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Atmospheric Transport Models for Hazardous Releases: Variability and Uncertainties – Findings of COST Action ES1006 and Operational Experiences

Kathrin Baumann-Stanzer^a, Paul Skomorowski^a, Erwin Polreich^a, Silvia Trini Castelli^b, Bernd Leitl^c, Peter Carny^d

^aCentral Institute for Meteorology and Geodynamics ZAMG, Vienna, Austria

^bInstitute of Atmospheric Sciences and Climate, National Research Council, Turin, Italy

^cMeteorological Institute of the University of Hamburg, Germany

^dABmerit GmbH, Slovenia

k.baumann-stanzer@zamg.ac.at

Atmospheric transport models are in use to model the airborne transport of toxic or radioactive gases or aerosols in large, regional or very local scale events. Different approaches are available, ranging from simple parametric models and Gaussian methods to Lagrangian dispersion models and advanced CFD-based modelling suites. The variety of the models implemented in today's emergency response systems, used in crisis management and emergency response planning, therefore ranges from very simple, robust and fast approaches to highly sophisticated model systems taking into account changes in the meteorological conditions in time and space, terrain and building effects etc. The various methodologies have advantages and disadvantages with respect to their computational efficiency, accuracy, reliability of the results and many more. For any accidental release scenario, authorities may come to different decisions and a variety of instructions may be given to emergency responders, depending on the simulation tools applied.

Which variability in model results can be expected in emergency cases depending on the atmospheric transport model used? How can these uncertainties be explained? How may these be handled in real time application? These questions are addressed in the paper.

The performance of different models for local hazardous releases in built-up areas is illustrated by selected results from model evaluation exercises undertaken in the frame of COST Action ES 1006: non-blind and blind test cases, for continuous as well as for puff releases, sensitivity studies and applications of the same model by different users. A comprehensive overview of all results of these model evaluation exercises is given by Baumann-Stanzer et al. (2015).

Regional to large scale atmospheric dispersion calculations from different emergency response tools, e.g. for radiological hazards, may also render significant differences in the simulated affected areas – due to different meteorological input but even in case of identical meteorological input and source term due to differences in the applied model physics. This is exemplified and discussed based on a model comparison study using the model systems TAMOS, RODOS and ESTE: comparisons of model results based on the same meteorological forecasts under various weather conditions and for different release scenarios.

1. Introduction

Whenever contaminated material is or might be dispersed in the atmosphere in the case of nuclear or chemical accidental releases, a quick and accurate prediction of the concentrations is crucial for emergency response (Gargoum, 2010). Both developers and users of airborne hazard dispersion models have a mutual interest in assessing the performance and reliability of tools applied for emergency management. In order to measure the quality of model results and to improve the implementation of dedicated local-scale models, a task-oriented validation and application procedure has been adopted by COST Action ES1006 (Baumann-

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Stanzer et al., 2015). An overview of the activities that were undertaken by COST Action ES1006 is given by Leitl et al. (2016).

1.1 Challenges and uncertainties

In the case of accidental releases, the source term itself is afflicted with large uncertainties. Furthermore, representative meteorological data are not (or not in time) available as input for dispersion modelling. Therefore, assumptions need to be made. In urban areas as well as in industrial regions, the presence of obstacles, the complexity of built environments as well as complex terrain additionally introduce substantial challenges to flow field simulation as well as to the modelling of local to regional-scale dispersion modelling. In general, the uncertainty of a model result is the sum of the following three components (e.g. Chang and Hanna, 2004):

- Model uncertainty mainly associated with limitations and simplifications inherent in model formulation and modelling set-up
- Input data uncertainty related to source term and meteorological input
- Inherent variability of stochastic processes as turbulence

The first two components may be reduced by the use of more sophisticated model approaches and (as far as possible) accurate, on-site, real-time measurements. The inevitable lack of information concerning the source term in the case of an accidental release may be countervailed by the use of inverse modelling approaches based on concentration measurements.

The third component is not reducible because stochastic fluctuations are inherent for atmospheric processes.

1.2 Test cases

Within COST Action ES1006, two comprehensive and quality controlled datasets were generated comprising continuous and puff releases in a simplified urban geometry 'Michelstadt' (wind tunnel data), in a Complex Urban Terrain Experiment ('CUTE' wind tunnel and field experiment). Furthermore, data from a real accidental gas release at an industrial plant was used for model testing ('AGREE'). A detailed description of the test cases is available in the corresponding document of the Action (Baumann-Stanzer et al., 2015). The validation data is available upon request via the Action website (www.elizas.eu).

In cooperation between ZAMG and ABmerit, 56 scenarios were selected for model comparison: 2 source terms for medium and heavy accident at the NPPs Dukovany, Krsko and Leibstadt, for release heights of 60m and 150m above ground. EZMW meteorological forecast data were prepared for 5 different weather periods.

1.3 Models

The models used at present for local scale emergency response modelling in the case of a harmful release into the atmosphere can be divided into three types according to the complexity of the flow and dispersion modelling approaches as listed in table 1 (Baumann-Stanzer et al., 2015). A typical representative of Type I is ALOHA. Examples for model Type II are LASAT and MSS models. Type III includes more sophisticated CFD (e.g. ADREA-HF) and LES (e.g. PALM) models.

Model type	Flow modelling							Dispersion modelling
Туре І	Impact of buildings and obstacles on flow is neglected.							Gaussian
Type II	Flow	between	buildings	is	considered	by	diagnostic/empirical	Lagrangian
	approach.							
Type III	Flow between buildings is resolved prognostically.							Eulerian (CFD, LES)

Table 1: Types of atmospheric flow and dispersion modelling approaches.

In regional up to large scale emergency response modelling, dispersion models are applied based on meteorological fields (mainly flow data) from meteorological forecast data. Examples for Type I applications in this context are the Gaussian puff models ATSTEP, RIMPUFF which are implemented in the emergency response system RODOS. Type II models applied for regional atmospheric transport modelling of hazardous (mainly radioactive) releases are DIPCOT (implemented in RODOS), FLEXPART and ESTE.

2. Results

2.1 Local-scale modelling of hazardous releases in urban environment

In the frame of COST Action ES1006, stakeholder opinions in several European countries were gathered by means of questionnaires and interviews. This review focused on the models and emergency response tools currently in use as well as on stakeholders' needs, expectations and requirements for advanced atmospheric dispersion models in the context of emergency response to accidental releases to the atmosphere.

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The practical limitations in using more complex tools in emergency response scenarios were expressed to be a major concern for end-users and decision makers. Documenting the limitations of different local-scale emergency response methodologies by assessing the actual uncertainty of model results is recognized as an important issue as well. Nevertheless only a minority of stakeholders answered that they would like to have confidence intervals provided in addition to predicted concentration values or hazardous areas.



Figure 1: Number of stakeholder interviews conducted by COST ES1006 (left) and preferred model simulation outputs as expressed by these stakeholders (right).

In the following, selected examples of model evaluation experiments undertaken by COST Action ES1006 are presented. Several groups applied models of different complexity to simulate releases in urban environment. The model results were compared to measurements from wind tunnel experiments as well as to field observations (in the case of 'CUTE').

All test cases from the model evaluation exercises conducted by COST Action ES1006 for continuous and puff releases in built-up environment reveal a general tendency of better agreement between model results and measured concentrations with increasing model complexity (Baumann-Stanzer et al., 2015). In practice, confidence lines are often added to the results of Type I models to account for uncertainties e.g. due to unknown wind direction fluctuations. An example is shown in Figure 2. In this case from the Michelstadt experiment, it is obvious that these standard confidence lines are not sufficient to cover the area reached by the plume in these complex urban surroundings. The release takes place in a large square. The wind tunnel measurements indicate that a large part of the plume is deflected into streets perpendicular to the main flow direction. Significant concentration values are observed south of the outer confidence lines of the model result shown on the left side of Figure 2. Based on cases with different source locations in the Michelstadt and CUTE experiments, Baumann et al. (2015) demonstrate that if the release is located inside a street canyon or a courtyard, an appropriate description of the building geometry becomes fundamental for reproducing the plume dispersion due to plume splitting and deflection. In these cases, more advanced models are clearly preferable.



Figure 2: Maximum tracer gas concentrations near ground (shaded areas) and wind direction confidence lines calculated with a Type I model (left) and from wind tunnel measurements (right: average concentration values at receptor points) for a continuous release scenario in the Michelstadt experiment.

Figure 3 presents scatter plots of simulated and measured mean dosages at receptor points from puff releases separated according to the model types defined in Table 1. The figures on the left side represent comparisons between simulated and observed mean dosages from the Michelstadt experiment, the figures on the right side those from the CUTE experiment.



Figure 3: Mean dosage values caused by puff releases in 'Michelstadt' (left) and in the 'CUTE' experiment (right) simulated by models of the three types (Table 1) compared to wind tunnel measurements at all available receptor points in a non-blind model evaluation exercise.

In both experiments, the Type I model results underestimate the measured mean dosages at most receptor points which were situated at places where a significant impact by the plume is expected in the experiments (upper pictures in Figure 3). The model results are even of about one order of magnitude less than the measurements. This is especially relevant in the context of emergency response planning as a conservative approach ('on the safe side') is usually preferred. Thus, these model results might be misleading when used as basis for emergency response planning in urban surroundings. Even the use of additional thresholds to account for these uncertainties is not sufficient as was explained before.

Both model evaluation exercises reveal that the agreement between model results and measurements increases significantly when the impact of obstacles on the flow is considered by empirical approaches (Type II) and even more if simulated prognostically (Type III). This is shown qualitatively by scatter plots as well as quantitatively by means of statistical metrics by Baumann-Stanzer et al. (2015).

In the 'CUTE' model evaluation exercise, the variability of puff releases due to the natural variability in the turbulent flow field was studied. For this purpose, 20 to 25 puff realizations were simulated with two different approaches of large eddy simulation. In the wind tunnel, data from at least 200 consecutive releases were collected for each measurement location in order to ensure sufficient statistical representativeness of the puff dispersion results. The resulting distribution of mean dosages and of peak concentrations at one single receptor point for one puff release scenario are depicted as histograms in Figure 4. For other receptor points, the histograms look different and the relative accuracy of the two LES models varies. This demonstrates that a single realization is not sufficient to correctly catch and characterize puff releases, and a statistical analysis of a larger number of releases is necessary.



Figure 4: Distribution of predicted and measured dosage (left), peak concentrations (right) at one receptor point from measurements and two LES models.

Dealing with accidental releases in real-time, it is at present not possible to account for this kind of intrinsic variability in a quantitative manner. This implies that the results of a single model run need to be used with the awareness that they cannot represent such variability and its related uncertainty.

2.2 Regional-scale modelling of hazardous releases

A comparison of Type I and type II model results for fictitious release scenarios from European nuclear power plants based on identical meteorological input data revealed that higher agreement is found in most cases within one class of model type. In the example depicted in Figure 5, the plumes simulated with Type I models stays in rather narrow shape while transported around the eastern edge of the Alps. The Gaussian puffs follow the main flow indicated by the ECMWF forecast fields in this case. Both models are based on the approximation of a homogeneous, stationary flow field. In distances of more than 10 km, this approximation causes a significant increase of the model uncertainty. The application of these two models therefore usually is suggested only for the near field up to 10 km. These model approaches are in general not applicable in complex terrain, with highly variable surfaces, flow and turbulence fields.

In the Type II model results in the lower pictures of Figure 5, a significantly increased plume spread is found as soon as the plume reaches the Alpine area. This results in a larger affected area with lower maximum concentrations in Austria, Slovenia and Italy in this scenario. Emergency response planning based on Type I results would lead to different counter-measures in different areas than those based on the results of the more sophisticated models. All three Lagrangian models used in this model comparison study are operationally used for regional-scale emergency response modelling. It is recommended to prefer these or similar models instead of Gaussian or similar simplified approaches in the context of regional-scale emergency response modelling especially in areas where the flow might be influenced by orography.

Within this model comparison study, differences are found between the Lagrangian models especially concerning the vertical transport, dry and wet deposition (not shown here). Especially with changing wind conditions and strong vertical movement (frontal passages) the results in some cases differ significantly even between models of type II which are in principle using a very similar physical representation of the plume. In emergency planning, these differences can be interpreted as indicator for model uncertainty especially if model ensembles are available to the decision maker.



Figure 5: Near ground Cs-137 concentrations [Bqs/m³] integrated for the first 24 hours of a fictitious release at Dukovany on 6.7.2013 3UTC simulated with Type I models (upper pictures: ATSTEP and RIMPUFF) and with Type II models (lower pictures: DIPCOT, FLEXPART and ESTE).

3. Conclusions

Exemplary results of several model evaluation studies for atmospheric transport models for hazardous releases shown in this paper indicate that the model performance increases with increasing model complexity. Confidence lines added to simplified model estimates are not sufficient in complex surroundings. The use of Lagrangian models with flow models taking into account obstacles or even more sophisticated CFD or LES models are absolutely recommended for local-scale applications in this context. The same applies if the hazardous gas dispersion is relevant in the regional scale and topographical effects have to be considered.

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