_n)/2$, and into the level z_{n-1} (downward) if $l_n(i)$ negative and $-l_n(i) > (z_n - z_{n-1})/2$. If the condition is not met, the i th package stays at the level z_n . From the top and bottom levels the vertical transport is one way.

During current model simulations, the dispersion of a radionuclide – ^{131}I – was considered. The emission was assumed to be from the Paks NPP (46°34'N, 18°51'E) as a point source. The radioactive decay and the change of activity of ^{131}I were simulated. Chemical reactions were not considered. However, the structure of the program allows simultaneous simulations of the dispersion of several hundred isotopes, taking into account all radioactive decays and reactions.

The deposition is handled as a first-order reaction, which decreases the amount of the radionuclide in the atmosphere. Dry deposition of radionuclides from the bottom layer is parameterized by a constant deposition coefficient ($3 \times 10^{-6} \text{ s}^{-1}$ for ^{131}I) based on *Baklanov and Sørensen* (2001). The wet deposition velocity was parameterized using a simple scheme to calculate the wet deposition coefficient k_w based on the relative humidity RH with the following parameterization (*Pudykiewicz, 1989, 1991; Brandt, 1998*):

$$k_w = 0, \quad \text{if } RH < RH_t$$

$$k_w = 3.5 \times 10^{-5} \left(\frac{RH - RH_t}{RH_s - RH_t} \right), \quad \text{if } RH \geq RH_t, \quad (8)$$

where RH is the current relative humidity, RH_s is the saturation relative humidity (100%), and RH_t is a threshold value of relative humidity (80%); above which the wet deposition of radionuclides from the bottom layer occurs. The radioactive decay is calculated by a constant rate: $k_c = \log 2 / t_{1/2}$, where the radioactive half life ($t_{1/2}$) of ^{131}I is $6.948 \times 10^5 \text{ s}$.

During the model computations, each process – horizontal spreading (advection and diffusion), vertical dispersion, source and sinks terms (deposition, radioactive decay, and emission processes) – are calculated separately using the operator-splitting approach. The model was coupled with the ALADIN mesoscale limited area numerical weather prediction model used by the Hungarian Meteorological Service.

2.2. The semi-adaptive method

In a previous investigation (*Lagzi et al., 2006*), an adaptive grid model has been presented to describe the formation and transformation of air pollutants based on triangular unstructured grids. This technique is based on the calculation of

spatial error estimations. The algorithm can then choose to refine the grid in regions of high spatial error by comparison with a user defined tolerance for radionuclides. Therefore, depending on the numerical error, the spatial resolution was varied. In this study, another effective way is presented to reduce the CPU time of model calculations. The model applies a semi-adaptive method to perform faster simulations. In contrast to the adaptive method, in the newly introduced semi-adaptive method, the spatial resolution remains constant but a concentration test is applied to determine if model calculations are to be performed in particular grid cells.

The main concept of the semi-adaptive method is that the model calculation is performed only in the grid cells, where a predefined condition is met. This condition is that the concentrations in the grid point in the previous time step must be greater than a user defined critical concentration. By this method, the accuracy and the CPU time depend on the critical concentration and the simulation period. At the beginning of the simulation, immediately after the accidental release, the efficiency of the acceleration is higher, since model calculations are performed only in a few grid points. With the development of the plume, the efficiency of the method decreases as the number of affected grid points increases. Through the choice of the critical concentration, the CPU time and the error of the method can be adjusted. By increasing the critical concentration, the CPU time can be significantly decreased, however, the calculation error increases.

3. Results and discussion

3.1. Modeling accidental release

The features of the transport model and the efficiency of the semi-adaptive method are illustrated by two simulations of a hypothetical nuclear accident in the Paks Nuclear Power Plant, in the central part of Hungary (46°34'N, 18°51'E). During the simulations, ^{131}I isotope was emitted into the atmosphere from the point source to the given grid cell with the rate of $10^{10} \text{ cm}^{-3} \text{ s}^{-1}$ between 00 and 12 UTC on December 2, 2005 and March 24, 2006. Meteorological fields (wind speed, wind direction, temperature, relative humidity, cloudiness, and mixing layer height) were obtained from ALADIN weather prediction model. Simulations were performed for 48 hours after the hypothetical accidents. The modeled area covered the region around Hungary (10.85°–25.1°E, 41.3°–52°N) and contained 8640 grid cells on each 32 vertical levels.

Fig. 1 depicts the horizontal structures of the radioactive plume originating from the Paks Nuclear Power Plant at the emission level (120 m above the surface), 12, 24, 36, and 48 hours after a hypothetical accident on December 2, 2005. The plume structure is predominantly determined by the wind field. However, other meteorological parameters can also influence the dispersion

(e.g., vertical temperature gradient, planetary boundary layer height, etc.). During this simulation period, the Carpathian Basin was affected by a Mediterranean cyclone and a warm front caused rainy weather. The variable wind field caused the plume to spread in south, south-western direction in the first few hours of the simulation, but as the wind direction changed, the radioactive cloud had moved in eastern, north-eastern, and finally, northern direction. Due to this variable wind field, a wide region (including all of Hungary) was affected by the plume. However, as the concentration was highest after the release, when the plume had moved in southern direction, the highest cumulative dry deposition of ^{131}I to the surface appeared to the south of the point source (*Fig. 2a*). The cumulative wet deposition (*Fig. 2b*) was also significant, because more than 15 mm precipitation occurred in some parts of central Hungary during two days after the hypothetical accident. Highest wet deposition was found around the point source (the maximum was higher than 10^9 cm^{-2}), where the largest amount of precipitation was fallen during 48 hours.

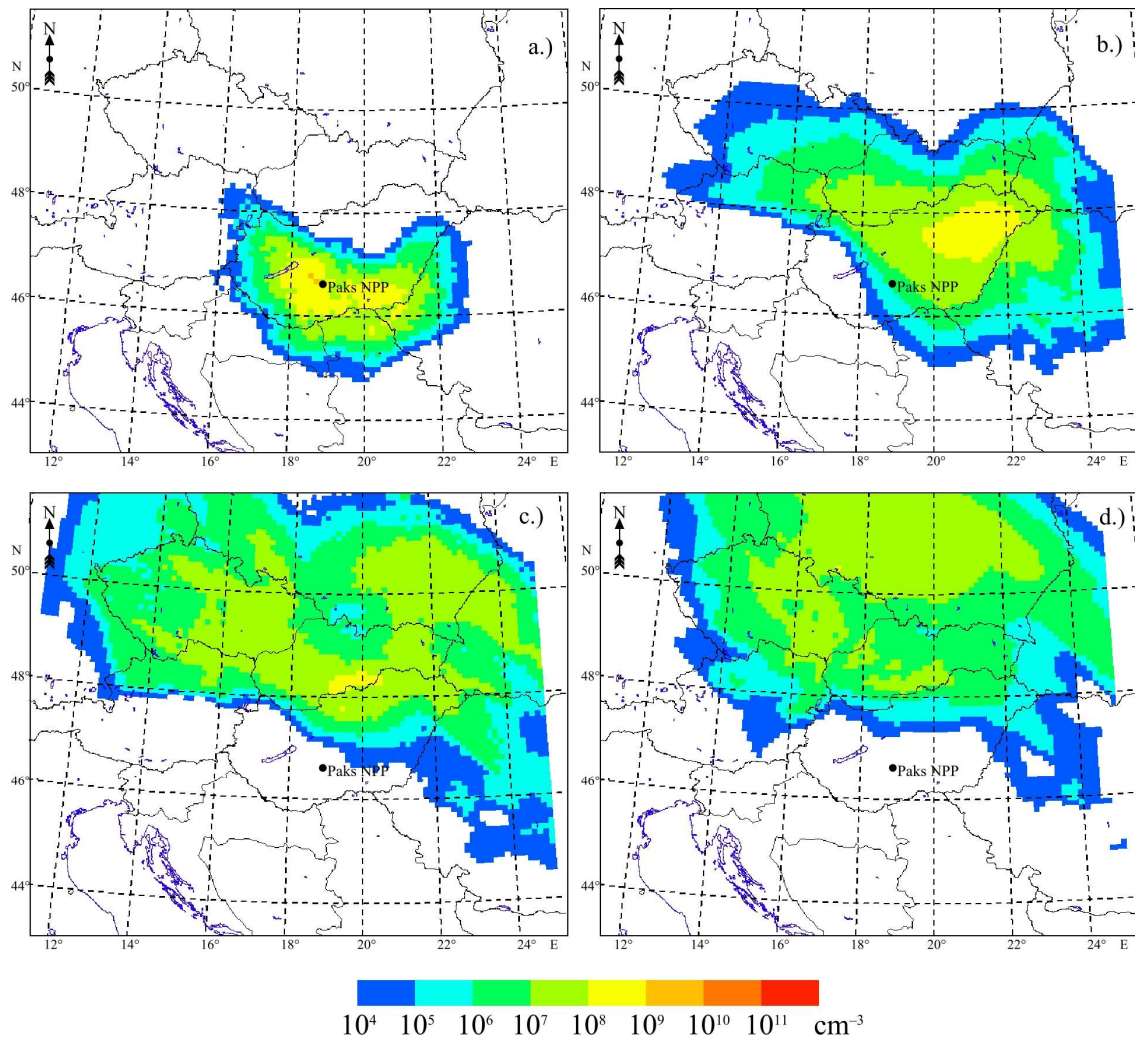


Fig. 1. Horizontal distribution map of ^{131}I concentration at 120 m above the surface, (a) 12, (b) 24, (c) 36, and (d) 48 hours after the hypothetical accident at 00 UTC, December 2, 2005.

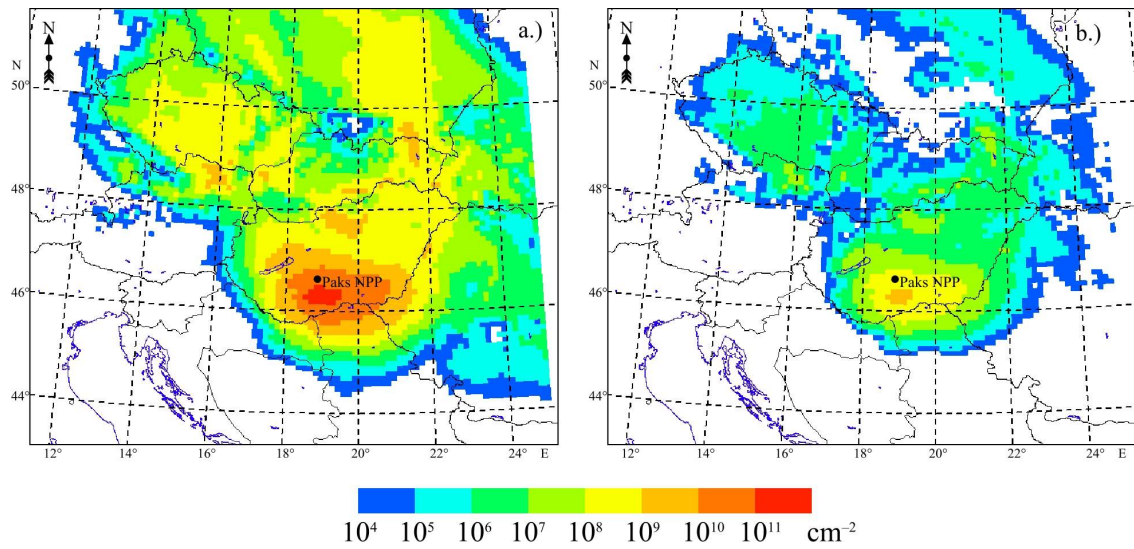


Fig. 2. Horizontal distribution map of cumulative (a) dry and (b) wet deposition of ^{131}I to the surface, 48 hours after the hypothetical accident at 00 UTC, December 2, 2005.

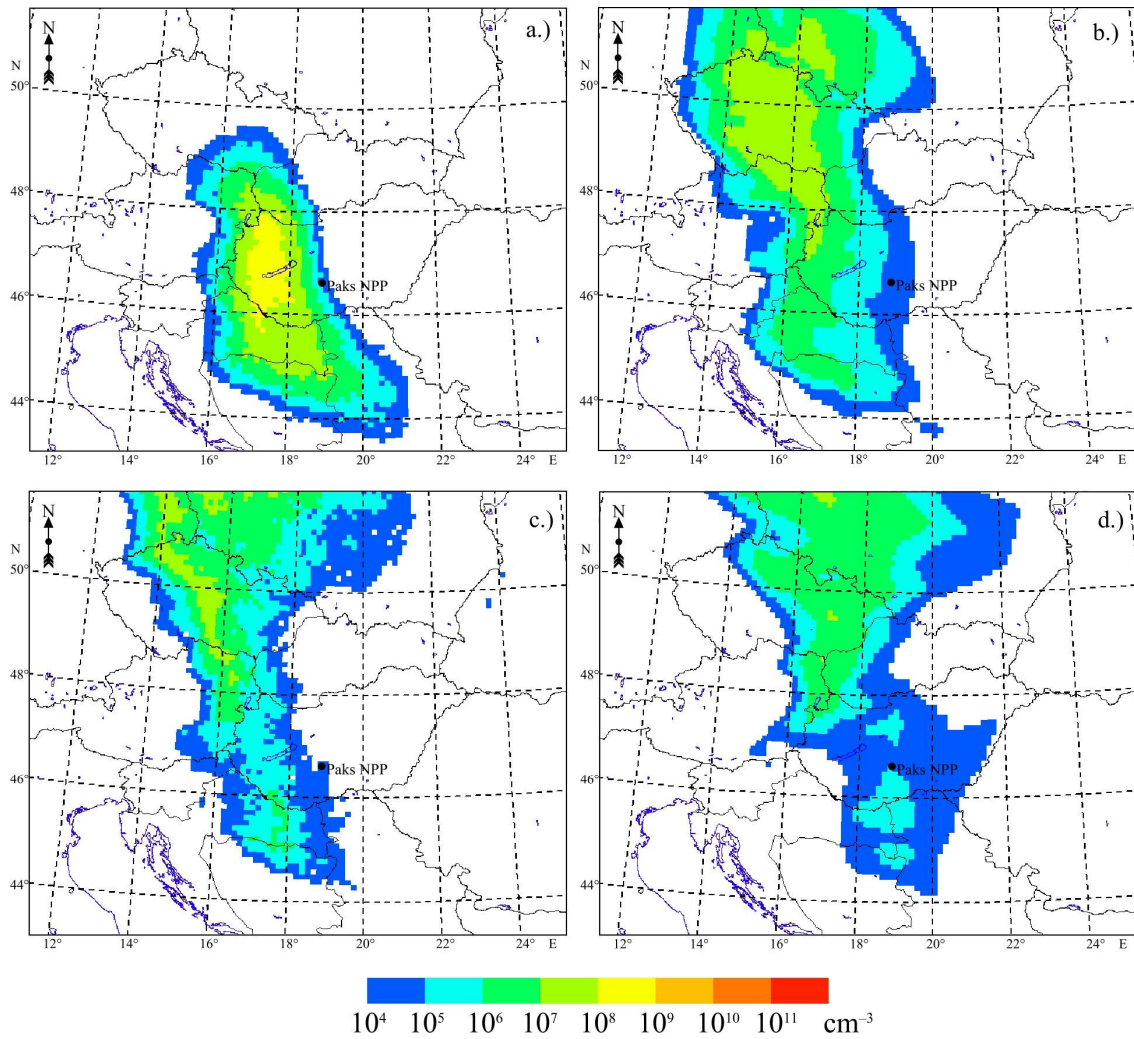


Fig. 3. Horizontal distribution map of ^{131}I concentration at 120 m above the surface, (a) 12, (b) 24, (c) 36, and (d) 48 hours after the hypothetical accident at 00 UTC, March 24, 2006.

During the period of the second simulation (March 24–25, 2006), an anticyclone was located over Central Europe, which caused sunny, dry weather. In the first 12 hours of the simulation, the plume was spread in a wide south-north belt, which had moved to the North and finally to the East (*Fig. 3*). Significant cumulative dry deposition was observed in south-northern axes (*Fig. 4a*), however, wet deposition (*Fig. 4b*) was very minor due to the dry weather conditions.

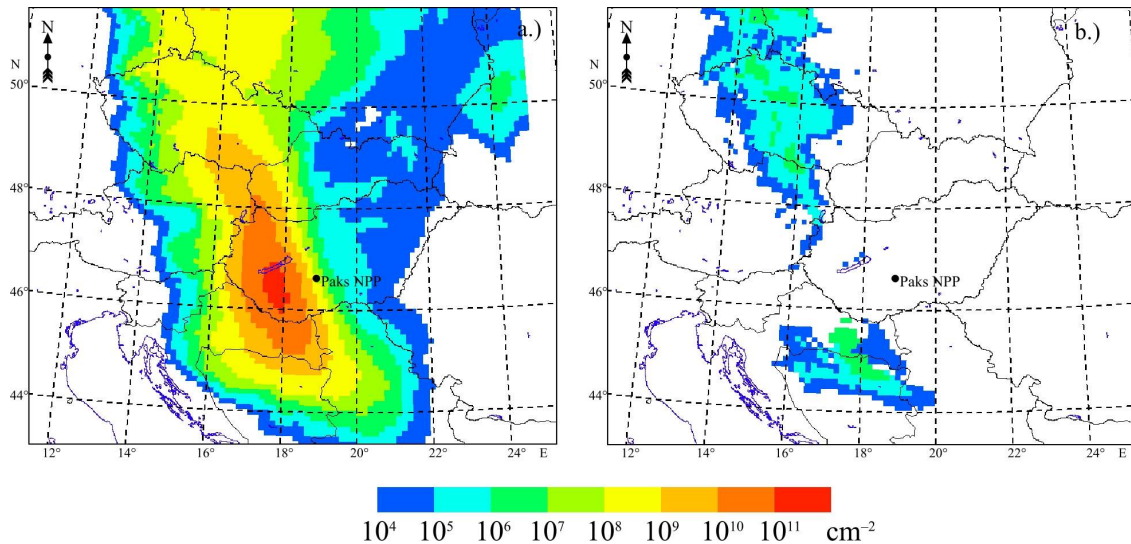


Fig. 4. Horizontal distribution map of cumulative (a) dry and (b) wet deposition of ^{131}I to the surface, 48 hours after the hypothetical accident at 00 UTC, March 24, 2006.

3.2. Efficiency of the semi-adaptive method

Efficiency of the semi-adaptive method is illustrated by running a set of simulations with the same meteorological and emission conditions used in the standard model runs described above, but during these simulations, the calculations have only been made on grid columns (on active cells), when the concentration of ^{131}I , at least at one grid cell in any of the 32 layers of a given grid column, exceeds a previously defined critical concentration. *Fig. 5* shows the number of active cells as a function of time, and critical concentrations. The higher the critical concentration is, the lower the number of active cells are. By increasing this critical concentration, higher acceleration can be achieved, since fewer calculations must be performed over the domain. In *Fig. 6*, the relative CPU time and the ratio of active cells can be seen as a function of the critical concentration for a 48-hour simulation (00 UTC, March 24, 2006–00 UTC, March 26, 2006). In case of relative CPU time, 1 refers to the CPU time of the simulation without the semi-adaptive method. The ratio of active cells is the maximum number of calculated horizontal grid cells during the whole simulation divided by the total number of horizontal grid cells 8640 (96×90). One can see that both the ratio of active cells and the relative CPU time

decreased with the increase of the critical concentration, but the size of the decreases are different. For lower critical concentrations (up to 10^7 cm^{-3}), the relative CPU time decreases rather than the maximum number of active cells during the simulation. The reason for this difference is that the number of active cells increases during the simulation. Accordingly, the acceleration is most effective after starting the simulation and decreases with time as the number of active cells increases.

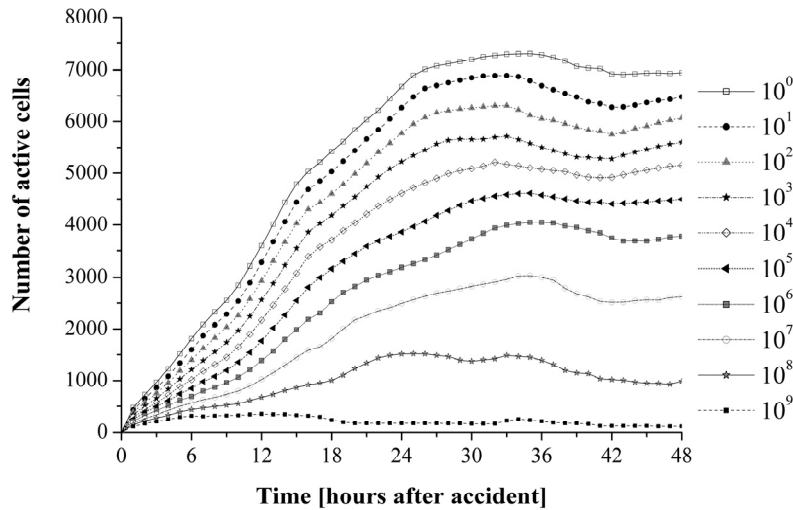


Fig. 5. Number of active cells during a 48-hour simulation after the hypothetical accident at 00 UTC, March 24, 2006 with different critical concentrations (in cm^{-3}).

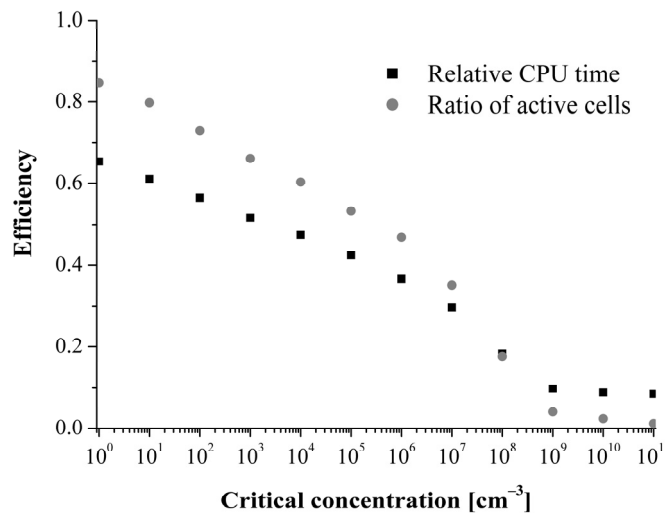


Fig. 6. Relative CPU time and ratio of active cells as a function of critical concentration. Test data: March 24–25, 2006.

In Fig. 6, the ratio of maximum number of active cells are presented, however, the relative CPU time corresponds to the whole period. In case of higher critical concentrations (from 10^9 cm^{-3}), with increase of the critical concentration the number of active cells slightly increases further, but it seems

that there is no further significant changes in the effective CPU time. This result suggests that there is a possible limit of the acceleration and any further increase of critical concentration will not increase the efficiency of the simulation. We should note that the CPU time also contains the time of unpacking, reading, and repacking of all meteorological datasets from the ALADIN model output files, and this time cannot be shortened by the semi-adaptive method.

The decrease of the simulation time of an accidental release model is crucially important and, at the same time, the method applied for the acceleration must be reliable. In *Fig. 7*, the horizontal distribution of the plume at the surface can be seen after 12 hours of a hypothetical accident using different critical concentrations. It appears that there is good agreement between maps with no critical concentration and lower critical concentrations (10^4 – 10^6 cm^{-3}). The polluted area and region with the highest concentrations can be captured similarly in all cases. However, some differences appear in the distribution, and these differences increase with increases in the critical value. For higher critical concentrations (10^7 – 10^9 cm^{-3}) the differences became significant, and only the most polluted area appears in the maps. Additionally, in some part of these regions, higher concentrations can be found as in case of standard model runs without the semi-adaptive method. Nevertheless, simulations using high critical concentrations can rapidly provide information about the direction of plume transport.

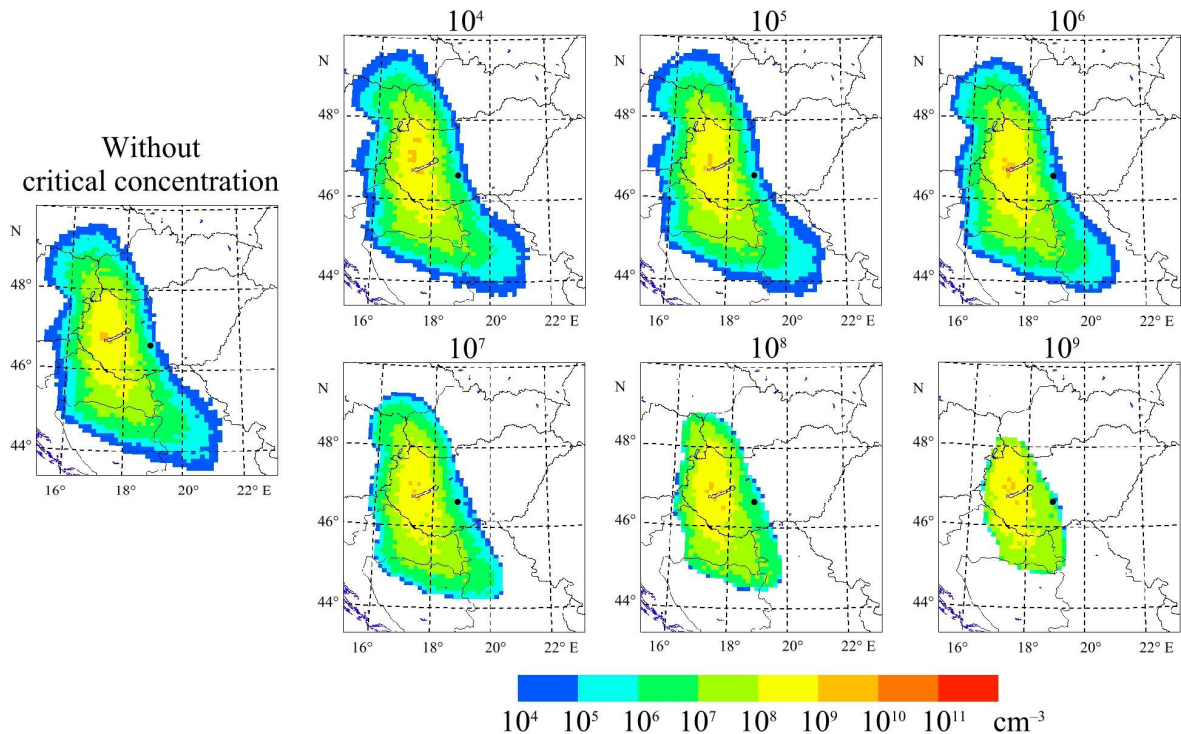


Fig. 7. Horizontal distribution map of ^{131}I concentration at the surface 12 hours after the hypothetical accident at 00 UTC, March 24, 2006 without and with different critical concentrations (in cm^{-3}). Same input meteorological and emission data were used in all cases. The black point denotes Paks NPP.

The differences depend not only on the choice of critical concentration but also on the simulation time. *Figs. 8a* and *b* present the relative differences of average and maximum concentrations of ^{131}I at the surface calculated without (c_1) and with (c_2) a critical concentration.

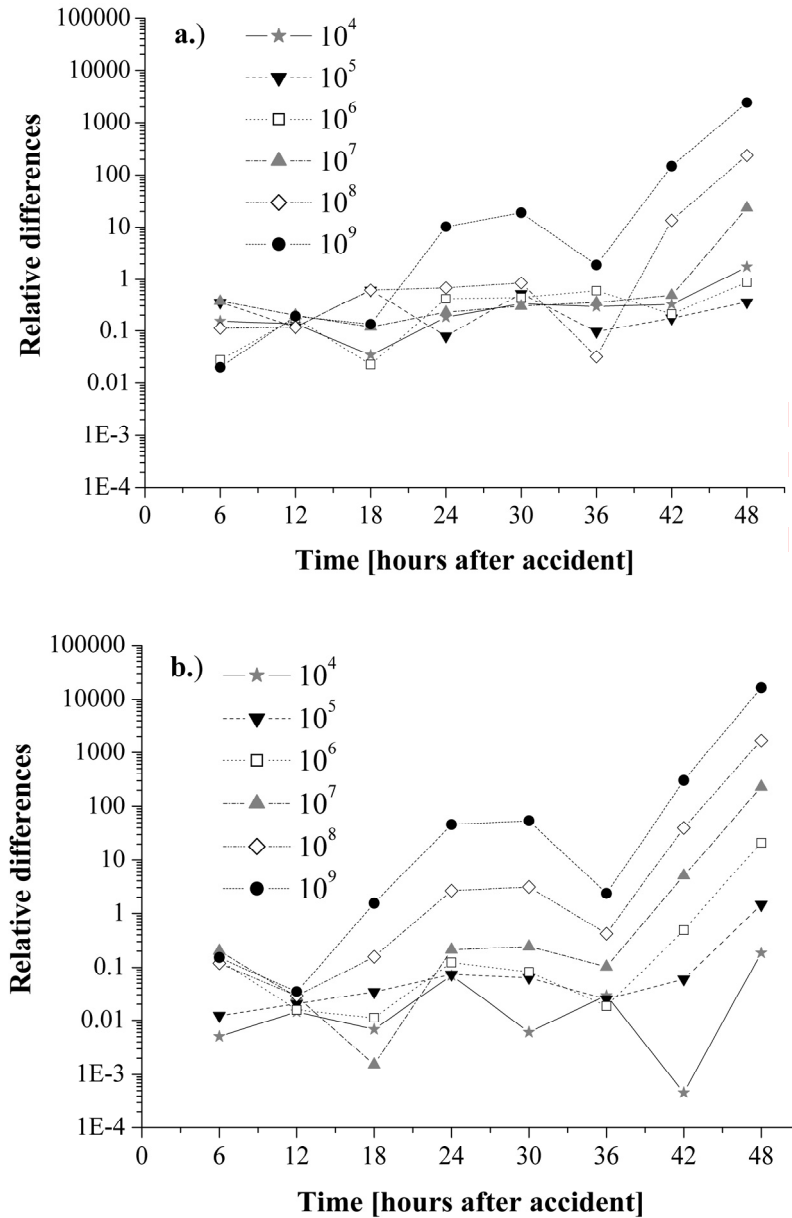


Fig. 8. (a) Relative differences of average ^{131}I concentration at the surface during a 48-hour simulation after the hypothetical accident at 00 UTC, March 24, 2006 in 6-hour time step. Values are calculated over the whole domain with and without semi-adaptive method with different critical concentrations (in cm^{-3}). (b) Same as Fig. 8a, but for maximum values.

The relative difference was calculated as $\text{diff} = |c_1 - c_2| / c_1$. Relative differences of average values (*Fig. 8a*) varied around 0.1 in general, but there are greater differences in case of 10^9 cm^{-3} critical concentration in the first

simulation day. From the 36th hour of the simulation, the differences became larger and the highest differences were found in case of higher critical concentrations. It is particularly noticeable, that differences decreased at 12 and 36 hours after the hypothetical accident (at 00 UTC). This is because of more turbulent conditions during daytime. Relative differences of maximum values (*Fig. 8b*) show greater variability. Nevertheless, if the critical concentration remains lower than 10^8 cm^{-3} till the 36th hour of the simulation, model estimation gives similar maximum values (the relative differences are small). It should be noted, that for a purpose of a shorter (for 12 hours) prediction of the maximum value, higher critical concentrations (10^8 – 10^9 cm^{-3}) should also provide appropriate results.

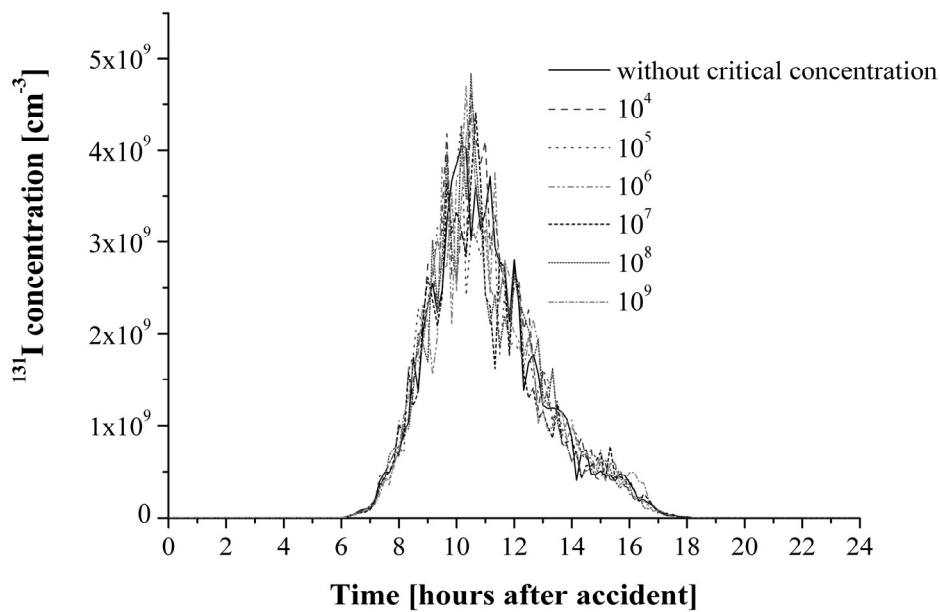


Fig. 9. Temporal variation of ^{131}I concentration at the surface over the city of Veszprém (47.1°N , 17.92°E) after the hypothetical accident at Paks NPP at 00 UTC, March 24, 2006. Values are calculated without and with different critical concentrations (in cm^{-3}).

The semi-adaptive method was also tested over given points. *Fig. 9* shows the temporal variations of ^{131}I concentration at the surface in Veszprém (47.1°N , 17.92°E , about 90 km to the NW direction of the point source) after a hypothetical accident in Paks NPP at 00 UTC, March 24, 2006, calculated with different critical concentrations. The plume passed over the city in the same interval, from 06 UTC to 18 UTC, and maximum concentrations appeared between 10 and 11 UTC in case of all different model runs with different critical concentrations. In the time series, about 20% variations on average can be found between values calculated with and without the semi-adaptive method. However, these differences are mainly caused by the stochastic calculation of the vertical transport term and not due to the different critical concentrations. This can be seen in *Fig. 10*, where two standard model runs without the semi-

adaptive method are compared. In spite of that in both cases the same meteorological and emission input fields were used, similar differences in concentration values can be seen similarly to *Fig. 9*, where model runs with different critical concentrations are presented. The differences between any two simulations should decrease with the use of more ‘packages’ in stochastic diffusion. These results also underline that the semi-adaptive method should be an effective way to accelerate the calculations.

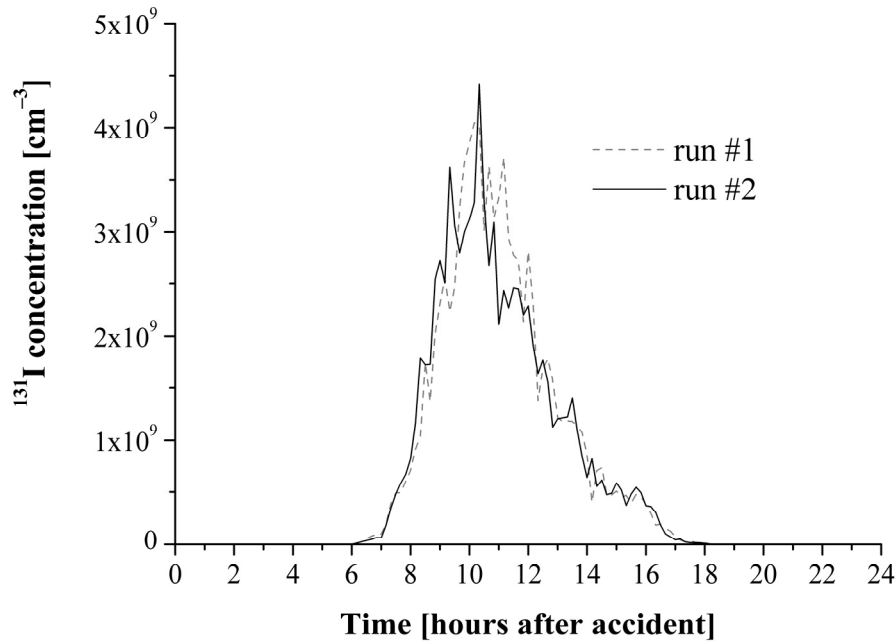


Fig. 10. Same as *Fig. 9*, but both time series were calculated without semi-adaptive method.

4. Conclusion

Modeling of the accidental release of radionuclides or highly toxic air pollutants requires fast and precise model estimations. In this study an Eulerian version of the TREX transport-exchange model is presented. We have also provided here a new method to accelerate the simulation, which is crucially important if a nuclear accident occurs, as we can gain time to prepare for the effects of the plume. With the semi-adaptive method, the efficiency of model simulations could be increased.

Two test simulations have been carried out for 48 hour periods. In case of each simulation, a hypothetical accident was assumed at the Paks Nuclear Power Plant, and the transport and deposition processes of ^{131}I have been estimated over a domain of $96 \times 90 \times 32$ grid cells. All meteorological fields for the simulations were obtained from the ALADIN numerical weather prediction model. Concentration fields, dry and wet deposition have been presented for two different meteorological conditions.

To apply the semi-adaptive method, the model simulations have been performed only on grid columns, where the concentration exceeds a predefined level in any of 32 layers in the column. The more efficient the method is, the most inactive cells are there, so the model became faster than without the semi-adaptive method, because less calculation is needed. The calculation time decreases with increasing critical concentration.

Based on our results, it seems that the semi-adaptive method could be an appropriate tool for accelerating the simulations. With high critical concentration, 10 times acceleration could be achieved compared to simulation without semi-adaptive method. However, there are some limits to this process. The higher the critical concentration is, the greater the differences are in the structure of the plume and in the estimated concentrations compared to the results obtained from normal simulation. The agreements between two cases are better in earlier part of simulation and generally decline with time, but more intense turbulence in daytime should be diminish the differences either during the latter part of simulation. Although high critical values (more than 10^7 cm^{-3} – compared to the emission rate used in this study) may cause large differences in simulated concentrations, it also should be usable for a fast, rough estimate for the direction of travel of the plume and the order of magnitude of the concentration. Determination of the critical concentration plays an important role of this method in decision support. It should be noted that further investigations should precede the implementation and any operational use of the semi-adaptive method in simulation of accidental release. Results of this study contribute to the further development of TREX dispersion model system.

Acknowledgements—The authors would like to thank *András Horányi* and *László Kullmann* for the ALADIN data. This research is supported by Hungarian Research Found (OTKA K68253, OTKA K81933 and OTKA K81975) and by SEE-GRID-SCI (SEE-GRID eInfrastructure for regional eScience) project, funded by the European Commission through the contract nr RI-211338.

References

- Alexandrov, V.N., Owczarz, W., Thomson, P.G. and Zlatev, Z., 2004: Parallel runs of a large air pollution model on a grid of Sun computers. Math Comput Simulat 65, 557-577.*
- Arya, S.P., 1988: Introduction to Micrometeorology. Academic Press, INC, San Diego. pp. 307.*
- Baklanov, A. and Sørensen, J.H., 2001: Parameterisation of Radionuclide Deposition in Atmospheric Long-Range Transport Modelling. Phys Chem Earth (B) 26, 787-799.*
- Baklanov, A., Sørensen, J.H., Hoe, S.C. and Amstrup, B., 2006: Urban meteorological modelling for nuclear emergency preparedness. J Environ Radioactiv 85, 154-170.*
- Bartnicki, J., Saltbones, J. and Foss, A., 2003: Performance of the SNAP model in an ENSEMBLE exercise of simulating real-time dispersion from a nuclear accident. Int J Environ Pollut 20, 1-6, 22-32.*
- Baumann, K. and Stohl, A., 1997: Validation of a long-range trajectory model using gas balloon tracks from the Gordon Bennett Cup 95. J Appl Meteor 36, 711-720.*
- Bellasio, R., Bianconi, R., Graziani, G. and Mosca, S., 1999: RTMOD: an Internet based system to analyse the predictions of long-range atmospheric dispersion models. Computers & Goesciences 25, 819-833.*

- Brandt, J., 1998: Modelling transport, dispersion and deposition of passive tracers from accidental releases. PhD thesis. Ministry of Environment and Energy National Environmental Research institute and Ministry of Research and Information Technology Risø National Laboratory, Denmark, Roskilde. pp 307.
- Brandt, J., Christensen, J.H., Frohn, L.M. and Zlatev, Z., 2000: Numerical modelling of transport, dispersion, and deposition – validation against ETEX-1, ETEX-2 and Chernobyl. *Environ Model Softw* 15, 521-531.
- Brandt, J., Christensen, J.H. and Frohn, L.M., 2002: Modelling transport and deposition of caesium and iodine from the Chernobyl accident using the DREAM model. *Atmosph Chem and Phys*, 397-417.
- Businger, J.A., Wyngaard, J.C., Izumi, Y. and Bradley, E.F., 1971: Flux-profile relationships in the atmospheric surface layer. *J Atmos Sci* 28, 181-189.
- Dabdub, D. and Seinfeld, J.H., 1996: Parallel computation in atmospheric chemical modelling. *Parallel Comput* 22, 111-130.
- Dimov, I., Georgiev, K., Ostromsky, T. and Zlatev, Z., 2004: Computational challenges in the numerical treatment of large air pollution models. *Ecol Model* 179, 187-203.
- Dombovári, P., Ranga, T., Nényei, Á., Bujtás, T., Kovács, T., Jobbágy, V., Vincze, Cs. and Molnár, F., 2008: Új terjedésszámító szoftver fejlesztése és bevezetése a Paksi Atomerőműnél. (in Hungarian) *Sugárvédelem I*, 30-36.
- Ehrhardt, J., Brown, J., French, S., Kelly, G.N., Mikkelsen, T. and Müller, H., 1997: RODOS: Decision-making support for off-site emergency management after nuclear accidents. *Kerntechnik* 62, 122-128.
- Ferenczi, Z. and Ihász, I., 2003: Validation of the Eulerian dispersion model MEDIA at the Hungarian Meteorological Service. *Időjárás* 107, 115-132.
- Galmarini, S., Bianconi, R., Bellasio, R. and Graziani, G., 2001: Forecasting the consequences of accidental releases of radionuclides in the atmosphere from ensemble dispersion modelling. *J Environ Radioactiv* 57, 203-219.
- Galmarini, S., Bianconi, R., Klug, W., Mikkelsen, T., Addis, R., Andronopoulos, S., Astrup, P., Baklanov, A., Bartniki, J., Bartzis, J.C., Bellasio, R., Bompay, F., Buckley, R., Bouzom, M., Champion, H., D'Amours, R., Davakis, E., Eleveld, H., Geertsema, G.T., Glaabl, H., Kollax, M., Ilvonen, M., Manning, A., Pechinger, U., Persson, C., Polreich, E., Potemski, S., Prodanova, M., Salton, J., Slaperj, H., Sofiev, M.A., Syrakov, D., Sørensen, J.H., Van der Auwera, L., Valkama, I. and Zelazny, R., 2004: Ensemble dispersion forecasting – Part I: concept, approach and indicators. *Atmos Environ* 38, 4607-4617.
- Gultureanu, D., Gultureanu, B., Mikkelsen, T., Thykier-Nielsen, S. and Matenciuc, M., 2000: Air pollution studies for the Romanian nuclear power plant – Cernavoda based on the RIMPUFF dispersion model. *Air Pollution Modeling and Its Applications XIII Book Series: NATO challenges of modern society* 13, 779-780.
- Holtstag, A.A.M. and De Bruin, H.A.R., 1988: Applied Modeling of the Nighttime Surface Energy Balance over Land. *J Appl Meteorol* 27, 689-704.
- Horányi, A., Ihász, I., and Radnóti, G., 1996: ARPEGE/ALADIN: A numerical weather prediction model for Central-Europe with the participation of the Hungarian Meteorological Service. *Időjárás* 100, 277-300.
- Horányi, A., Kertész, S., Kullmann, L. and Radnóti, G., 2006: The ARPEGE/ALADIN mesoscale numerical modeling system and its application at the Hungarian Meteorological Service. *Időjárás* 110, 203-227.
- Jones, A., Thomson, D., Hort, M. and Devenish, B., 2007: The UK Met Office's next-generation atmospheric dispersion model, NAME III. *Air Pollution Modeling and Its Applications XVII Book Series: NATO challenges of modern society* 17, 580-589.
- Lagzi, I., Tomlin, A.S., Turányi, T., Haszpra, L., Mészáros, R. and Berzins, M., 2001: The simulation of photochemical smog episodes in Hungary and Central Europe using adaptive gridding models. *Lect Notes Comput Sc* 2074, Part II, 67-70.
- Lagzi, I., Kármán, D., Tomlin, A.S., Turányi, T. and Haszpra, L., 2004: Simulation of the dispersion of nuclear contamination using an adaptive Eulerian grid model. *J Environ Radioactiv* 75, 59-82.
- Lagzi, I., Mészáros, R., Ács, F., Tomlin, A.S., Haszpra, L. and Turányi, T., 2006: Description and

- evaluation of a coupled Eulerian transport-exchange model: Part I: model development. *Időjárás* 110, 349-363.
- Lagzi, I., Tomlin, A.S., Turányi, T. and Haszpra, L., 2009: Modelling photochemical air pollutant formation in Hungary using an adaptive grid technique. *Int J Environ Pollut* 36, 44-58.
- Langner, J., Robertson, L., Persson, C. and Ullerstiga, A., 1998: Validation of the operational emergency response model at the Swedish Meteorological and Hydrological Institute using data from etex and the chernobyl accident. *Atmos Environ* 32, 4325-4333.
- Larson, D.J. and Nasstrom, J.S., 2002: Shared- and distributed-memory parallelization of a Lagrangian atmospheric dispersion model. *Atmos Environ* 36, 1559-1564.
- Lovas, R., Patvarczki, J., Kacsuk, P., Lagzi, I., Turányi, T., Kullmann, L., Haszpra, L., Mészáros, R., Horányi, A., Bencsura, A. and Lendvay, Gy., 2006: Air pollution forecast on the HUNGRID infrastructure. In *Parallel Comput: Current & Future Issues of High-End Computing*, (eds.: G.R. Joubert, W.E. Nagel, F.J. Peters, O.G. Plata, P. Tirado, E.L. Zapata). John von Neumann Institute for Computing Series, Vol. 33, Jülich, Germany, 121-128, ISBN 3-00-017352-8.
- Martin, M., Oberson, O., Chopard, B., Mueller, F. and Clappier, A., 1999: Atmospheric pollution transport: the parallelization of a transport & chemistry code. *Atmos Environ* 33, 1853-1860.
- Martin, M.J., Parada, M. and Doallo, R., 2004: High performance air pollution simulation using OpenMP. *J. Supercomput* 28, 311-321.
- Mészáros, R., Lagzi, I., Juhász, Á., Szinyei, D., Vincze, Cs., Horányi, A., Kullmann, L. and Tomlin, A.S., 2006: Description and evaluation of a coupled Eulerian transport-exchange model: Part II: Sensitivity analysis and application. *Időjárás* 110, 365-377.
- Mikkelsen, T., Thykier-Nielsen, S., Astrup, P., Santabarbara, J.M., Sørensen, J.H., Rasmussen, A., Robertson, L., Ullerstig, A., Deme, S., Martens, R., Bartzis, J.G. and Pasler-Sauer, J., 1997: MET-RODOS: A comprehensive atmospheric dispersion module. *Radiat Prot Dosim* 73, 45-56.
- Molnár, F. Jr., Szakály, T., Mészáros, R. and Lagzi, I., 2010: Air pollution modelling using a Graphics Processing Unit with CUDA. *Comput Phys Commun* 181, 105-112.
- Ostrowsky, T., Dimov, I.T. and Zlatev, Z., 2005: Parallel implementation and one year experiments with the Danish Eulerian Model. *Lect Notes Comput Sc* 3401, 440-447.
- Paulson, C.A., 1970: The mathematical representation of wind speed and temperature profiles in the unstable atmospheric surface layer. *J Appl Meteorol* 9, 857-861.
- Pechinger, U., Langer, M., Baumann, K. and Petz, E., 2001: The austrian emergency response modelling system TAMOS. *Phys. Chem. Earth (B)* 26, 99-103.
- Pudykiewicz, J., 1989: Simulation of the Chernobyl dispersion with a 3-D hemispheric tracer model. *Tellus* 41B, 391-412.
- Pudykiewicz, J., 1991: Environmental prediction systems: Design, implementation aspects and operational experience with application to accidental releases. In *Air Pollution Modeling and Its Applications VIII. NATO challenges of modern society* (eds.: H. van Dop and D.G. Steyn). Vol. 15. Plenum Press, New York and London, pp. 561-590.
- Ryall, D.B. and Maryon, R.H., 1998: Validation of the UK Met. Office's name model against the ETEX dataset. *Atmos. Environ.* 32, 4265-4276.
- Saltbones, J., Foss, A. and Bartnicki, J., 1998: Norwegian Meteorological Institute's real-time dispersion model SNAP (severe nuclear accident program): Runs for ETEX and ATMES II experiments with different meteorological input. *Atmos. Environ.* 32, 4277-4283.
- Singh, D.E., Garcia, F. and Carretero, J., 2006: Parallel I/O optimization for an air pollution model. *Parallel Comput: Current & Future Issues of High-End Computing. Proceedings of the International Conference ParCo 2005* (eds.: G.R. Joubert, W.E. Nagel, F.J. Peters, O. Plata, P. Tirado, E. Zapata), 33, 523-530.
- Sørensen, J.H., Rasmussen, A., Ellermann, T. and Lyck, E., 1998: Mesoscale influence on long-range transport – evidence from ETEX modelling and observations. *Atmos Environ* 32, 4207-4217.
- Sørensen, J.H., Baklanov, A. and Hoe, S., 2007: The Danish emergency response model of the atmosphere (DERMA). *J Environ Radioactiv* 96, 122-129.
- Srinivas, C.V., Venkatesan, R., Muralidharan, N.V., Das, S., Dass, H. and Kumar, P.E., 2006: Operational mesoscale atmospheric dispersion prediction using a parallel computing cluster. *J Earth System Science* 115, 315-332.

- Stohl, A. and Wotawa, G., 1997: Validation of the Lagrangian particle model FLEXPART using ETEX data. ETEX symposium on long-range atmospheric transport, model verification and emergency response. *European Commission* EUR 17346, 167-170.
- Stohl, A., Hittenberger, M. and Wotawa, G., 1998: Validation of the lagrangian particle dispersion model FLEXPART against large-scale tracer experiment data. *Atmos Environ* 32, 4245-4264.
- Stohl, A., Forster, C., Frank, A., Seibert, P. and Wotawa, G., 2005: Technical note: The Lagrangian particle dispersion model FLEXPART version 6.2. *Atmos Chem and Phys* 5, 2461-2474.
- Zegeling, P.A. and Kok, H.P., 2004: Adaptive moving mesh computations for reaction-diffusion systems. *J. Comput Appl Math* 168, 519-528.