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INVESTIGATION OF THE DISPERSION OF AIR POLLUTANTS BY THE REPLAT MODEL

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Abstract: Lagrangian dispersion models are useful for simulating the trajectories of pollutants from single sources. A class of these models uses "real particles": particles with fixed, realistic size and density, and the particles are tracked individually. In the presentation we introduce the Real Particle Lagrangian Trajectory (RePLaT) dispersion model. As an extension to other real particle models, RePLaT takes into account the effect of turbulent diffusion and the scavenging of particles by precipitation. A novel feature of the model is the application of the impact of precipitation on individual particles by a random process which depends on precipitation intensity. Since RePLaT tracks realistic particles, it is also suitable for the investigation of the chaotic behavior in dispersion and deposition processes from a dynamical systems point of view. In order to validate RePLaT, we simulated the dispersion of volcanic ash from the Eyjafjallajökull eruptions and the dispersion and deposition of the radioactive particles released during the accident of the Fukushima Nuclear Power Plant. The results of the simulations indicate good agreement with satellite and surface measurements.

Key words: *RePLaT, dispersion model, realistic particles*

INTRODUCTION

In the last decades the demand for precise tracking and forecasting of atmospheric pollutants has increased due to the growing interest in environmental problems and, consequently, requirements for detailed prediction of health and economic hazards. Lagrangian models are useful for simulating the trajectories of pollutants from single sources.

A class of the Lagrangian particle-tracking models tracks "ghost particles" (computational particles): any of these particles carry an artificial mass which is determined by the emitted mass and the number of particles used in the simulation. The properties of these particles usually do not coincide with the ones of any real pollutant particle. The mass attributed to the ghost particle decreases exponentially due to dry and wet deposition (e.g. FLEXPART (Stohl, A. et al., 2005)). In this approach a ghost particle is considered to be the centre of mass of a large amount of adjacent pollutants. As the trajectory of these pollutants is represented by a single trajectory, the method of ghost particles tacitly supposes that these neighbouring particles remain together forever. However, the chaotic nature of the advection dynamics implies that an initially small, compact ball of particles in the atmosphere becomes rapidly deformed into a complicated, filamentary shape of large extent (Haszpra, T. and T. Tél, 2013b).

Another class of the Lagrangian models follows "real particles": the particles in these models have fixed, realistic size and density (e.g. VAFTAD (Heffter, J.L. and B.J. Stunder, 1993), PUFF (Searcy, C. et al., 1998)). However, the recently available models of this type do not take into account the deposition and the scavenging of particles by precipitation. The aim of our work was to develop a relatively simple Lagrangian dispersion model which is easy to understand and which, at the same time, considers the atmospheric physical processes in a realistic manner. The Real Particle Lagrangian Trajectory (RePLaT) model tracks individual aerosol particles with realistic size and density, and takes into account more processes than other models which also follow real particles. The model was evaluated by simulating historical events and comparing the results to observations. Since RePLaT describes the motion of realistic aerosol particles, it is suitable for the investigation of the dispersion and deposition processes from a dynamical systems point of view (Haszpra, T. and T. Tél, 2013a,b).

THE REPLAT LAGRANGIAN DISPERSION MODEL

Advection

The simulated pollutant clouds contain several particles with realistic radius (on the order of a few μm) and density (on the order of 2000 kg m^{-3}). The equation of motion of the particles is derived from Newton's equation. Scale analysis reveals that the horizontal velocity of a particle takes over the actual local wind speed within a fraction of a minute, while in the vertical direction the terminal velocity also has to be taken into account besides the vertical velocity component w of air. Therefore a particle is advected by the wind components u, v in the horizontal direction and its vertical motion is, in addition, influenced by its terminal velocity w_{term} which depends on the size r and density ρ_{p} of the particle and the density ρ and viscosity ν of the air at the location $\mathbf{r}_{\mathrm{p}}$ of the particle:

$$\frac{\mathrm{d}\mathbf{r}_{\mathrm{p}}}{\mathrm{d}t} = \mathbf{v} + w_{\mathrm{term}}\mathbf{n}, \tag{1}$$

where

$$w_{\mathrm{term}} = -\frac{2}{9}\frac{\rho_{\mathrm{p}} r^2 g}{\rho \nu}. \tag{2}$$

This follows from Stokes's law which is valid for small particles. In equation (1) $\mathbf{r}_{\mathrm{p}}(t)$ denotes the particle trajectory, $\mathbf{v} = (u, v, w)$ is the velocity of air, g is gravitational acceleration and $\mathbf{n}$ is the vertical unit vector pointing upwards.

Turbulent diffusion

Since the meteorological data utilized by the dispersion model have coarse resolution without resolving turbulent diffusion, the effect of small-scale turbulence on the particles is built into the model as a stochastic term. In the planetary boundary layer the computation of the vertical turbulent diffusivity is based on the Monin–Obukhov similarity theory (see e.g. Dyer, A.J. (1974), Troen, I.B. and L. Mahrt (1986)), while the horizontal turbulent diffusivity is assumed to be constant in both this layer and the free atmosphere. The equation of motion completed by the impact of turbulent diffusion is

$$\frac{\mathrm{d}\mathbf{r}_{\mathrm{p}}}{\mathrm{d}t} = \mathbf{v} + w_{\mathrm{term}}\mathbf{n} + \boldsymbol{\xi}\cdot\mathbf{K}, \tag{3}$$

where ξ is a random walk process and $\mathbf{K}$ represents the turbulent diffusivity in the different directions, which might be location- and time-dependent. For more details, see Haszpra, T. and T. Tél (2013a).

Scavenging by precipitation

The main novel feature of the model is the application of the impact of precipitation on individual particles by a random process which depends on precipitation intensity. The parameterisation of wet deposition is motivated by the general Eulerian approach (Seinfeld, J.H. and S.N. Pandis, 1998). There the impact of wet deposition is taken into account via the following equation:

$$\frac{\mathrm{d}m}{\mathrm{d}t} = -k_{\mathrm{w}} m, \tag{4}$$

where m is mass and k_{w} is the wet deposition coefficient (or scavenging coefficient). This implies that after a short time Δt, locally a fraction of $1-\exp(-k_{\mathrm{w}}\Delta t)$ of mass is deposited. We use this relationship to incorporate wet deposition into our model. Wet deposition is considered in RePLaT as a random process that results in a particle being captured by a raindrop within time Δt with certain probability (depending on precipitation intensity via k_{w}; for a detailed description, see Haszpra, T. and T. Tél (2013a)):

$$p_{\mathrm{r,rain}} = 1 - \exp(-k_{\mathrm{w}}\Delta t). \tag{5}$$

Thereby the radius and density of the particle change suddenly to that of the raindrop ($\rho_{\mathrm{rain}} = 1000$ kg/m^3, r_{rain} o r). The trajectory of the "new" particle (a particle that turned into a raindrop) is computed using the terminal velocity based on the new properties of the particle, typically using a terminal velocity w_{term} derived from the quadratic drag law for large particles:

$$w_{\text{term}} = -\frac{8}{3}\frac{\rho_{\text{rain}} r_{\text{rain}} g}{\rho C_{\text{d}}}, \tag{6}$$

where $C_{\text{d}} = 0.4$ is the drag coefficient for spheres. The transformed particle does not leave the atmosphere instantaneously, but as a raindrop falling through the air according to equation (3).

There are different parameterisations available for the typical radius of the raindrops (Sportisse, B., 2007). In RePLaT we use the Pruppacher–Klett parameterisation (Pruppacher, H.R. and J.D. Klett, 1997):

$$r_{\text{rain}} = 0.488 P^{0.21}, \tag{7}$$

where the unit of r_{rain} is mm and the unit of rain intensity P is mm·h^{-1}. For simplicity, at present the effect of wet deposition is taken into account only below the 850 hPa level.

CASE STUDIES

In order to validate the RePLaT model we simulated the volcanic ash dispersion from the Eyjafjallajökull's volcanic eruptions and the dispersion and deposition of the radioactive particles released during the accident of the Fukushima Nuclear Power Plant.

The Eyjafjallajökull's eruptions

We simulated the dispersion of volcanic ash from the Eyjafjallajökull's eruptions in 2010 from May 8 to 19.

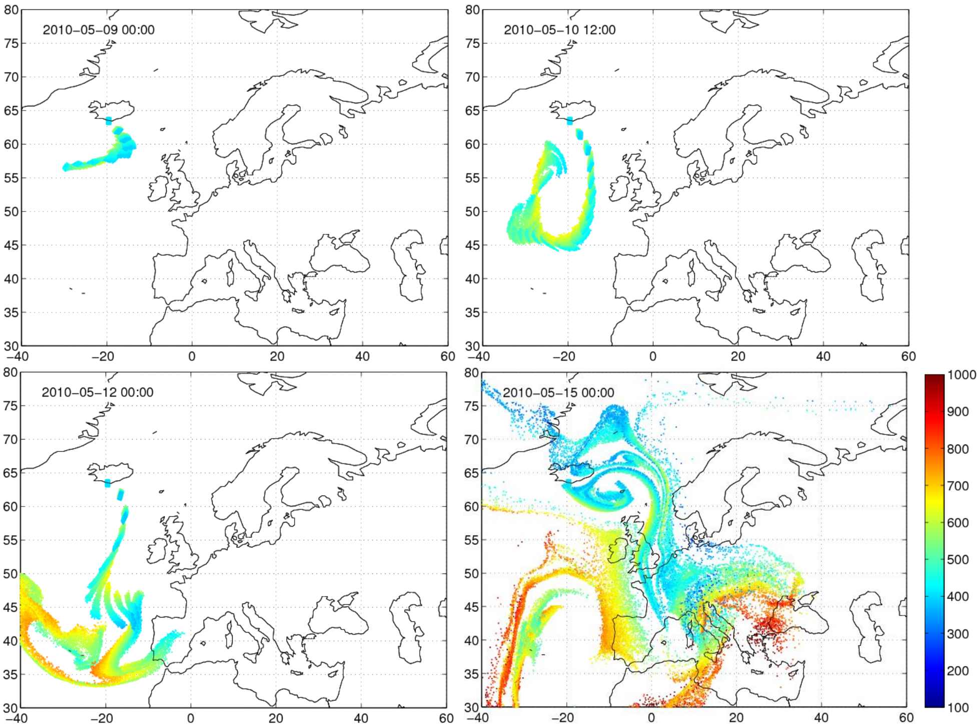

Figure 1: The dispersion of a sequence of volcanic ash puffs from the Eyjafjallajökull's eruption in RePLaT simulation at the times indicated in the panels. Each volcanic ash puff consists of 10^3 particles with $r = 1$ μm. The initial altitude of the centre of puffs is $p_0 = 500$ hPa, the initial extension is 1°×1°×200 hPa. The puffs are emitted in every 6 hours from May 8, 00 UTC on. The colorbar indicates the altitude of the particles in hPa (Haszpra and Horányi, 2014).

In the beginning of this period, northern flows were dominating south to Iceland, and a high pressure area was located in the Atlantic region. Figure 1 shows that the volcanic ash is dispersing in a filamentary structure and becomes transported to south, firstly, following the anticyclonic flow. It is also due to the northerly winds that the volcanic ash can reach even the Iberian Peninsula located about 2000 km away from Iceland. Some days later the volcanic ash is dispersed all over Europe. In the 4th panel of Figure 1 particles are tracing out a cyclone developing west to Iceland and a high pressure system located east to Portugal. The colors of the figure from red to light blue draw attention to the fact that particles with exactly the same radius can reach quite different altitudes in the atmosphere within the same time even if it is a not too long period.

We compared the results of the simulation with satellite observation on May 10 (2nd panel of Figure 1). The shape of the ash cloud was found to be similar in the simulation and in the satellite image. Even the fat patch at the southwest "edge" of the ash cloud found here appears in the satellite image. According to the comparison, there seemed to be a satisfying agreement between the simulation and the measurement.

The Fukushima Nuclear Power Plant accident

In order to validate RePLaT we also simulated the dispersion of two radioactive material, the aerosol-bound caesium-137 isotope (^{137}Cs) and the noble gas xenon-133 isotope (^{133}Xe) released during the accident of the Fukushima Nuclear Power Plant in the spring of 2011 (Haszpra, T. and T. Tél, 2014). Wind data are taken from the ERA-Interim database, and the data of local emission are based on the literature (Stohl, A. et al., 2012). The dispersion of the radioactive material is tracked over several weeks. The radius and density of ^{137}Cs carrier particles is estimated to be $r = 0.2$ μm and $\rho_{\mathrm{p}} = 1900$ kg m^{-3} based on Stohl, A. et al. (2012), while the noble gas component was treated formally as $r = 0$ μm particles (i.e. particles with zero terminal velocity) in equation (3).

Figure 2 illustrates the geographical distribution of ^{137}Cs one week after the accident. The simulation shows that the particles are transported principally to the east, southeast and northeast directions over the Pacific Ocean. In mid March a fraction of the radioactive material is captured by the steering flow of two cyclones near Japan and at the coast of North America. These particles were lifted to the free atmosphere (see the particles in blue on the right hand side of Figure 2) and reached even Europe about a week later.

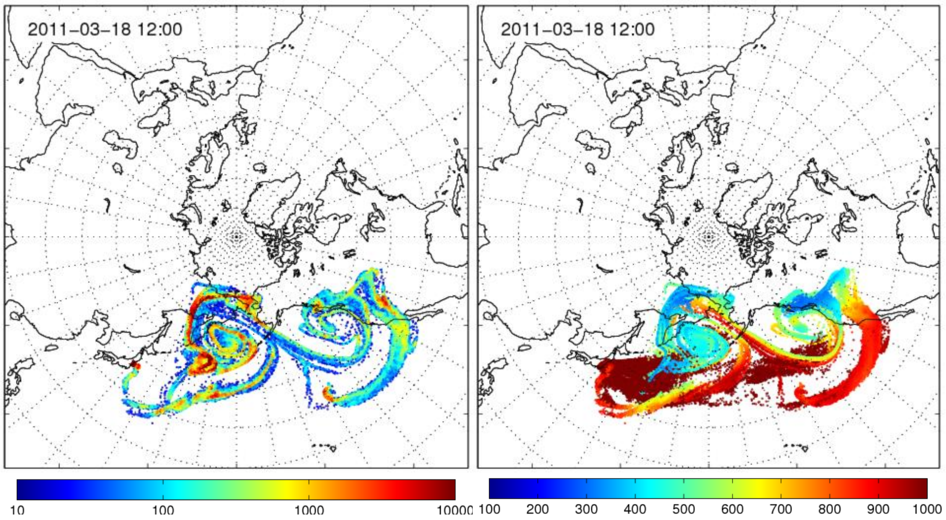

Figure 2. The dispersion of ^{137}Cs from the Fukushima accident on March 18, 2011. Initial conditions on March 11: $r = 0.2$ μm particles initiated in a volume of 1°×1° area and height of about 300 m according to the *a posterior* estimation of (Stohl, A. et al., 2012). Left: Radioactivity in air columns over a grid of about 0.5°×0.5° resolution in the unit of Bq m^{-2}. Right: Altitude of the particles in hPa.

Figure 3 shows the radioactivity in the first few days after the arrival of the ^{137}Cs cloud to different locations. It is remarkable that the arrival times of the pollution coincide reasonable well with the measured data (dashed lines). The deviations in the intensities might be related to at least two important factors: firstly, the emission data were estimated and can be subject to considerable uncertainties, and secondly, the relatively coarse resolution of the meteorological data (6 hours) used in the simulation can also be responsible for the difference, because it smoothes out heavy precipitation events, therefore fewer particles fall out from the atmosphere.

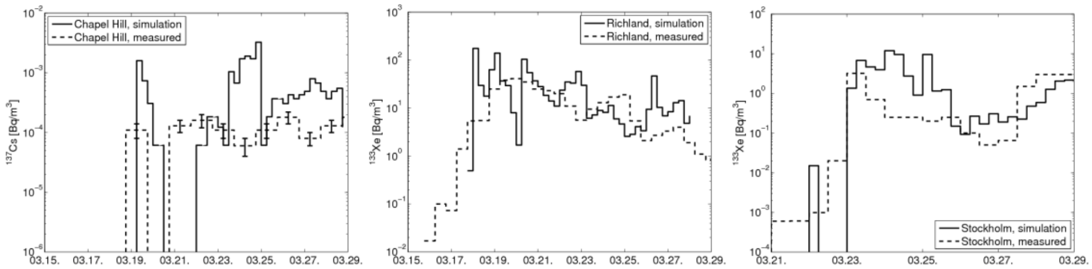

Figure 3. The radioactivity of ^{137}Cs (left) and ^{133}Xe (middle and right) simulated by RePLaT (solid line) and the measured data (dashed line) as a function of the days of the year (month.day.) at Chapel Hill, Richland and Stockholm, respectively.

SUMMARY

We developed the RePLaT Lagrangian dispersion model. In order to refine the simulations, in the future the model should be improved by additional factors related mostly to a more detailed description of the wet deposition. The separation of the in-cloud and below-cloud scavenging and the distinction between scavenging by rain and scavenging by precipitation can be some of the main aspects of the improvement.

In conclusion, we can say that the simulations carried out by the RePLaT model agree reasonably well with observations, and additionally, the model provides opportunity for a novel study of the chaotic behaviour of dispersing aerosol particles in the atmosphere.

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