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EXTENDED ABSTRACT

Validation of Lagrangian Particle Dispersion Models in the EXPO-URB Project

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Abstract. The first results of the model intercomparison and validation program carried out in the frame of the EXPO-URB project, presented at the HARMO23 Conference, are discussed. The main project's goal is to evaluate the capability of Lagrangian dispersion models in calculating long-term radiation exposure in urban environments, considering potential leakages from radionuclide sources. Four modelling systems are applied and findings from one of the test experiments carried out in the Environmental Wind Tunnel are illustrated. The results from the Lagrangian particle models are analysed and their performances are addressed based on graphical and statistical analysis. The differences among the model outputs enable assessing the critical aspects in modelling flow and dispersion in a complex built environment and the potential of the models in reproducing the observed fields.

Keywords: *Lagrangian particle models, Wind Tunnel expxeriments, Release in Built Environment, Model Intercomparison*

INTRODUCTION

The EXPO-URB project is presented at Harmo23 Conference, and the current work is connected to it. The main project's goal is to evaluate the capability of Lagrangian dispersion models in calculating long-term radiation exposure in urban environments. Radionuclide sources, characterized by low momentum and no-buoyancy, are considered.

Multiple experimental datasets have been collected and processed through extensive boundary layer wind-tunnel simulations, reproducing the flow and tracer release in the mock-up of a typical European city. Different test cases have been elaborated, varying wind direction, building complexity and source location. Here we consider a test case, coded T1.1, where the most dense building configuration is used, with a north wind direction. Four meteo-dispersive modelling systems, based on the interface of meteorological codes and Lagrangian particle dispersion models, were applied and tested against the experimental data: TalDia-ARTM, MISKAM-LASAT, GRAL-system and MicroSwiftSpray.

The concentration values predicted by the models in the T1.1 test case are compared to the observed data at 72 points, in 51 locations and at different heights. The statistical analysis is based on protocols developed during COSTES1006 and COST732 Actions. Metrics like Fractional Bias (FB), Normalised Mean Square Error (NMSE), Index of Agreement (IA), Geometric Mean bias (MG) and Geometric mean Variance (VG) are considered. Illustrative results of the model intercomparison and evaluation are presented, highlighting the possible critical items encountered. The applicability of the different metrics in such a complex urban configuration, with concentrations ranging over different orders of magnitude, is evaluated and discussed. The sensitivity of the modelled concentration fields to the meteorological input considering two different grid resolutions, is analysed. An interpretation of the results, based on the differences of the modelling systems, is offered.

The potential of the Lagrangian dispersion models in dealing with long-term predictions is addressed, together with their usability in terms of computational demand and runtime needs.
The simulation results of the single modelling systems are submitted as separate contributions and presented as posters during the Harmo23 conference.

THE EXPERIMENTAL SETUP

The experiments have been carried out in the Environmental Wind Tunnel Laboratory (EWTL) at Hamburg University. In Table 1 and Figure 1 the setup of the wind tunnel experiment for the selected test case T1.1 is reported and illustrated.

Table 1. Setup of the wind tunnel experiment for the T1.1 test case

Geometry	Level 2 - dense
Stability	Neutral
Source	Coordinates: 430.4 North/Lat/Y [m]; 2.4 East/Lon/X [m] 20 Height/Z [m]
	Type: stack
	Diameter: D = 2 m
	Height over (flat) roof: 2 m
	Emission rate: 2 g/s (= kBq/s) (WT)
Flow	Exit temperature: 20 °C
	Exit velocity: 2 m/s
	Roughness: z_0 = 0.6 m
	Reference height: 100 m
	Reference wind speed: 10 m/s
	Wind direction: 0° (360°)

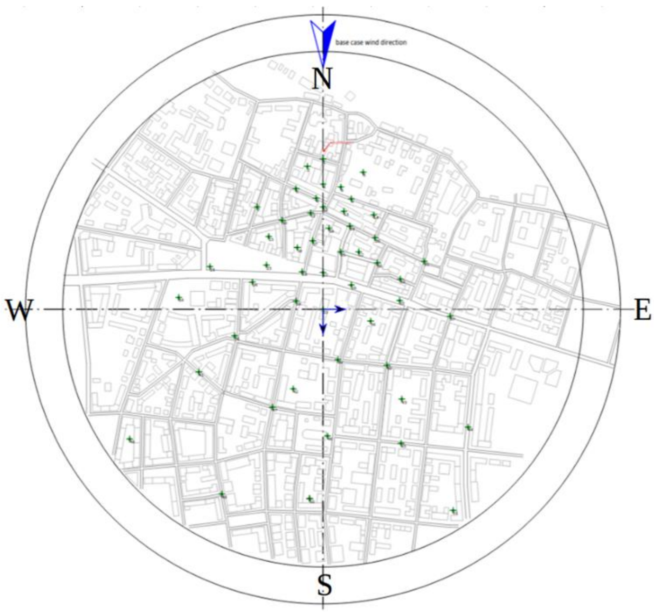

Figure 1: Setup of the T1.1 test case, as in Table 1. The red point shows the source position, the green crosses indicate the locations of the measuring points. The blue arrow shows the wind direction, from north (0°).

THE MODELS AND THE SIMULATIONS

Here we present the results of simulations performed for test case T1.1 using as input to the models the flow field produced on a grid of 5 m and 2 m resolutions, on a domain of about 1600 × 1600 m.
The **ARTM** model (Hanfland et al., 2022) operates typically on 0.5 km^2 – 10 km^2 scale and simulates atmospheric dispersion of radionuclides released during routine operation of nuclear facilities. In this work the ARTM Version 3.1.0 was applied. The model uses the diagnostic wind field model TALdia in cases where buildings of orographic features are present. The vertical wind-profile is given by a logarithmic function. This model delivers a divergence-free flow field and turbulence parameter for the whole domain. Obstacle-induced turbulence is also included. The discharged radionuclides are simulated by numeric particles moving according to these pre-calculated fields and undergo radioctive decay, as well as dry and wet deposition (if applies).
LASAT version 3.4 (Janicke Consulting, 2019) simulates pollutant plumes as clouds composed of numerous small particles, each representing a defined pollutant mass. Their transport accounts for spatial and temporal variations in wind conditions. Here, the flow fields were calculated using the microscale flow and dispersion model MISKAM (Eichhorn and Kniffka, 2010), then properly converted for use in the LASAT model. MISKAM is a model designed to calculate wind fields and pollutant concentration distributions in areas with complex building structures, typically on spatial scales of a few hundred meters. The flow simulation in MISKAM is based on the full set of three-dimensional momentum equations.

MicroSPRAY is the microscale version of the Lagrangian particle dispersion model SPRAY, accounting for the presence of buildings. A detailed description of the model can be found in Tinarelli et al. (2012). Here MicroSPRAY is driven by the flow field produced by the diagnostic code MicroSWIFT, solving the obstacles. A logarithmic wind profile is used as input to MicroSWIFT; the turbulence is calculated as the sum of a background term, calculated using Hanna (1982) parameterisation, and a term based on a deformation tensor and a mixing length, used to model the turbulence generated by the obstacles.
GRAL (https://gral.tugraz.at/) is a Lagrangian particle model and is frequently used for atmospheric dispersion modelling of air pollutants and odour for regulatory purposes. GRAL has an inherent flow solver to compute flow in the vicinity of obstacles such as buildings (Öttl, 2015). Although a standard k-ε turbulence model is available an algebraic mixing length model was utilized here. GRAL uses standard wind profiles that follow nearly those proposed by US-EPA, and special turbulence algorithms to account for low wind or calm conditions in complex terrain. Plume rise is based on Hurley (2005) model.

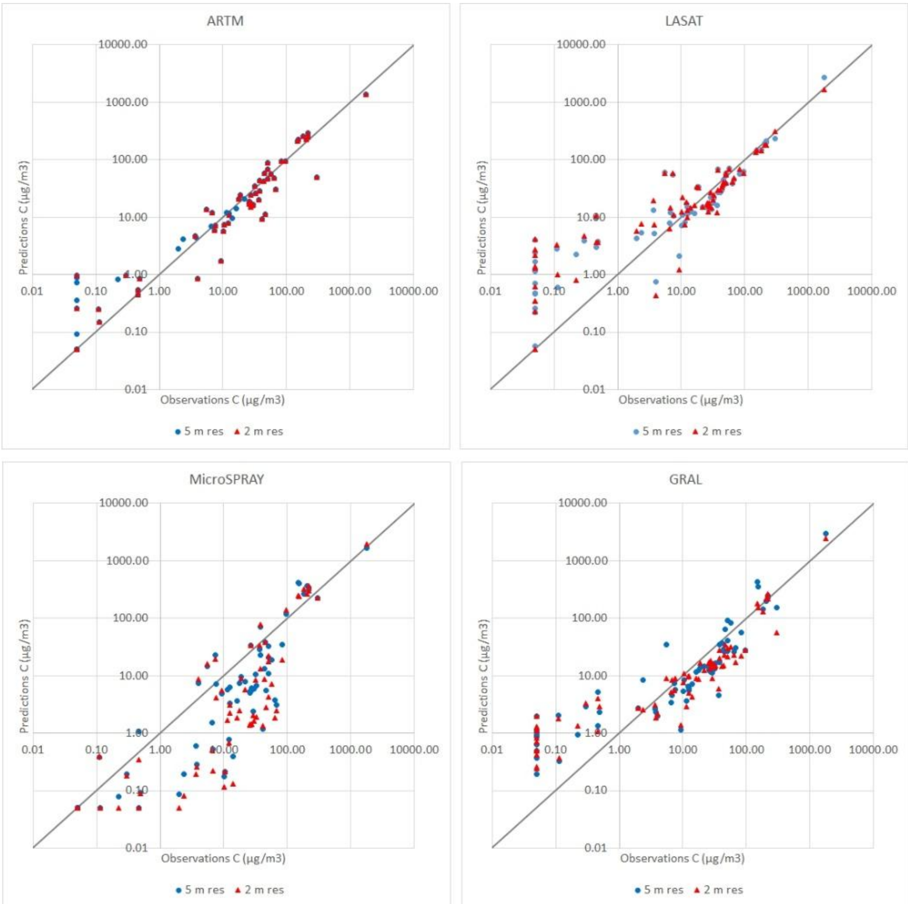

Figure 2: Scatter plots for the four models of the predicted concentration versus the observed one, using input meteorological fields at 5 m (blue dots) and 2 m (red triangles) horizontal grid spacing, for a 0° deg wind direction in the most dense building configuration.

RESULTS AND DISCUSSION

To compare predictions and observations, and to estimate the corresponding statistics, a minimum threshold concentration value is assigned to both of them when they are lower than the sensitivity/precision of the measurements. This is particularly important when calculating the MG and the VG, since they are strongly influenced by extremely low values and are undefined for zero values. It is recommended (Hanna and Chang, 2012) to take into consideration an instrument threshold, such as the limit of detection, which should be used as the lower bound for both predicted and observed values.
In Figure 2, the scatter plots of the predicted versus observed concentrations at the measuring points are reported. In general, the agreement between predictions and observations is analogous and relatively good

for both 5-m and 2-m resolutions, and the highest concentration values are well captured. In particular, ARTM, LASAT and GRAL show some values over the threshold where the measurement takes the threshold value. MicroSPRAY tends to underestimate the concentration in the medium range, 10-10^2 µg/m^3, whereas all threshold values for the observed data correspond to threshold values in the predictions.

The formulas of the statistics are recalled hereafter.

$$FB = \frac{\overline{\Phi_o} - \overline{\Phi_p}}{0.5\left(\overline{\Phi_o} + \overline{\Phi_p}\right)}; \; NMSE = \frac{\overline{\left(\Phi_o - \Phi_p\right)^2}}{\overline{\Phi_o} \cdot \overline{\Phi_p}};$$

$$MG = exp\left(\overline{\ln \Phi_o} - \overline{\ln \Phi_p}\right); \; VG = exp\left[\overline{\left(\ln \Phi_o - \ln \Phi_p\right)^2}\right]$$

$$IA = 1 - \left[\frac{\sum_{i=1,N}\left(\Phi_{pi} - \Phi_{oi}\right)^2}{\sum_{i=1,N}\left(\left|\Phi_{pi} - \overline{\Phi_o}\right| + \left|\Phi_{oi} - \overline{\Phi_o}\right|\right)^2}\right]$$

The following reference acceptance criteria were defined by Hanna and Chang (2012) for built environments: |FB| < 0.67; NMSE < 6, i.e.; 0.5 < MG < 2.0; VG < 75.
The dataset is composed of 72 observations, thus the limited number of values for this single test case has to be accounted for when evaluating the model performance through the metrics. These last reflect the dispersion of the predictions with respect to the observations.

Table 2. Statistics for test case T1.1 as in Table 1, for meteorological input at 5 m and 2 m grid spacing

	ARTM		LASAT		µSPRAY		GRAL	
	5 m	***2 m****	***5 m***	***2 m***	***5 m***	***2 m***	***5 m***	***2m***
FB	0.11	-0.11	-0.14	0.07	-0.03	0.01	-0.22	0.03
NMSE	1.13	1.16	2.70	0.14	0.84	0.51	4.37	2.03
MG	0.90	0.59	0.56	0.55	2.44	3.56	0.73	0.84
VG	2.13	1.79	8.77	9.71	11.55	50.91	7.05	6.89
IA	0.97	0.97	0.96	0.99	0.98	0.99	0.93	0.97

***reduced domain**

Most models have excellent FB and IA values. Moving from 5 m to 2 m grid resolution does not necessarily lead to improved performances. The best agreement is found for high concentration values, and this is confirmed also by a significant improvement in the statistics when considering the subset of the ten highest values (not shown). In particular, ARTM, LASAT and GRAL fulfil all the above criteria. MicroSPRAY fulfils all criteria apart from MG and has high VG values: this is due to the underestimation of the concentration values in the medium range and has been thoroughly investigated.
In Figure 3, the contour plots for test case T1.1 are reported for all models. They depict the distribution of the concentrations and add a spatial description of the outcomes described by the analysis of the results.
Note that during the conference, specific contributions present the results and sensitivity analyses for the single model considered in the intercomparison, together with the related interpretation.

CONCLUSIONS

A first evaluation of Lagrangian particle dispersion models applied to a release in a complex built environment enables a preliminary discussion of the ability, reliability and limitations of this kind of modelling approach. Beyond the specific result for the single model, the validation proves the robustness of the Lagrangian approach and, based on the criteria established for built environments, the models can be considered ‘good models’. The highest concentration values are well captured by all models, and this aspect is important in view of population protection and response to accidental releases.
Besides EXPO-URB specific research plan, the final aim of presenting this work is to open the intercomparison and evaluation program to other groups that may be interested in validating their models in the context of the project’s goal.

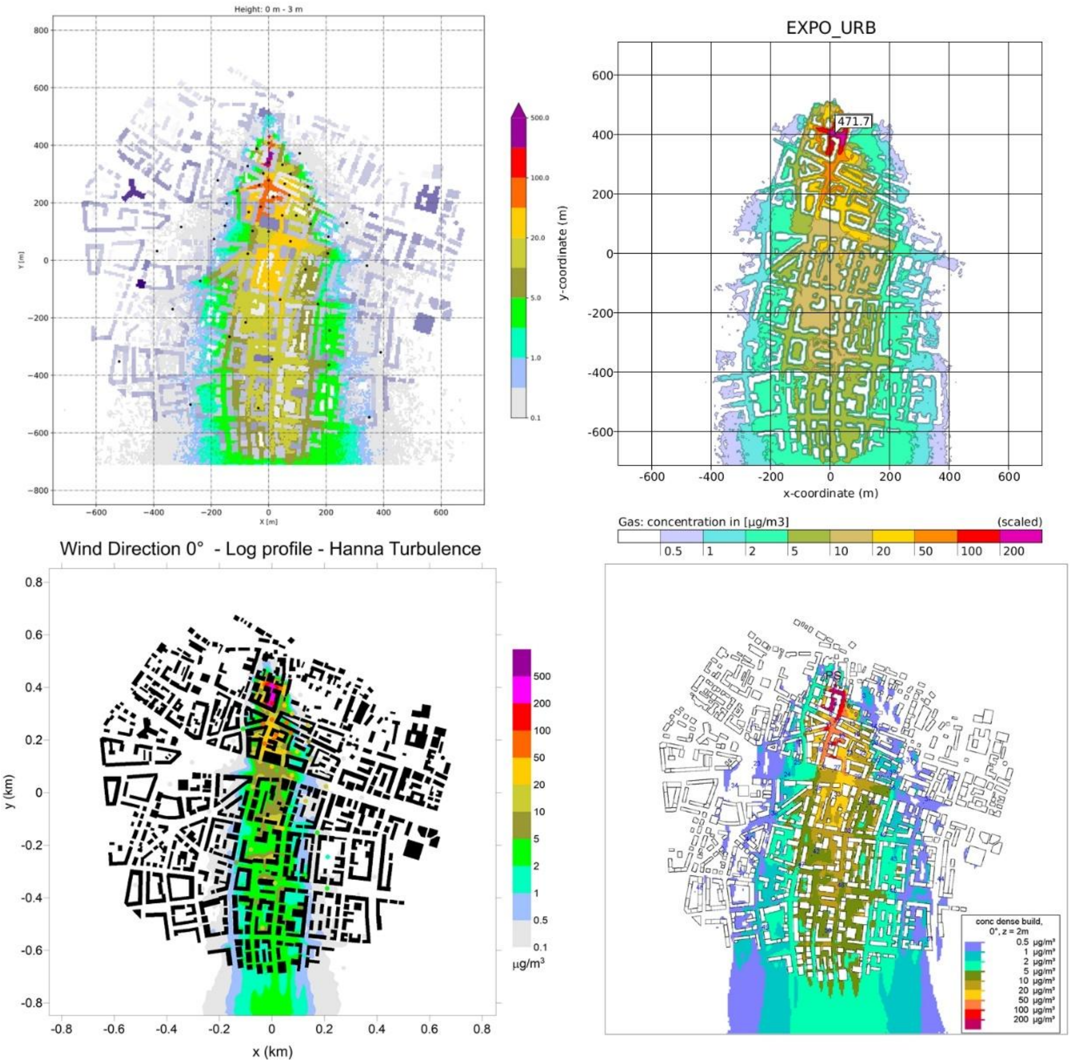

Figure 3: Contour plots of the concentration field at 2 m height for the four models, for a 0° deg wind direction in the most dense building configuration, with input meteorological fields at 5 m grid spacing: From top left to bottom right: ARTM, LASAT, MicroSPRAY, GRAL

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