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BEST PRACTICE GUIDELINES FOR THE USE OF ATMOSPHERIC DISPERSION MODELS AT LOCAL SCALE IN CASE OF HAZMAT RELEASES INTO THE AIR

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Abstract: The last decade witnessed noteworthy progress in both atmospheric dispersion modelling in industrial or urban environments and access to computational power. Although the problem is still challenging, there are now reliable methods for predicting the turbulent flow around the buildings in an uneven terrain and the dispersion and deposition of possibly toxic gases or particles following an accidental or malevolent release. Moreover, some of these Atmospheric Dispersion Models (ADMs) can produce operational information like exposure and dose indexes in a time consistent with crisis management when integrated in Emergency Response Tools (ERTs). However, most practitioners still have reservations about modelling in general or use over-simplified models which are neither accurate, nor systematically conservative. In an important step to bridge the gap between the scientists, model developers and emergency players (plant operators, first responders, public authorities...), COST Action ES1006 undertook the development of Best Practice Guidelines (BPG) for the use of ADMs and ERTs within the framework of emergency preparedness and response. This was deemed essential by experts in the Action for promoting the use of up-to-date models inside ERTs used by the practitioners. This paper presents an overview of the content and main conclusions of the BPG.

Key words: *atmospheric dispersion models, emergency preparedness and response, best practice guidance*.

INTRODUCTION

COST Action ES1006 dedicated to the “evaluation, improvement and guidance for the use of local-scale emergency prediction and response tools in case of airborne hazards in built environments” (called “the Action” in this paper) took place between 2011 and 2014. The activities were divided between Working Groups: WG1 aimed to catalogue the threats likely to impact an industrial site or an urban district, and the experiments and models devoted to the local scale atmospheric dispersion; WG2 aimed to benchmark the performance of various models when compared to wind tunnel and real scale experiments; and WG3 was an application oriented sub-project aiming to bridge the gap between model developers and end-users.

A key output from the Action was a document entitled “Best Practice Guidance” (BPG) produced by Working Group 3. These guidelines apply to the usage of Atmospheric Dispersion Models (ADMs) and Emergency Response Tools (ERTs) in support of decision-making in an emergency involving the release of hazardous materials (“hazmat”) into the atmosphere. The following paper strives to (1) exemplify the differences in modelling the same situation using different types of models, (2) explain and briefly illustrate what can be found in the BPG, and (3) summarize the conclusions drawn by the BPG experts.

WHY IS IT CRUCIAL TO USE UP TO DATE DISPERSION MODELS?

In the framework of the Action, questionnaires were distributed to first responders and stakeholders in several European countries with the objective of identifying their perception of, use of, needs and requirements for ADMs in ERTs. According to some of the responses, the available ADMs are perceived as having low accuracy and significant limitations due to lack of confidence in the input data, lack of modelling of critical phenomena, and lack of standardization in the application of modelling procedures. Several stakeholders did not trust ADM results unless they were presented along with *in-situ* measurements. From these statements, it was clear that there was a huge gap between the stakeholders' perception or state of mind regarding ADMs, the present capabilities of the models, and the efforts of developers to verify and validate model results and adapt ADMs to the practical needs of first responders and decision-makers.

On one side, considerable progress has been made in the last decade on parameterizing physical processes and implementing efficient numerical methods in ADMs. Advanced "4D" models are now available, that enable scientists and engineers to produce realistic and accurate simulations of the air flow and the dispersion. Moreover, the results of these models may be post-processed to provide operational results (danger zones, intervention zones...) when ADMs are integrated in ERTs.

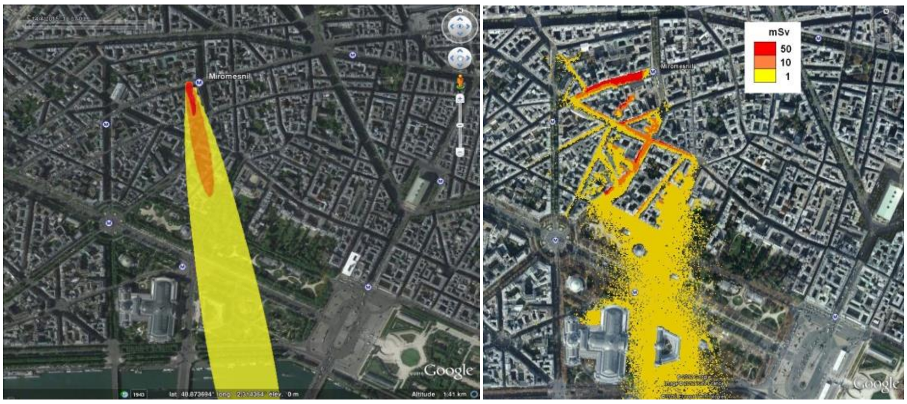
On the other side, most of the first responders and decision makers still use or are provided with the results of simplified models which ignore the local effects of the topography and obstacles such as buildings, and so are not adapted to application in built-up environments. Even when the time constraint is not as stringent as in an emergency, ADMs used by risk assessors and, in general, by stakeholders to establish consequence assessments, emergency planning and management procedures or even urban planning are often over-simplified and do not accurately represent dispersion in complex urban or industrial environments.

It is indisputable that different models are far from being equivalent as illustrated by the Figures 1-a) and 1-b) which were produced by the French Atomic and alternative energies Commission (Armand et al., 2013) as part of a fictitious "dirty bomb" exercise organised with Paris Fire Brigade. Figures 1-a) and 1-b) show the total effective dose (for an adult) predicted due to the hypothetical dispersion of 10 TBq of cobalt-60 in Paris city centre (8th district) following explosion of the dirty bomb The dose is representative of the radionuclide integrated concentration in a horizontal plane near ground level. The 3D computations were done in real time using dispersion solvers implemented in the CERES® CBRN-E (CEA modelling and decision-support system): a Gaussian puff model Figure (1-a) and a Lagrangian Particle Dispersion Model coupled to a diagnostic flow model (influenced by the buildings) Figure (1-b).

The differences between the model solutions are obvious. The simple Gaussian model which ignores the obstacles predicts a simple dispersion downwind. However, the diagnostic wind field and LPDM model predicts the dispersion to be strongly influenced by the street network, and concentration gradients between the sides of some streets can be seen as the upwind propagation of the contaminant. What is not visible in the figures is that the plume travel time through the domain and its residence time in the streets is also much longer when predicted by the LPDM.

In this fictitious situation developed for emergency preparation training, the results were not of course compared against measurements. However, the LPDM embedded in CERES® CBRN-E was validated in the frame of the Action WG2 (Duchenne et al., 2016). These demonstrate that that the LPDM results are more realistic and relevant than the Gaussian ones. Moreover, they also demonstrated as shown here, that the Gaussian model is not systematically conservative contrary to the widespread belief among first responders.

Finally, the computational time of the LPDM was no more than 10 minutes on an octa-core server, which is an acceptable duration to provide a more accurate and informative prediction of the dispersion and exposure. This example and many others provide evidence for why first responders and decision makers should use up-to-date flow and dispersion modelling, whether they undertake it themselves or receive it from scientific advisers.



Figures 1-a) and 1-b). Total effective dose due to the fictitious release of 10 TBq of ^{60}Co in Paris city center(emergency response exercise).Prediction by a Gaussian model (a) and by diagnostic flow and LPDM models (b).S is the source location.

THE JUSTIFICATION AND CONTENT OF THE BPG

Many human beings live in urban industrialized environments where both accidents and emerging threats (like terrorist attacks) may occur which lead to releases of hazardous materials into the air. While fortunately these events are quite seldom, they cannot be ignored. This is the reason why the COST Action ES 1006 focused on the threats to human life posed by hazmat releases in complex built environments. The most severe consequences of such events are likely to occur in the vicinity of the source and up to a few kilometres. At this local scale, it is critical to accurately model the dispersion and deposition of airborne materials in order to reliably assess the health effects on the population and first responders.

This provides the justification for the development and detailed verification and validation of the various kinds of atmospheric dispersion models. However it would be pointless to develop sophisticated dispersion models adapted to complicated environments that are unknown or not used by the people actually facing emergency situations (like the fire fighters, the representatives of public authorities, etc.). Thus, it was considered that to raise awareness the final part of the COST Action ES 1006 should try to establish the BPG for using different ADMs whether they were integrated or not into ERTs.

The BPG strives to organize guidelines with the aim of promoting effective and efficient knowledge transfer from the scientific community to plant operators, first responders, public local and national authorities, and all professionals routinely or occasionally involved in the preparedness and response to potentially hazardous dispersions of Chemical, Biological, or Radiological (CBR) species. The BPG is based on consideration of a range of ADMs and ERTs which have been used for a long time or are at the leading edge of the technology.

In order to establish a common understanding of the fundamental principles, the BPG identifies the key issues linking modelling and emergency preparedness and response. These issues relate to:

- The different types of ADMs, their main features, advantages and drawbacks;
- The position of the ADMs in the chain of assessment in ERTs;
- The estimation of exposure or dose indexes (giving an assessment of the health consequences) produced by post-processing the outputs of ADMs;
- The reference threat scenarios identified by the Action to illustrate the potential use of ADMs and ERTs;

- The people involved in the different phases of the response (risk assessors, experts, emergency responders, decision makers…), their roles and their interest in ADMs and ERTs;
- The results provided by ADMs which can be used in an operational situation and distributed to the emergency responders and / or decision-makers (danger zones, intervention zones...).

As an illustration, Figure 2 presents a simplified organizational diagram applicable to a radiological or chemical emergency involving an accidental or deliberate hazmat release. While national peculiarities might exist in the organization, it appears that as different as an accidental and a terrorist attack are, the organisation of the emergency response is likely to be similar. Figure 2 identifies the points at which the use of ADMs and ERTs may assist during the course of an emergency. For example, at field level, they may support the operational decisions of emergency responders. At local or intermediate level, they may provide information to better understand the situation and anticipate its evolution. At the highest decision making level, the results can be used to better handle the emergency and communicate with the population.

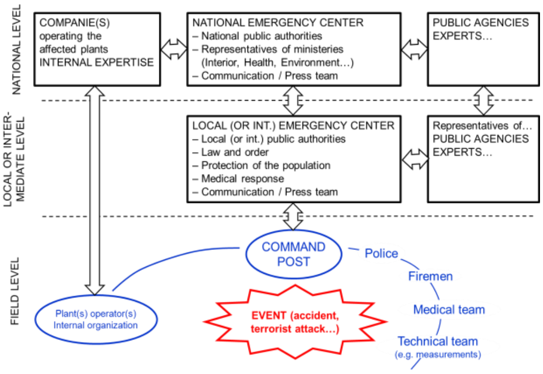


Figure 2. General sketch-up of the organization for handling an emergency.

Atmospheric dispersion models require meteorological inputs which may be observations and / or provided by flow models. Flow and dispersion models are connected, and the Action identified the general types of models listed in Table 1 and their typical execution times.

The BPG points out that ADMs and ERTs can provide supporting information whether the releases are long (some hours for continuous releases) or short (some seconds or minutes for puff releases) as, in the latter case, the end of the release is definitely not the end of the crisis.

Table 1. The classification by types of flow and dispersion models with their typical execution times (on adapted computational resources, e.g. a basic laptop for type 1 to a large workstation for type 3).

Model type	Flow model	Dispersion model	Execution time
1	No computation of the flow	Gaussian plume / puff model standard or with possible sophistication taking account of buildings	Seconds to minutes
2	Resolution of the flow with simplifications (limited set of equations and / or semi-analytical relations around the buildings…)	In general, Lagrangian particle dispersion model	Minutes to hours
3	Resolution of the flow around the buildings with the complete set of equations (CFD methods such as RANS or LES)	In general, Eulerian transport and dispersion model	Hours to days

Experts commonly agreed that throughout the emergency, a major challenge for the actors is to have the best possible representation of past events and the anticipated evolution of the situation. In this regard, the BPG highlights that even if the nature of the release is not precisely known, a preliminary flow and dispersion computation is instructive. A realistic calculation performed during the early stages of an emergency can provide useful information regarding features of the dispersion that may occur in complex industrial or urban environments that are not intuitive. This information can be valuable to decisions regarding the intervention of rescue teams, even if the exact concentration levels are not yet known.

A new aspect was also to give recommendations on ADMs or ERTs use from different perspectives:

- The first one takes account of the available level of information regarding the complexity of the situation, the environmental data, the release source, the meteorological input and all features of the event. This is related to the available models and computational resources, resulting in a proposal for a harmonized response-practice procedure and flow of actions (see the companion paper Herring *et al.*, 2016).
- The second one considers and separates the successive pre-event, event, and post-event phases of the emergency, the operators of the ADMs or ERTs and the final users of their results with the goal of answering the questions: "what to produce, when, and for whom?"
- The third one makes use of the relevant threat scenarios identified by the Action to give practical guidelines in case of (i) a neutrally buoyant release exemplified by the release of a small amount of chlorine within an urban area, (ii) a positive buoyancy release, as exemplified by a toxic plume produced by a fire in a warehouse, (iii) a dense gas release, exemplified by the leakage of many tonnes of (pressurized) chlorine or LPG, involving the flashing and pooling of material, and (iv) a "dirty bomb" that produces an explosive release of radionuclides.
- The fourth one is based on the results of the three model comparison exercises conducted by the Action, reported in "ES1006 Model Evaluation Case-Studies" (Baumann-Stanzer *et al.*, 2015) and summarized hereafter (see also Trini Castelli *et al.*, 2014; Baumann-Stanzer *et al.*, 2014).

Comparisons between ADM predictions and data from the Michelstadt and CUTE wind tunnel experiments in the Action showed that model performance increased with model complexity (i.e. a higher level of physical description). The improving performance trend was observed qualitatively from scatter plots, quantitatively by comparing the validation metrics, and from examination of scatter plots created for the set of ensembles produced by averaging over all results for a given model type. The type 3 CFD models were in general superior to the type 2 Lagrangian stochastic models and the type 1 Gaussian models (some of which were limited to modelling continuous plume releases).

Computational times are different for each model type as indicated in Table 1. Type 3 models typically involve long computation and preparation times and are not readily applicable during the emergency phase where a quick simulation is required. Type 2 models are usually significantly faster than type 3 ones and render a satisfying agreement with measurements that suggests they can be used with a reasonable level of confidence. A possible way to reduce the computational time for type 3 models is to provide access to pre-processed meteorological data that is statistically representative of the typical conditions at the site of interest. This would save time in generating the meteorology, and an answer could be obtained quickly because it is only necessary to undertake the dispersion modelling.

Whatever the model, the availability of proper inputs plays a crucial role for obtaining reliable results. As seen from the sensitivity analyses, the more detailed these are, the better the models perform. Nevertheless, the models appeared robust even when dealing with poor driving information, as will be the general case following accidental releases. Thus, they are valid tools to support the handling of emergencies and can be applied with reasonable confidence, even considering the uncertainties when dealing with unexpected situations.

The choice of the modelling approach involves a balance between the model performances, its reliability, and the run-time effort. Different modelling approaches can be used in different phases of the response process: the preparatory phase, the emergency response phase and during a post-accidental analysis. However, another criterion to be considered when making decisions on what modelling tool to adopt.is that a fast but inaccurate model output can compromise the effectiveness of a response action.

In its final part, the BPG addresses commonly asked difficult questions such as:

- How to deal with the uncertainties of the input parameters (source term, meteorological data…)?
- How to produce reasonably conservative results?
- How to overcome different results obtained by different models or operators?
- How to reconcile the modelling results and the field measurements?
- How to reconcile the needs and demands of the emergency players? Etc.

The reader is referred to the BPG for the answers to these given by the group of experts.

While it is essential to provide exposure or dose indexes since they are the practical measurement of the risk and cannot be ignored, it was beyond the scope of the Action to study the health and environmental impacts of hazmat releases. There is on-going research work whose aim is to improve the existing methods and the parameterisations associated with them. These topics are not covered by the Action and the BPG does not discuss the methods or parameters used to convert concentrations into exposures or doses.

The aim of the BPG is to provide a comprehensive yet focused document giving essential information for potential users in a straightforward manner. For this reason, the most important aspects of the guidance are summarized, while the reader is referred to other documents prepared in the frame of the Action for in-depth analysis. These include the Background and Justification Document, the Models and Emergency Response Tools Inventory, the Threats and Scenarios Catalogue, the Model Evaluation Protocol for Emergency Response, and the modelling exercises and inter-comparisons conducted by the Action (www.elizas.eu).

CONCLUSIONS

A summary of the BPG statements and recommendations built on the consensus among the international experts involved in the COST ES1006 Action is as follows:

- The use of ADMs in an emergency response does not correspond to the state-of-the-science of the 4D dispersion modelling in complex environments and more efforts should be done to promote the use of up-to-date models for emergency preparedness and response.
- Simple Gaussian models are still the models most often used for risk assessment and emergency response. These models do not resolve the detail of local-scale dispersion and without enhancements to predict dispersion in industrial or urban built environments may provide misleading outputs. Moreover, contrary to a common opinion of stakeholders, these models do not always provide conservative results.
- Simple Gaussian models might be advisable only on condition that they take account of buildings in some simplified way and are applied in the configurations for which they have been established.
- Lagrangian models taking account of the buildings may give accurate results in the order of 10-30 minutes with moderate computational resources. Input turbulent flow data models including buildings effects may be provided on-line by diagnostic flow or by CFD RANS models with some approximations, or off-line by pre-computed and tabulated CFD approach (RANS or LES).
- Eulerian models with the same input turbulent flow data as for Lagrangian models may be used when they are able to meet the time constraints of the event phase (although it is more practical to apply them in the pre- or post-event phases than in the emergency phase).

The Action identified the necessity for scientists and modelling experts to be engaged with the stakeholders, as this is a major condition for ensuring that the results from ADMs or ADMs results are trusted, and thus used by emergency responders and decision makers. It means that the development of ADMs in ERTs should not solely respect scientific criteria (like verification and validation), but also meet practical criteria (about the response time, interface, outputs, etc.). R&D in the field of atmospheric dispersion and health impact assessment should not only focus on physical modelling, but also consider the adequacy of the decision-support tools to meet the needs of the user organizations and civilian security missions. It seems to the experts within the Action that this approach is essential to promote the usage of state-of-the-art models inside the operational computational tools used by practitioners.

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