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Modelling air pollution around nuclear power plants: validation of dispersion models using tracer data

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Abstract

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The Šoštanj exercise of the Modelling and Data for Radiological Impact Assessments I Urban Environments Working Group took advantage of a set of measurement data from a 1991 tracer experiment to test atmospheric dispersion models for emissions from point sources over complex terrain. The data set included emissions of SO₂ from the stacks of the Šoštanj Thermal Power Plant in Slovenia, measurements of the SO₂ at a number of locations in the surrounding area up to 7 km from the plant, and meteorological data from several monitoring stations, all as measured half-hour average values. Two sets of meteorological conditions were modelled: (a) a simple situation with a strong wind blowing from a point source directly towards a monitoring station; and (b) a complex situation involving a temperature inversion and convective mixing. The modelling results enable the assessment of the capabilities of various dispersion models in handling both complex terrain and complex meteorological situations.

1. Introduction

In the event of a release of radioactivity from a nuclear facility, the first direct exposures of the surrounding population would typically result from atmospheric releases. Thus, the ability to generate reliable model predictions of atmospheric dispersion is essential to assessing potential effects of a facility on local populations. The goal of this exercise in the Modelling and Data for Radiological Impact Assessments I (MODARIA I) programme was to validate atmospheric dispersion models for use in the vicinity (tens of kilometres) of nuclear power plants, with validation involving the comparison of model predictions with measurements from an appropriate experimental situation (IAEA 2021). The emphasis has been on short-term releases, such as those that would occur in an accident, but the findings are also applicable for assessment of routine emissions. An experimental situation appropriate for such an exercise requires emissions data for a suitable tracer, environmental measurements of the tracer in the region surrounding the emissions source, and detailed meteorological data. It is also essential that other regional sources of the same tracer be minimal.

A data set obtained in 1991 at the Šoštanj Thermal Power Plant (TPPŠ) in Slovenia meets all of these requirements for use in a model validation exercise (Mlakar *et al* 2015). This time period predates the installation of desulphurisation units at the power plant, so emissions of SO₂ were very high, and were easy to measure with minimal measurement error. Other sources of SO₂ in the area were considerably lower, and thus, did not confound environmental measurements of SO₂ as a tracer for TPPŠ emissions. The data set consists of a three-week period in 1991 during which automatic measurements of SO₂ emissions from the TPPŠ chimneys, automatic measurements of SO₂ concentrations in air at several environmental monitoring

stations in the surrounding area up to 7 km from the plant, and detailed measured meteorological data were taken. Both simple and complex meteorological patterns occurred during the time period. The location of TPPŠ in an area of complex terrain means that a model validation exercise has to account for both complex terrain and complex meteorology, both of which affect the real-world dispersion of atmospheric pollutants. The exercise was also intended to facilitate evaluation of both spatial and temporal errors in the modelling.

2. Description of the exercise

This modelling exercise was developed and conducted within Working Group 2 of the MODARIA I programme, which was entitled 'Exposures in contaminated urban environments and effect of remedial measures' as part of a larger thematic heading 'Remediation of Contaminated Areas' (IAEA 2021, Thiessen *et al* 2022). The exercise was intended as a mid-range atmospheric dispersion exercise, applicable for a situation in which radioactive material is transported to an urban area from a distant source, such as a nuclear power plant. Participants in the exercise were requested to model the dispersion of an airborne tracer (in this case, SO₂), given starting information on emissions, meteorology, and terrain. Model calculations (time-dependent concentrations of SO₂ in air, with no time shift of emissions and meteorological data) were then compared with time-dependent measurements of the tracer in the environment at given locations. A full description of the modelling exercise and results from individual models is provided in the Working Group 2 report (IAEA 2021).

2.1. Data set

An experimental measurement campaign was conducted from 15 March to 5 April 1991, in the vicinity of the TPPŠ in the Šaleška region of Slovenia. The purpose of the campaign was the assessment of air pollution from the power plant, with an emphasis on meteorological conditions contributing to episodes of severe air pollution. At the time, prior to the installation of wet desulphurisation units, TPPŠ emitted about 100 000 tons of SO₂ per year, and concentrations of SO₂ in air could exceed 1 mg m⁻³. The campaign was conducted by researchers from ENEL-CRAM and CISE in Milano, Italy, and the Jozef Stefan Institute in Ljubljana, Slovenia; full details are provided by Elisei *et al* (1991). Results from the campaign were used to evaluate several air pollution models available at the time (Brusasca *et al* 1992, Božnar *et al* 1993, 1994).

Measurements of the emissions from all three stacks (chimneys) operating at TPPŠ were made automatically, with SO₂ emissions rates of 0.01–0.24 kg s⁻¹ (stack height, 100 m), 0.87–2.05 kg s⁻¹ (stack height, 150 m), and 0.53–2.46 kg s⁻¹ (stack height, 230 m). Emission rates were available as half hour values for modelling purposes. In addition the temperature of the gaseous emissions was given for plume rise calculation. The temperatures were in the range 155 °C–171 °C (stack height, 100 m), in the range 155 °C–183 °C (stack height, 150 m) and in the range 172°C–202 °C (stack height, 230 m). The temperature of the gaseous emissions is essential for plume rise calculation and should be measured or estimated also for the use of models for radiological emergency releases. Exit velocities for all there stacks were in the range 0.7–2.9 m/s (stack height, 100 m), 8.8–12.3 m/s (stack height, 150 m) and 8.6–12.7 m/s (stack height, 230 m).

Measurements of SO₂ concentrations in air were made automatically at six stations in the area surrounding TPPŠ. Meteorological stations conforming with World Meteorological Organization standards were operated at the same six locations. Air temperature, relative humidity, and wind were measured at all stations, while precipitation and air pressure were also measured at one station, and global solar radiation was measured at another station. A mobile Doppler sonic detection and ranging (SODAR, used for wind profiling) and differential absorption lidar (used for SO₂ remote sensing) were also operated during the campaign. All data were provided as half-hour average values.

2.2. Complexity of terrain and meteorology

TPPŠ is located in the centre of the Šaleška valley, which is also called the Velenje basin because of its shape. The average altitude of the valley is 400 m above sea level. The valley is surrounded by hills on the south side and by high mountains (Karavanke Alps) on the west, north and east sides. There are two towns (Šoštanj and Velenje) and several small villages in the valley and its surrounding area, where approximately 36 000 people lived at the time the campaign was performed (Elisei *et al* 1991). Some of the hills are much higher than the TPPŠ stacks (figure 1).

Based on an analysis of wind fields at five meteorological stations during 1991–1993, Mlakar and Božnar (2011) characterised the meteorology over the Šoštanj area in terms of ten classes, which could be further subdivided for more detail. The area is prone to the development of temperature inversions and consequent episodes of high air pollution. Two cases, reflecting different meteorological situations, were selected for the modelling exercise, as described below. In one case, there was a direct wind from the chimney toward a single measuring station, and in the other case, there was a complex wind situation.



Figure 1. Šoštanj Thermal Power Plant (2010).

2.3. Case 1 (30 March 1991)

The first case selected for the modelling exercise was a situation with simple meteorology, with a strong wind blowing directly from the chimney of height 100 m toward a measuring station atop a hill in the nearby area, 2.5 km away and 87 m higher than the top of the chimney. Case 1 utilised data from a single day (30 March 1991) when only one emission source was active. Measurements showed high concentrations of the tracer at the Veliki Vrh monitoring station, while measured concentrations at the other monitoring stations were low or negligible.

2.4. Case 2 (1-2 April 1991)

The second case selected for the modelling exercise was a complex situation, involving a night-time temperature inversion (stability class could be estimated as Pasquill–Gifford classes E–F, with low winds; detailed data were given to participants for calculation of Monin–Obukhov length), accumulation of air pollution below the inversion, and convective mixing (estimated class B with low and moderate winds) of the polluted air on the following day. This situation resulted in near simultaneous contamination being measured at the monitoring stations surrounding the power plant, including very different locations in different directions. Case 2 utilised data from a two-day period (1–2 April 1991) with two active emission sources. This was a very difficult situation to model (Grašič *et al* 2007).

3. Models used in the exercise

Six models were used during the course of the exercise, including models intended for different purposes (e.g. emergency assessment, research). Two major types of modelling approaches (Gaussian and Lagrangian particle models) were represented. Table 1 summarises the models, which are described in more detail in an IAEA Working Group 2 report (IAEA 2021).

4. Results of the exercise

Full descriptions of the results of the modelling exercises are provided in the IAEA Working Group 2 report (IAEA 2021). Selected results are described below, with respect to particular aspects of the modelling approaches or results. Most examples discussed are based on the results of Case 1.

		lable I.	Summary of models and selected parameter	ers as used for the Sostanj exercise.		
Model name	SPRAY	CERES®CBRN-E Parallel Micro-SWIFT- SPRAY PMSS	RASCAL 3.0.5	ARTM	LASAIR	NFS_Vinca
Participant(s)	M Z Boznar, P Mlakar, B Grašič	L Patryl	F Mancini	S Hettrich	S Hettrich	Z Grsic
Country	Slovenia	France	Italy	Germany	Germany	Serbia
Purpose of model	Air contamination dispersion modelling	Hazmat atmospheric dispersion modelling and impact assessment	Radiological emergency assessment	Long term dispersion modelling, annual dose calculations near nuclear facilities	Short term dispersion modelling, sudden releases	Research and operational use in Public Company Nuclear Facilities of Serbia
Type of model	Lagrangian particle dispersion model	Lagrangian particle dispersion model	Gaussian plume (TADPLUME) and Lagrangian puff (TADPUFF) models	Lagrangian particle dispersion model	Lagrangian particle dispersion model	Gaussian plume model (for continual releases); Gaussian puff model (for instant and continual pollutant releases)
Number of particles (Lagrangian models only)	$10-30 \text{ s}^{-1}$	$10^7 (60 \text{ s}^{-1})$	Not applicable	$1.008\times10^9\mathrm{h}^{-1}$	$1.008 \times 10^{6} \mathrm{h}^{-1}$	Lagrangian model of Gaussian type, 1 puff min ⁻¹
Domain size/calculation range	$15 \text{ km} \times 15 \text{ km}$	$15 \text{ km} \times 15 \text{ km}$	$15 \text{ km} \times 15 \text{ km}$	$15 \text{ km} \times 15 \text{ km}$	$15 \mathrm{km} \times 15 \mathrm{km}$	$15 \text{ km} \times 15 \text{ km}$
Grid size Grid height	150 m × 150 m 20 layers	$100 \text{ m} \times 100 \text{ m}$ 25 grid layers; ground layer up to 13 m height; last layer up to 6000 m height	150 m \times 150 m Not used	150 m \times 150 m Model simulates 19 grid layers up to 1500 m height; here used ground layer from 0 to 3 m	150 m × 150 m Model only outputs ground layer 0–3 m	150 m × 150 m Not used in this exercise
						(Continued.)

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			Table 1. (Continue	.d.)		
Model name	SPRAY	CERES®CBRN-E Parallel Micro-SWIFT- SPRAY PMSS	RASCAL 3.0.5	ARTM	LASAIR	NFS_Vinca
Release height	Actual stack + dynamic plume rise	Effective height, accounting for dynamic and buoyant sources	Effective release heights: Case 1, 100 m; Case 2, Stack 1-2-3, 100 m; Stack 5, 200 m	Actual stack height, multiple stacks possible, model calculates plume rise	Stack height maximum 200 m (model only supports building heights up to 200 m); only one stack per simulation, multiple stacks had to be calculated and results manually combined; plume rise had to be calculated and added manually; emission height limited to maximum 300 m, as model	Physical stack height, 100 m; effective stack height, time dependent
Model name	SPRAY	CERES®CBRN-E Parallel Micro-SWIFT-SPRAY PMSS	RASCAL 3.0.5	ARTM	was ucvertoped for freat ground emissions LASAIR	NFS_Vinca
Receptor height	First cell is 0–10 m above the ground	Ground level, 13 m in height	10 m height	Ground level	Ground level	2 m above ground level
Stability class	Dynamic, Monin–Obukhov length	Dynamic, Monin–Obukhov length	Defined by time period, using wind speed and solar radiation	Klug/Manier dispersion dasses, based on SODAR data; Monin–Obukhov length	Klug–Manier dispersion classes based on SODAR data	Pasquill stability class C
						(Continued.)

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Model name	SPRAY	CERES®CBRN-E Parallel Micro-SWIFT- SPRAY PMSS	RASCAL 3.0.5	ARTM	LASAIR	NFS_Vinca
Wind speed and direction	Mass consistent wind field based on several ground level measurements and SODAR vertical profile	Vertical wind profiles, interpolated as needed	Hourly data from Šoštanj location and SODAR location, uniform wind field	Hourly data required by model derived from SODAR, two modes: excluding half-hourly data and vector-adding half-hourly data to hourly data	Model could take higher resolved wind data; for comparison, same data were also used for ARTM	Case 1, TPP Šoštanj, SODAR multi-level wind data; Veliki Vrh, wind data at a height of 10 m above the ground
Dispersion parameters	Calculated by meteorological pre-processor	Wind field model PSWIFT (Oldrini <i>et al</i> 2013, Tinarelli <i>et al</i> 2013)	NRC parameterisation, function of Pasquill–Gifford stability class and distance, Gaussian puff model was used for simulations presented in this paper	Integrated wind field model using Klug–Manier dispersion dasses	Integrated wind field model using Klug–Manier dispersion classes	Briggs sigma parameters for rural area, Gaussian dispersion of puffs using the trajectories
Time step for meteorological data	Half hour	Half hour	Half hour or hour	Hour	Hour	1 min or 10 min
Terrain/ topography	Digital model of the heights	Shuttle Radar Topography Mission (SRTM) database	Surface roughness length and orographic data are used	Adapted orographic data; with and without buildings	Orography imported from OpenStreetMaps, with and without buildings at emission site	Egan's theory (Egan 1975)

Table 1. (Continued.)





4.1. Comparison of measurements and model results

A simple comparison of time-dependent measurements of SO₂ concentrations in air at a given monitoring station with time-dependent model predictions shows the difficulty of such modelling, even for the simple meteorological conditions of Case 1. Two examples are the results of the RASCAL 3.0.5 (figure 2) and SPRAY (figure 3, upper left) models. RASCAL 3.0.5 is a Gaussian plume/Lagrangian puff model intended for use in assessing a radiological emergency; it was run using hourly meteorological data. SPRAY is a Lagrangian particle model and is intended for more elaborate air contamination modelling; it uses more detailed meteorological data, updated every half hour. RASCAL 3.0.5 predicted a peak concentration much higher than any of the measured peaks for Case 1 and did not predict the correct timing of the peak. The SPRAY model reproduced the noon peak of Case 1 with respect to timing, although not fully in magnitude, but missed most of the other measured peaks.

During the period 11:00–13:00 the wind direction at the TPPŠ stack varied in the range $(13^{\circ}-38^{\circ})$; the Veliki Vrh station is in the direction 17° from the TPPŠ stack. The wind speed was in the range $(2.5-3.7 \text{ m s}^{-1})$. The SO₂ emissions were in the range $(1.53-1.64 \text{ t h}^{-1})$.

4.2. Adjustment of the model's sigma values

SPRAY was run again using 20% higher sigma values in all three directions. Measurements showed that the plume is more dispersed than the model showed, so we did an experiment to examine the influence of higher sigma values on the results. Sigma values are input parameters for the SPRAY model (Tinarelli *et al* 2000). This adjustment of the sigma values improved the predicted noon peak and some of the small morning peaks (figure 3, upper right 'new sigmas').

4.3. Allowance for spatial and temporal error

To allow for the possibility of the model predictions being off slightly in either direction or timing, predictions generated using the SPRAY model for Case 1 were also made for an additional five cells in each horizontal direction (S–N and E–W) and for adjacent time periods (Grašič *et al* 2011). The size of the initial cell as well as each additional cell was 150 m \times 150 m. The initial cell included the Veliki Vrh station in its territory.

The best fits of those predictions are shown in the lower graphs of figure 3 (operational version on the lower left, reconstructed 'new sigmas' on the lower right). This approach provided much better fits to the noon peak (both versions) and to the main morning peak (lower right), but did not greatly improve the modelling results for other parts of the time period. The label 'new sigmas' stands for 20% higher sigma values in all three spatial directions.



Figure 3. Comparison of model predictions (red) generated using the SPRAY model with the measurements (green) of SO₂ (μ g m⁻³) for the 30 March 1991 case (Case 1) at the Veliki Vrh station. Graphs on left show the operational version of the SPRAY model; graphs on right show results with revised values (20% higher) for the sigma terms. Upper graphs show predictions for the specified location and time; lower graphs show the best fit to the measurements for a range of locations (five cells in each direction) and time periods ($\pm \Delta t = 0.5$ h).



4.4. Use of detailed wind fields

The CERES®CBRN-E (Parallel Micro-SWIFT-SPRAY, PMSS) model used a detailed wind field (as did all other models except RASCAL) produced for the whole time period, together with an approach allowing for spatial and time error (figure 4). This approach resulted in predicted concentrations for Case 1 that were in good agreement with the measurements for the three largest peaks (7:30, 12:00, 22:30; figure 3), but not for all of the smaller peaks.



Figure 5. Measurements of SO₂ (μ g m⁻³) at the Veliki Vrh Station for the 30 March 1991 case (Case 1) compared with predictions from ARTM, both without accounting for buildings at the emission site (top) and with accounting for buildings at the emission site (bottom). The measurements have been averaged to show an hourly resolution. The error bars show the deviation range of the five-by-five cells target grid around the Veliki Vrh station to allow for slight deviations in the model predictions with respect to the location of the measurement points.

4.5. Model adaptations

The atmospheric radionuclide transport model (ARTM) and lagrangian simulation of the dispersion and inhalation of radionuclides (LASAIR) models (figures 5 and 6) were used by the same participant. ARTM is primarily intended for long-term dispersion modelling of ongoing releases, while LASAIR is intended primarily for short-term modelling of sudden releases. LASAIR required a number of adaptations or approximations to be used for this exercise, including allowing for more than one emissions source, adjustment for plume rise, and extension of the duration of the simulation time (Hettrich 2017). In addition, wind speeds <0.5 m s⁻¹ were assumed by LASAIR to equal 0.5 m s⁻¹. ARTM allowed only for hourly meteorological data input, which needed some consideration. It was run in two different modes; for the first attempt ('old'), the half-hour values were simply excluded, and for the second attempt ('averaged'), a vector addition was used to include and average the half-hour values into hourly ones for input into the model (Hettrich 2017). For direct comparison, the same two modes were also used in LASAIR, despite the model not being restrained to just hourly inputs (Hettrich 2017).

4.6. Accounting for effects of buildings

Predictions with ARTM and LASAIR were used to compare two methods of handling the meteorological data and approaches with and without accounting for buildings at the emission site, as well as accounting for



adjacent cells in the modelling domain (spatial error) (Hettrich 2017). The graphs (figures 5 and 6) show the range of values generated at each time point for each approach. The noon peak was reproduced reasonably well by both ARTM and LASAIR. In general, accounting for buildings produced lower predicted concentrations.

4.7. Use of meteorological forecasting

Prognostic weather information (weather forecasting) from the Weather Forecasting Model⁷ was used with the SPRAY model for an additional set of runs for Case 2, with varying combinations of measurements from the ground stations (including SODAR) and prognostic wind and temperature information (figure 7). Prognostic data were used in addition to measured data for higher levels of the atmosphere and for the vertical temperature profile, neither of which was measured. Prognostic data were input to the model in the same way as if they had been measured data. The model combined prognostic and measured data as if they were from the same measuring device. Prognostic data were used with no time shift compared with measured data—as the best reconstruction for the given time period. Prognostic data were not used as the only source









of meteorological data, and forecasting of air contamination concentrations was not the intention of this exercise. For this particular situation, the best results for the main peaks (approximately 07:00–12:00) were obtained when prognostic wind and temperature information for higher altitudes (>800 m for RUN 04 and >1100 m for RUN 05) was used along with the measurements from the ground stations. The results may reflect both the importance of the SODAR data for high level winds and the limitations of that data.

4.8. Simulation of the maximum concentration of SO₂

The NFS_Vinca model was used to simulate the maximum concentration of SO₂ in the air at the Veliki Vrh monitoring station during the noon peak on 30 March 1991 (Case 1). The measured peak of 288 μ g m⁻³ represented the cumulative concentration between 11:30 and 12:00. For this simulation, the vertical profile of

the wind (at 104, 158, and 213 m, from SODAR) at the emissions point and the temperature at 2 m above ground level at the emissions point were used to estimate the atmospheric stability class at the monitoring station, accounting for the difference in elevation (186 m) between the emissions point (360 m above sea level) and the monitoring station (546 m above sea level). A wind field was calculated from a linear combination of the vertical wind profile near the emissions point and the measured wind at the monitoring station (figure 8, left panel). The wind field was adjusted to the terrain using the Vinca diagnostic wind model. This calculated wind field, together with a Gaussian puff model, provided an estimated maximum concentration of SO₂ at the monitoring station of 308 μ g m⁻³ (figure 8, right panel).

5. Findings and recommendations

The TPPŠ modelling exercise made use of an extensive set of meteorological data, emissions data, and monitoring data to test the predictive capabilities of models for a situation with complex terrain and complex meteorology. An area up to 7 km from the plant was examined. This is the area where harmful effects of radionuclides released from the nuclear power plant would be first expected in the event of an nuclear or radiological emergency. A major goal of the exercise was to improve the understanding of the capabilities of particular models, the conditions for which they can be used, and the approximate spatial and time error of the models in the representation of the dispersion of the cloud of pollution over complex terrain. The exercise also included assessment of the spatial and temporal error of model predictions. In addition, this exercise provided an initial opportunity to test models using prognostic meteorological information (weather forecasting), such as might be used in an emergency. The prognostic modelling and a third test case based on the data set were further explored during the MODARIA II programme (IAEA in preparation).

Several sets of recommendations came out of the exercise (IAEA 2021):

- (a) To support the necessary meteorological and dispersion modelling for a given facility, it is essential to have a sufficient number of meteorological stations (e.g. 3–10, depending on the terrain), with automatic data collection and processing, at appropriate intervals. At least one location should include SODAR or radio acoustic sounding system, to provide vertical profiles of wind and temperature. This recommendation is also supported by previous results on the same data sets (Božnar *et al* 1993, 1994).
- (b) The meteorological model for a facility must be suited to the purpose and to the complexity of the site. It must be able to generate a three-dimensional numerical representation of the meteorological conditions and must be consistent with the available measurements. For complex terrain, such as that around the TPPŠ, mass-consistent wind models are recommended. Care must be taken not to unrealistically 'smooth' the terrain.
- (c) The atmospheric dispersion model must be appropriate for the complexity of the modelling domain. Simple Gaussian models are not suitable for complex terrain. A Gaussian puff model (or a Lagrangian puff model with Gaussian parameters of turbulence) may be useful for simple cases under strong wind conditions as can be seen from the Vinča model results, but are not suitable for more complex cases. Numerical Lagrangian particle models are presently the best suited for modelling dispersion over complex terrain. The models must account for transitions between surface water and land (e.g. as shown in figure 8, there are two lakes east of the TPPŠ), and between rural and urban environments, if used on such areas, and they must accurately account for effective plume rise. This recommendation is also supported by previous results on the same data sets (Božnar *et al* 1993, 1994, Grašič *et al* 2011).

For the assessment of the quality of the model predictions for areas over complex terrain, a suitable methodology should include assessment of temporal and spatial error. One possible methodology is used in this paper and is explained in detail by Grašič *et al* (2011). The building wake effect at the emission site can be handled with land use data (as shown with the SPRAY model) or with direct modelling of buildings (as shown with the ARTM and LASAIR models).

Future efforts in this area should include improved models for forecasting dispersion of contaminants, based on meteorological forecasts. Meteorological forecasts should be enhanced and validated for fine resolution over complex terrain (Mlakar *et al* 2017). The data set available for this exercise did not include deposition; prediction of contaminant deposition, in addition to dispersion, remains a challenge for future research.

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