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MODELLING 3D DRY DEPOSITION OF PARTICULATE MATTER FOR MICRO-SCALE AIR QUALITY: COUPLING A NEW SCHEME WITH AN EXISTING LAGRANGIAN STOCHASTIC MODEL

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Abstract: The numerical coupling of the code SPRAY-WEB (Università del Piemonte Orientale et al.) with the software library DePaSITIA (RSE SpA) represents an Open-Source numerical solution for 3D height-dependent dry deposition of atmospheric Particulate Matter (PM). An incremental validation on the scaled spruce forest of Ould-Dada (2002) is reported.

Key words: dry deposition; particulate matter; SPRAY-WEB; DePaSITIA; FOSS; Lagrangian Stochastic Models; canopy boundary layers; deposition velocity; pollutant dispersion.

INTRODUCTION

The numerical modelling of PM deposition is a key tool in assessing the effects of such process on both the concentration fields in the atmospheric domain and the cumulated mass on the deposition surfaces.
The current document briefly recalls the main features of the library DePaSITIA for PM deposition and its coupling with the Lagrangian Stochastic Model SPRAY-WEB (a dispersion model). An incremental validation on the scaled spruce forest of Ould-Dada et al. (2002) is reported, by comparison with Amicarelli et al. (2021). An improvement in the vertical profile of the deposited mass is achieved be means of a better setting of the bottom boundary conditions. The current modelling solution focuses on the following features: advanced formulations for the dry deposition mechanisms from Computational Fluid Dynamics mathematical models; a 3D multi-level dry deposition software for vegetation canopies; no need for input tuning parameters on dry deposition.

THE SOFTWARE LIBRARY DEPASITIA AND ITS NUMERICAL COUPLING WITH THE CODE SPRAY-WEB

SPRAY-WEB v.1.0 (2021, Università del Piemonte Orientale et al.) is a Lagrangian Stochastic Model for the dispersion of atmospheric pollutants (e.g., Tinarelli et al., 1994; Alessandrini & Ferrero, 2013; Bisignano et al., 2017) and represents the Open-Source version of the code SPRAY, which had been validated on a very large number of test cases (e.g., Tinarelli et al., 2000; Alessandrini et al., 2005; Alessandrini et al., 2013; Tomasi et al., 2019; among the others).
DePaSITIA v.1.0 (2019, RSE SpA) is a PM dry deposition scheme modelling the following deposition mechanisms: Sedimentation, Inertial impaction, Turbulent impaction and Interception. The process of Adhesion (i.e., missing bouncing) is also taken into account.
The software library DePaSITIA had been coupled with SPRAY-WEB to provide it with a 3D multi-level deposition scheme with multiple deposition mechanisms and an explicit dependence on the following

quantities: Leaf Area Density; leaf equivalent diameter; leaf ratios; mean velocity; friction velocity (Amicarelli et al., 2021). Few key features of this solution are recalled in the following.
In the presence of dry deposition, the balance equation for the mean concentration discretized in a Lagrangian Stochastic Model can be rearranged as follows:

$$\overline{\frac{dC}{dt}} = -\frac{\overline{F_d}}{\Delta z} \tag{1}$$

where C (kg×m^{-3}) is the instantaneous concentration, t (s) is time, Δz (m) is the depth of the current cell in the concentration statistics grid, the over-bar symbol represents the Reynolds' average and F_d (kg × s^{-1} × m^{-2}) is the dry deposition specific flux. This is the deposited mass per unit of time and unit of "horizontal area", which is defined as the projection of the monitored volume along the horizontal.
The formula for the dry deposition flux reads:

$$\overline{F_d} = u_d \overline{C} \cdot LAD \cdot \Delta z \tag{2}$$

where LAD (m^{-1}, Leaf Area Density) is the one-sided area of all the vegetation surfaces per unit of volume and u_d (m/s) is a quantity called deposition velocity (Sip & Benes, 2017):

$$u_d = R_a\left(u_{IN} + u_{IM} + u_{TI} + u_{SE}\right) \tag{3}$$

where u_{IN} (m/s) is the interception velocity, u_{IM} (m/s) is the inertial impaction velocity, u_{TI} (m/s) is the turbulent impaction velocity and u_{SE} (m/s) is the sedimentation velocity. The adhesion coefficient R_a is defined by Zhang et al. (2001). Both interception and turbulent impaction are associated with passive PM particles following the streamlines or the trajectories of the fluid particles, respectively. Inertial impaction and sedimentation refer to non-passive behaviours of the PM particles. As a first approximation, the deposition velocity depends on the mean velocity instead of the instantaneous velocity to avoid modelling the pollutant turbulent flux by means of a concentration fluctuation model (e.g., Cassiani et al., 2007; Amicarelli et al., 2011; Amicarelli et al., 2017).
DePaSITIA is coupled with SPRAY-WEB as a library integrated within a reference code. The input quantities of DePaSITIA are associated with meteorology, vegetation canopy and PM. They are available in the input files of SPRAY-WEB. Only the mean concentration is calculated by SPRAY-WEB and provided to DePaSITIA.
Time integration of the system (1)-(3) for a generic deposition time step Δt_d (s) is based on the following expression, computed by SPRAY-WEB only when DePaSITIA is activated:

$$C(t + \Delta t_d) = C(t) e^{-\left(LAD \cdot u_d \cdot \Delta t_d\right)} \tag{5}$$

More details are available in Amicarelli et al. (2021), whereas some additional information is provided hereafter.
The coupled solution SPRAY-WEB - DePaSITIA permits the simultaneous deposition of multiple species. For each pollutant, SPRAY-WEB produces both the 2D horizontal field for the Reynolds-averaged time-cumulated deposition mass per unit of horizontal surface $M_{d,2D}$ (kg×m^{-2}):

$$M_{d,2D}(x,y,t) = \int_{t_0}^{t} \int_{z_{c,\min}(x,y)}^{z_{c,\max}(x,y)} \frac{\overline{F_d}(x,y,z,t)}{\Delta z(x,y,z)} dz dt \tag{6}$$

and the 3D field of the quantity $M_{d,*}$ (kg×m^{-2}):

$$M_{d,*}(x,y,z,t) = M_{d,3D}(x,y,z,t) \Delta z(x,y,z), \qquad M_{d,3D}(x,y,z,t) = \int_{t_0}^{t} \frac{\overline{F_d}(x,y,z,t)}{\Delta z(x,y,z)} dt \tag{6}$$

where $M_{d,3D}$ (kg×m^{-3}) is the Reynolds-averaged time-cumulated deposition mass per unit of volume. For both $M_{d,2D}$, $M_{d,3D}$ and $M_{d,*}$, the over-bar symbol is omitted for simplicity of notation. The initial time is denoted by t_0 (s). The local minimum and maximum heights of the canopy layer are $z_{c,min}$ (m) and $z_{c,max}$ (m), respectively. After a full discretization, it follows that the sum of the $M_{d,*}$ values over the cells of the same grid column equals $M_{d,2D}$:

$$M_{d,2D}\left(x_0, y_0, t_j\right) = \sum_{i=1}^{n_{z,c}} M_{d,*,i}\left(x_0, y_0, z_i, t_j\right) \tag{6}$$

where the subscripts "$_0$", "$_i$" and "$_j$" refer to the on-going grid column, level and time, respectively.

INCREMENTAL VALIDATION ON A SCALED SPRUCE FOREST

The numerical coupling SPRAY-WEB - DePaSITIA was recently validated on the scaled spruce forest of Ould-Dada (2002) in the reference simulation of Amicarelli et al. (2021), which is here updated with original results after a minor improvement in the bottom boundary conditions. This is associated with a correction on the particle bouncing scheme at ground. The test case represents the dispersion of PM from two line sources in a canopy neutral atmospheric boundary layer. Regarding the experimental test case and the numerical setup, the reader might refer to Ould-Dada (2002) and Amicarelli et al. (2021), respectively.

Figure 1 shows the stationary field of the concentration mean. At the spatial resolution of the concentration grid, the two source plumes seem a unique plume emitted from an Elevated Source. The plume centreline lifts towards the emission height of the upper pollutant source, increasing x values. The plume is more dispersed within the canopy where the Reynolds number reaches local maxima.

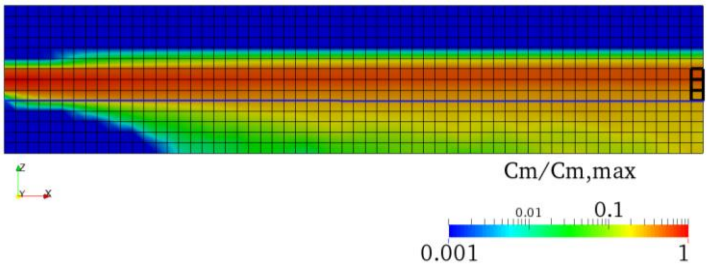

Figure 1. Width-averaged stationary field of the normalized mean concentration (SPRAY-WEB & DePaSITIA): current updated simulation. The mean concentration is normalized by its maximum value. The cells belonging to the monitoring regions of the mean concentration scale are highlighted (3 cells above the canopy, in the outlet region). The blue horizontal line represents the canopy top.

The plume begins to interact with the ground upstream the monitoring region for the deposited mass, which is highlighted in Figure 2. The stationary field of the deposition quantity $M_{d,*}$ (kg×m^{-2}) is reported as the product of the cell depth times the Reynolds-averaged time-cumulated deposition mass per unit of volume. The vertical evolution of $M_{d,*}$ depends on the mean velocity, the mean concentration and the Leaf Area Density. $M_{d,*}$ generally increases with height, except for the upper canopy level where *LAD* reaches its minimum value within the canopy. The longitudinal variability of $M_{d,*}$ is only associated with the evolution of the mean concentration field.

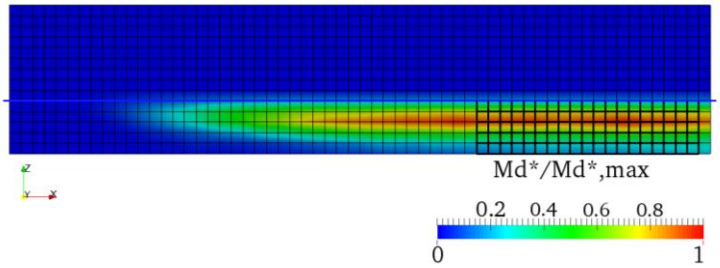

Figure 2. Width-averaged stationary field of the normalized values of $M_{d,*}$ (the cell depth times the Reynolds-averaged time-cumulated deposition mass per unit of volume) at $t=t_f$ (SPRAY-WEB & DePaSITIA): current updated simulation. $M_{d,*}$ is normalized by its maximum value. The cells belonging to the monitoring regions of the deposition mass are highlighted (most downstream part of the canopy, but the outlet section). The blue horizontal line covering the whole domain length represents the canopy top.

The experimental quantity used for comparison is the deposition velocity scale $u_{d,*} = \frac{u_d \overline{C}}{\overline{C_*}}$ (m/s), where $\overline{C_*}$ (kg×m^{-3}) is a concentration scale equal to the mean concentration averaged over 0.450m≤z≤0.700m at the outlet section (Ould-Dada, 2002). The monitoring region for the deposition velocity scale is limited by 4.000m≤x≤5.818m. Figure 3 shows the comparisons between the simulated profiles of the deposition velocity scale and the available measurements of Ould-Dada (2002). The current numerical solution (subscript "$_{sim}$") shows a profile shape similar to the experiment; $u_{d,*}$ increases with height, except for the top canopy level, where a relevant underestimation is noticed. This is related to the large sensitivity of this vertical level to the Leaf Area Density, as in Amicarelli et al. (2021). The simulated deposition velocity scale averaged over the canopy depth $u_{d,*,sim,avg}$=7.705×10^{-4}m/s provides an underestimation of 23%, with respect to the experimental value $u_{d,*,meas,avg}$=9.952×10^{-4}m/s. With respect to the reference simulation in Amicarelli et al. (2021), the current updated simulation takes advantage from a minor improvement to the bottom boundary conditions and a computational speedup factor of ca.4, reached by means of the *-O2* optimization compilation flag. Stationary conditions are dynamically achieved. They are associated with the elapsed time t_e=46s (single core of an Intel processor i5-8250U at 1.60 GHz). The current updated simulation provides a better match with the experimental profile; the improvements reduce with the distance from the bottom.

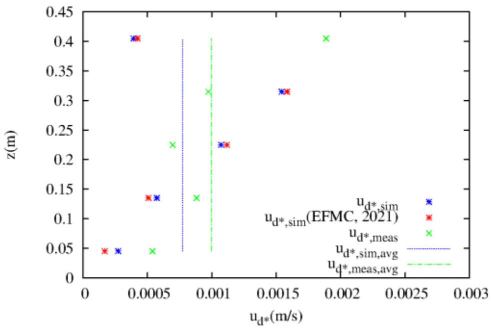

Figure 3. Vertical profiles of the deposition velocity scale. Comparisons between the available measures ("$_{meas}$", Ould-Dada , 2002), the current updated simulation ("$_{sim}$") and the reference simulation in Amicarelli et al. (2021). Width-averaged values.

CONCLUSIONS

The numerical coupling of the code SPRAY-WEB (Università del Piemonte Orientale et al.) with the software library DePaSITIA (RSE SpA) represents an Open-Source numerical solution for 3D height-dependent dry deposition of PM, validated on the scaled spruce forest of Ould-Dada (2002). This solution is based on advanced formulations for the deposition mechanisms of sedimentation, inertial impaction, turbulent impaction and interception. Bouncing effects are also considered and no input tuning parameter is requested. The input quantities include canopy quantities (Leaf Area Density, leaf equivalent diameter, leaf shape, orientation and roughness parameters), information on the transporting fluid (local mean velocity, friction velocity), and PM variables (local mean concentration, median diameter, density). The validation test case is also disseminated as an Open-Source tutorial to prove the repeatability of the results. Potential application fields are: soil/water/forest/food contamination; vegetation barriers as pollution-control protection actions; forest acidification; micro-scale dry deposition of atmospheric PM on 3D elevated and ground-level obstacles (e.g., PM deposition on people skin and respiratory system, electric insulators, buildings and architectonic works).

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The contributions of S. Alessandrini to the current study were made before January 2014 as an employee of RSE SpA, except for the manuscript's co-revision carried out under his current affiliation at NCAR.

REFERENCES

Alessandrini S., et al.; 2005; Comparison of different dispersion models with tracer experiment; Nuovo Cimento C, Geophysics Space Physics C, 28:141. doi:10.1393/ncc/i2005-10187-0

Alessandrini, S., Ferrero, E., Anfossi, D.; 2013; A new Lagrangian method for modelling the buoyant plume rise Atmospheric Environment, 77:239-249.

Amicarelli A., et al.; 2021; Environmental Fluid Mechanics; A dry deposition scheme for particulate matter coupled with a well-known Lagrangian Stochastic Model for pollutant dispersion; published online 8 March 2021; https://doi.org/10.1007/s10652-021-09780-y

Amicarelli A., et al.; 2017; A stochastic Lagrangian micromixing model for the dispersion of reactive scalars in turbulent flows: role of concentration fluctuations and improvements to the conserved scalar theory under non-homogeneous conditions; Environmental Fluid Mechanics 17(4):715-753; DOI 10.1007/s10652-017-9516-1

Amicarelli A., et al.; 2011; LAGFLUM, a stationary 3D Lagrangian stochastic numerical micromixing model for concentration fluctuations: validation in canopy turbulence, on the MUST wind tunnel experiment; International Journal of Environment and Pollution, 47, n.1/2/3/4, 317-325.

Bisignano, A., Mortarini, L., Ferrero, E., Alessandrini, S.; 2017; Model chain for buoyant plume dispersion. Int. J. Environ. Pollut. 62(2/3/4):200-213.

Cassiani, M., Radicchi, A. and Albertson, J.; 2007; Modelling of concentration fluctuations in canopy turbulence; Boundary-Layer Meteorology, 122, 655-681.

DePaSITIA v.1.0 (RSE SpA); 2019; https://github.com/AndreaAmicarelliRSE/DePaSITIA

Ould-Dada Z.; 2002; Dry deposition profile of small particles within a model spruce canopy; The Science of the Total Environment, 286:83-96.

Sip V., L. Benes; 2017; Dry deposition model for a microscale aerosol dispersion solver based on the moment method; Journal of Aerosol Science, 107:107-122.

SPRAY-WEB (Università del Piemonte Orientale et al.); 2021; http://sprayweb.isac.cnr.it/

Tinarelli, G., et al.; 1994. Lagrangian particle simulation of tracer dispersion in the lee of a schematic twodimensional hill. J. Appl. Meteorol. 33, 744–756.

Tinarelli G, et al.; 2000; A New High Performance Version of the Lagrangian Particle Dispersion Model Spray, Some Case Studies; In: "Boston, MA": "Springer US":499-507. doi:"10.1007/978-1-4615-4153-0_51"

Tomasi E., et al.; 2019; Turbulence parameterizations for dispersion in sub-kilometer horizontally non-homogeneous flows; Atmospheric Research, 228:122-136

Zhang L., S. Gong, J. Padro, L. Barrie; 2001; A size-segregated particle dry deposition scheme for an atmospheric aerosol module; Atmospheric Environment, 35 (3): 549-560.