Evaluation of meso-scale dispersion modelling for accidental release

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Abstract

A modelling system, PERLE, has been developed at Meteo-France, for the Crisis Meteorological Cell (CMC) of atmospheric accidental release, in case of emergency. Mesoscale meteorological fields are simulated by the non-hydrostatic MESO-NH model (8km and 2km resolution nested grids), that also supply an overview of the plume on a regional scale with an eulerian passive tracer. The dispersion model is a lagrangian particle model, to describe the pollutant cloud in the vicinity of the release during the first critical few hours. Two stochastic dispersion models have been evaluated and compared: DIFPAR and SPRAY. The performance of PERLE is tested against a large range of stability and turbulence conditions. A set of fourteen test cases has been conducted on ⁸⁵Kr measurements, released in La Hague plant gaseous waste and measured in the surrounding near field (<5km) by IRSN. Most of the meteorological conditions concern a marine BL, with neutral static stability and a small diurnal variability. In these situations, both models have shown quasi-similar and correct results beyond 800m from the source. Below that, modelling ATC are largely underestimated, partly due to insufficient meteorological horizontal resolution. The system is also applied to the Toulouse Sud campaign (1993), capturing the essential features of the plume. However the 2km meteorological resolution is not sufficient to capture the topographic influence on the flow structure with accuracy. A sensitivity study on the height release has been performed for the neutral and convective boundary layer on Toulouse: the asymmetric structure of turbulence in the CBL appears correctly with SPRAY. PERLE is able to yield reliable simulations of atmospheric dispersion in inhomogeneous turbulence, for emergency purposes, with competitive computation time (< 30min).

Keywords: dispersion; turbulence; meso-scale.
1 Introduction

The growing concern for environmental problems underlines the importance of correctly predicting the fate of pollutants released into the PBL, and calls for more reliable models. Combination of meteorological and dispersion models are currently used to help direct emergency response following a hazardous material release. They must be able to model the airborne pollutant dispersion on any complex terrain, influenced by meso-scale effects (topography, urban, coastal) with a reasonable degree of confidence.

Firstly, dispersion models need realistic three-dimensional atmospheric fields as input for transport and dispersion studies of atmospheric pollutants. Secondly, the conventional gaussian and eulerian K-theory models are inadequate for modelling dispersion in complex terrain, or convective boundary layer. Alternatively, lagrangian particle models and higher-order closure models are able to yield reliable simulations of atmospheric turbulent dispersion. To examine the local scale in an emergency purpose, only lagrangian particle models are suitable for computation time. This type of models also reduces the close-to-source artificial diffusion, resulting from the smoothing inherent to the eulerian grid. Many authors have shown that Monte-Carlo models are promising for inhomogeneous turbulence (Thomson [1]; Weil [10]).

The integrated modelling system PERLE has been developed to simulate and track accidental airborne pollutant at meso-scale, for emergency purposes. PERLE is based on a combination of the non-hydrostatic mesoscale meteorological model Meso-NH (Lafore et al. [2]), and a lagrangian particle model SPRAY (Tinarelli et al. [3]) or DIFPAR (Wendum [4]).

A description of the system is given in section 2. Section 3 deals with the comparison between simulations and experiments. In section 4, the practical use of PERLE in emergency context is outlined.

2 Description of the models

2.1 Meso-NH

Meso-scale meteorological fields are simulated by Meso-NH [2], a model jointly developed by Meteo-France and Laboratoire d’Aérologie (http://www.aero.obs-mip.fr/mesonh). The model is based upon the Lipps and Hemler anelastic system, and is able to simulate all scales ranging from synoptic scale to turbulent large eddies, owing to interactive grid-nesting technique. Initial and boundary conditions of the larger domain are provided by NWP models ALADIN, ARPEGE or ECMWF.

Physical parametrizations are advanced and validated: the one-and-a-half-order closure turbulence scheme with the Bougeault-Lacarrere [5] mixing length, a warm microphysical scheme, the Kain-Fritsch-Bechtold convection scheme, the ECMWF radiation, a soil and vegetation scheme and the Town Energy Balance scheme [6].
2.2 Particle models SPRAY and DIFPAR

The dispersion model in PERLE is a lagrangian particle model, where the evolution of the cloud of pollutant is simulated by tracking a large number of particles, following a lagrangian formulation of advection and turbulent diffusion (given by Meso-NH) with an added random walk formulation for turbulent behaviour. Two lagrangian dispersion models have been evaluated and compared: DIFPAR and SPRAY.

SPRAY is based on a three dimensional form of the Langevin equation for the random velocity [1], and an accurate description of the model is given in [3]. The lagrangian time scales, the skewness and the variances are assigned from $u^*$, $w^*$, $L_{MO}$, $H_{mix}$, the turbulent kinetic energy and the dissipation, given by the one-and-a-half-order closure Meso-NH scheme.

DIFPAR is presented in [4] with a formulation based on the Fokker-Planck equation. The diagonal diffusivity components are calculated from Meso-NH wind and turbulent kinetic energy.

3 Simulation results

3.1 La Hague release

Test cases have been conducted on $^{85}$Kr measurements, a chemically rare inert gas, released in La Hague plant gaseous waste (stack 100m high) and measured in surrounding near field (<5km) by IRSN (Institute for Radiological Protection and Nuclear Safety) as a plume tracer. Air samples were collected downwind of the discharging stack, at a distance between 300m and 3500m, at different levels from the ground to 100m height. Fourteen measurements, carried out between 1998 and 2002, have been simulated by DIFPAR and SPRAY, using meso-scale meteorological fields from Meso-NH (2km resolution). Dispersion simulations are compared to observations in terms of Atmospheric Transfer Coefficient $(ATC)$ over sampling duration $(ATC = \frac{\int_{T_0}^{T_1} C(x,y,z,t)dt}{Q})$, with C the concentration, Q the total quantity of emitted gas, and T0 and T1 the instants of beginning and end of samplings), and standard deviation of the horizontal plume spread $\sigma_y$, as observations have shown that the plumes were approximately gaussian on the ground. DIFPAR and SPRAY results were also compared to classical Pasquill [7] and Doury gaussian plume models, the latters using meteorological input data from emission site location.

The plant gaseous waste is located on the west arm of Cotentin peninsula (Fig.1). The series of measurements concerns a broad range of direction flux, but most of the plumes are influenced by a marine boundary layer, prevailing neutral or weakly convective static stability and a small diurnal variability, in windy conditions (between 5m.s$^{-1}$ and 10m.s$^{-1}$ at 10m height).
Figure 1: Orography of Meso-NH domain (extension 120×120km²) around La Hague release, with the wind arrows of the 2001/02/16.

Figure 2: Simulated vertical cross-sections of the plume with SPRAY (left) and DIFPAR (right) with height measurements superimposed for 01/02/16 case.

Simulation results are shown on Figure 3, in terms of ATC and $\sigma_y$. In these situations, DIFPAR and SPRAY have shown quasi-similar and correct results beyond 800m from the source. Bellow that, modelling ATC are largely underestimated, especially for SPRAY, as Figure 2 is representative of the set of results, for close-to-source measurements.

Beyond 1000m from the source, SPRAY underestimates the horizontal spread (Fig.3b), as the vertical extension of the plume is larger than DIFPAR in most of the cases. Below 500m-700m, both models largely overestimate the horizontal dispersion.

Pasquill plume model, and moreover Doury, largely underestimates the ATC for all the range of distances, especially under 1000m. The horizontal spread is in
good agreement with measurements above 500m with Pasquill model, as we consider the gaussian horizontal diffusion assumption. On the contrary, Doury model shows systematic important under-estimations with measurements.

![Graph showing comparison between measurements and models](image)

Figure 3: ATC (at the top) and Standard deviation of the horizontal plume spread $\sigma_y$ (at the bottom) at ground level as a function of the downwind distances (between 300m and 3500m), for measurements, SPRAY, DIFPAR, PASQUILL and DOURY modelling.

The ability of PERLE to simulate dispersion for neutral and weakly convective situations, over gentle topography, has been shown, beyond 1km from the source. Below that, it is necessary to reduce Meso-NH resolution, and to take into account the influence of the buildings. However, the aim of PERLE, in a context of emergency, is to model the airborne pollutant dispersion with a reasonable degree of confidence beyond 1km from the source, as the close-to-source area has already been touched before giving the emergency response. On the contrary, gaussian models are not likely to capture the essential features of dispersion characteristics, even in gentle topography.

### 3.2 South-Toulouse experiment

In 1994 has been led an in-situ dispersion experiment in South -Toulouse, with SF6 release in the industrial area, for the two main wind directions of the climatology (SE and NW). This experiment turned out to be relevant, as an
accidental release (AZF) occurred on September 2001, the 21st, on the same location, in very similar SE meteorological conditions, and resulted in casualties and major damages.

Figure 4: (a) Orography around the source (zoom of 40×40km²). (b) Horizontal cross section at 10m of the Meso-NH vertical velocity (contour interval of 0.01m.s⁻¹, negative values in dot lines) with wind arrows, and the hill contour. (c) Vertical profile of the Meso-NH wind speed until 1200m height. (d) Vertical profile of the potential temperature.

For the SE release, the source is located downstream of an hill of 250m height (Fig.4a). Meso-NH reproduces a subsidence around the release (Fig.4b), and a mechanical turbulence, associated to a strong wind shear and neutral static stability (Fig.4.c-d). The model reproduces quite well the flow characteristics, with the exception of the subsidence, largely underestimated, and the absence of rotation wind downstream (132° instead of 118° observed). Therefore, the wind direction error is transferred on the dispersion plume axis of SPRAY and DIFPAR (Fig.5). Beyond this error, concentrations are in good agreement with
measurements for both models. The use of a 500m resolution nested grid in the Meso-NH model improves significantly the direction flow, and consequently the plume modelling (not shown).

For the NW situation, the topographic influence effects on the flow structure are also important, with a lateral spread at the bottom of the hill, that is lightly underestimated by Meso-NH at 2km resolution, and better reproduced at 500m resolution.

Due to the 2km resolution of the meso-scale model, which is not sufficient to characterise the complex turbulence of the PBL at the edge of the hill, the lagrangian particle models were not able to describe the overall structure of the dispersion phenomena. However, they were able to describe the overall structure of the plume in a reasonable way.

Figure 5: DIFPAR modelling ATC on a 3km×3km domain, with SF6 measurements superimposed.

3.3 Height release sensitivity study

Turbulent diffusion in a convectively unstable boundary layer is of interest both for practical and scientific reasons, as maximum ground level concentrations of pollutants emitted from tall stacks usually occur under such conditions. And it has been recognised that Gaussian and eulerian K-theory models are not suitable in this case. A test has been led on the real case of 2002/07/22 at the same location than the previous experiment (Fig.6a), as vertical meteorological profiles were available to validate Meso-NH results, although there has been no pollutant release. The ability of the system to simulate a real CBL, with comparison with the Willis and Deardorff [8] water tank experiments, is tested with a sensitivity study to the height release.

At 5TU, the turbulent heat flux is overall negative, except on Toulouse city core, where the urban effects, taken into account by TEB [6], induce turbulent buoyant production (Fig.6b). The release source is located at the edge of the mixing height development area (Fig.6c), and the static stability is quasi neutral.
Consequently, the Obukhov length scale appears negative, representative of a convective instability (Fig. 6d).

Figure 6: (a) Orography of the Meso-NH 2km-resolution domain (72×72km²), with the urban core area. (b) Turbulent heat flux (contour interval of 0.001 K.m.s⁻¹). (c) Mixing height (contour interval of 10m, from 50 to 180m). (d) Obukhov length scale (contour intervals of −1500, -100, 0, 10 and 600m).

The 130m mixing height is well reproduced by both lagrangian models, whereas there are differences regarding the plume behaviour: for SPRAY, the plume reaches the ground with significant concentrations; on the contrary, DIFPAR develops a weak vertical diffusion. Unfortunately, the lack of dispersion measurement prevents a selection between the two models.

At 12TU, the BL is convective on the overall domain, with a mixing height of 1000m around the release. For the case of low-level source (Fig. 8a-b), the plume rises strongly, especially with SPRAY, and causes an elevated concentration maximum near the top of the BL. The plume from the elevated source (Fig. 8c-d) descends and impinges on the ground for SPRAY, whereas the DIFPAR plume...
Figure 7: Vertical cross section of ATC in the plume axis for SPRAY (a) and DIFPAR (b).

Figure 8: Vertical cross section of ATC in the plume axis for SPRAY (left) and DIFPAR (right), for a low-level source (top) and an elevated source (bottom).
raises. SPRAY is in better agreement with [8] than DIFPAR, diagnosing the asymmetry in bottom-up and top-down diffusion for the CBL.

3.4 PERLE in the operational context

For emergency response, two interactive nested models of Meso-NH are used, with a first domain covering 240km*240km area (8-km resolution) and a second domain covering 60km*60km area (2-km resolution). The vertical grid includes 40 levels until 16km. The initial and boundary conditions of the larger domain are defined by ALADIN (0.1° resolution) for an accident in Western Europe. The initialisation by meteorological forecasts instead of measurements is essential, as the experience shows that meteorological measurements are in most of the cases not available in the vicinity of the source when an accident occurs. Furthermore, a passive tracer is simulated by the eulerian model on both grids, to provide a regional description of the pollutant cloud.

The area of the lagrangian particle model is 30km*30km. Five particles per time step (1s) are emitted during the release. Concentration fields are estimated from the spatial distribution of the set of particle positions, on a grid with 100m horizontal resolution and 10m vertical resolution. Each of the particles is assigned a mass, yielding the total observed release mass.

As DIFPAR is more costly than SPRAY, the latter has been preferred in a first step for PERLE in CMC. An improvement of DIFPAR computation time would allow its integration in PERLE for emergency. Meso-NH is started with a [3-4] hour time lag before the release instant. For a release duration of 1 hour and a SPRAY run of 2 hours, the computation time for the entire PERLE run is of 25 min. Based on research tools, the system PERLE has been developed into a reliable software package, prompting for user-input in the context of an emergency response situation.

4 Conclusion

The PERLE system, based upon the meso-scale model Meso-NH and a lagrangian particle model SPRAY or DIFPAR, demonstrate its ability to model the airborne pollutant dispersion with a reasonable degree of confidence.

Because of its realistic representation of atmospheric dynamics and physics, the prognostic meteorological model is flexible, and has no limitation of terrain application: from flat to complex terrain, with a capability of forecasting flow features driven by diurnal heating cycle, or by surface and urban effects, that are of main interest for dispersion phenomena. The emergency framework implies timeliness and accuracy: the “cheap” configuration of Meso-NH in PERLE is able to reproduce correctly the meso-scale turbulence features. However, in complex flow, the 2km horizontal resolution can be insufficient, and 500m resolution highlights an improvement.

Both DIFPAR and SPRAY models demonstrate their ability in reproducing the complete 3D concentration fields. Despite some differences, neither of them
highlights a systematic error for a type of BL. In a first stage of PERLE as an operational tool, SPRAY has been chosen for its economic computation cost.

The behaviour of PERLE for stable low wind speed conditions still needs to be evaluated, as development of BL schemes for stable conditions is an ongoing area of investigation [9]. Dispersion in a stable BL will be explored during the CAPITOUL campaign, which takes places in 2004 in Toulouse for urban BL, with tracer release experiments.

Acknowledgements

We wish to thank EDF Research Environment Team, especially D. Wendum and E. Gilbert for the use and their help with DIFPAR.

References