EFFECTS OF RELEASED HAZARDOUS GASES (EFRHA) MODEL: DEVELOPMENT AND VALIDATION

Richard Tavares[1] *and Ana Isabel Miranda*[2]

[1]Hydrodynamics, Energetics and Atmospheric Environment Research Laboratory, Institute of Research in Urban Sciences and Techniques, École Centrale de Nantes, Nantes, France
[2]Centre for Environment and Marine Studies & Department of Environment and Planning, University of Aveiro, Aveiro, Portugal

Abstract

The renewed concern in assessing consequences from technological hazards in industrial and urban areas continues emphasizing the development of local-scale consequence analysis (CA) modelling tools able to predict short-term pollution episodes and exposure effects on humans and the environment in case of accident with hazardous gases (hazmat). In this context, this work presents the development and validation of the EFfects of Released Hazardous gAses (EFRHA) model. This integrated CA modelling tool is designed to simulate the outflow and atmospheric dispersion of heavy and passive hazmat gases in complex and build-up areas, and estimate the exposure consequences of short-term pollution episodes in accordance to regulatory/safety threshold limits. Five main modules comprising up-to-date methods constitute the model: meteorological, geo-information, source term, dispersion, and effects modules. Different initial storage/transportation physical states and accident scenarios can be modelled. Considered EFRHA's main core, the dispersion module comprises a shallow layer modelling approach capable to account the main influence of obstacles during the hazmat gas dispersion phenomena. The validation exercise of EFRHA modelled results shows the consistent description of ambient conditions, hazmat gas release and dispersion variation. Dispersion modelled results were compared against measurements observations for different release and dispersion conditions. An acceptable agreement was obtained, demonstrating its capability to reasonably predict hazmat gas accidental release and dispersion in industrial and urban areas. Overall the work shows that EFRHA model can be used as a straightforward tool to support CA studies for training and planning, as well as to support decision and emergency response in case of hazmat gases accidental release in industrial and built-up areas.

Key words: *Accidental release, atmospheric modelling, consequence analysis, hazardous gases*

INTRODUCTION

Although not considered an everyday phenomenon, accidents involving the release of hazardous gases (hazmat) are continuously reported worldwide with significant impacts on human health and environment, which has led to an increased awareness of the consequences from exposure to hazmat released into the atmosphere in industrial and urban areas over the last decades. This renewed concern in assessing consequences from technological hazards, gave numerical tools a unique value and large efforts have been taken in the development and implementation of local-scale consequence analysis (CA) modelling tools able to predict short-term pollution episodes and exposure effects on humans and the environment in case of accident with hazardous gases (hazmat) (Tavares R., 2011). The intent to understand and numerically describe the various stages of accident scenarios involving the outflow, dispersion and consequences of hazmat gases accidental releases, continues emphasizing the development of new and more accurate modelling techniques. Despite the variety of existing CA modelling tools/software packages, most of these comprise either simple modelling approaches that cannot properly represent the actually occurring real conditions in industrial and built-up areas, or complex modelling systems that turn the tool powerless to provide fast response information (*see* Mannan S., 2005; Hanna S.R. *et al*., 2008).

Endorsed by the continuous improvements on computational hardware capacity, state-of-the-art modelling techniques, reviews and/or guidelines for hazmat gas release and dispersion modelling, the EFfects of Released Hazardous gAses (EFRHA) model was developed and validated. This integrated CA modelling tool was designed to predict short-term pollution episodes in case of hazmat gas accidental release and dispersion into the atmosphere in industrial and built-up environments.

OVERVIEW OF EFRHA MODEL

Aiming to overcome some of well-known constrains of existing CA models/software packages, the EFfects of Released Hazardous gAses (EFRHA) model was developed to predict short-term pollution episodes and consequences from accident scenarios involving the release and dispersion of hazmat gases in industrial and urban areas. EFRHA's design kept a compromise between the simplicity of simple dispersion models and an increased modelling capability to account the influence of obstructions on dispersion, even considered a 'non-CFD model', according to Britter R. and Schatzmann M. (2007).

Five main and interdependent modules comprising up-to-date methods/models, usually applied separately in the various CA modelling elements, constitute the model: meteorological (EMM), geo-information (EGIM), source term (ESTM), dispersion (EDM), and effects/consequences (EEM) (see Figure 1).

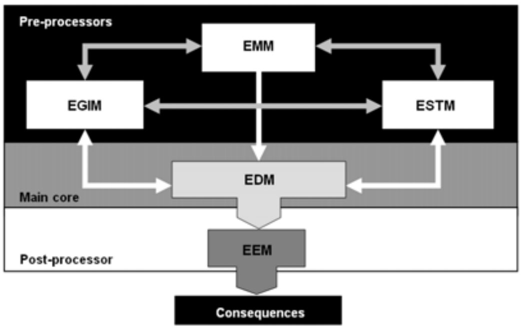

Figure 1. Schematic representation of EFRHA modules structure and data flow along the simulation process.

The organization of the modules follows the needs of information processing flow, to properly describe hazmat gas accident scenario release and dispersion phenomena, without forgetting the influence of surrounding environment. Considered the main core of EFRHA model, EDM is supported by additional related models integrated in the form of pre- (EMM, EGIM and ESTM) and post- (EEM) processors. The EMM is designed to numerically describe the atmospheric boundary layer (ABL) conditions based on the quantitative Monin-Obukhov Similarity Theory approach. Surface momentum and energy fluxes relationships and the logarithmic profile for mean wind profile with an adjustment for diabatic flows are implemented in EMM algorithm. Topographical, land-use and obstructions data, in addition to, receptors and sources spatial distribution are processed in EGIM. Accounting for Geographical Information System tools formats, a regular Cartesian coordinate system is assumed, in which, regular and discrete gridded data can be used to characterize terrain, receptors and sources. In case of obstructed areas, quasi-steady-state average gridded wind fields are estimated based on the Diagnostic Wind Model principles (Douglas S. and Kessler R., 1990). Mean wind fields are adjusted based on the obstructions spatial distribution and a divergence minimization is performed to ensure mass conservation. Different initial storage/transportation physical states and accident scenarios can be processed in ESTM to numerically describe hazmat gas outflow. Instantaneous, continuous and transient release phenomena can be defined, as well as different initial hazmat physical state and scenario conditions (compressed gas, non-boiling liquid, two-phase pressurized liquefied gas (PLG), and evaporation of liquid pool).
Considered the *main core* of EFRHRA model, EDM comprises an up-to-date Shallow Layer modelling approach to quantitatively describe the hazmat passive and dense gas transport and dispersion phenomena on simple or complex topography. The EDM modelling approach is based on the TWODEE-2 model (Folch A. *et al*., 2009). Shallow water equations are adapted to predict hazmat gas cloud behaviour during the dispersion phenomena. Assuming an incompressible homogeneous fluid behaviour and a hydrostatic pressure distribution, shallow water equations are adapted to hazmat gases having a non-uniform vertical profile as given by Hankin R. and Britter R. (1999). Predicted the 2D hazmat concentration fields as a function of time, potential consequences on human health from the exposure to levels of hazmat gas concentration of concern are predicted in the EEM post-processor. Direct comparisons between simulated concentrations fields and reference safety threshold limits are performed to determine threat and damage temporal and spatial distribution, according to the application purposes and post-processing options.

EFRHA’s main outputs can be presented in different formats, from summary text files to table information, as a function of time and/or spatially distributed data to make the format compatible with other visualization and plotting tools. Concentration and exposure consequence (threat) contour maps can be generated at different periods. Additionally, time evolution of gas concentrations for specific spots of interest and peak concentrations can be graphically plotted. If spatial distribution of population is available, a direct overlap of information allows estimating the total number of people (potentially or effectively) exposed to certain levels of hazmat gas concentrations after the accident event.

VALIDATION OF EFRHA MODEL

Qualitative and quantitative analyses validation techniques suggested in the *Model Evaluation Guidance Protocol* (MEGP) (Britter R. and Schatzmann M., 2007) were applied to evaluate EFRHA aptness to produce quality assured results, but also to identify its main features and weaknesses. A preliminary individual analysis of EFRHA’s pre-processors outputs was carried out (see Tavares R., 2011), showing the consistent description of ambient meteorological and terrain conditions, as well as, the variation of the hazmat gas release phenomenon. To evaluate EFRHA’s performance in its entire scope, the model was applied to the set of Validation Test cases (VT) summarized in Table 1. Well-established full-scale field experimental test trials: Thorney Island (TI), Burro (B) and Desert Tortoise (DT) trials, extensively used in model validation studies were selected based on reviews and databases (see Mannan S., 2005).

Table 1. Overview of experimental data sets considered in EFRHA model validation exercise

ID	Test Trial	Substance	Spill Flow (kg/s)	Duration (s)	Release Type	Meteorological Conditions
VT1	TI 8	Freon12-N_2	3967.0	1.0	Puff	T_a = 17.2 ºC; P=1 bar; u_{ref} = 2.4 m/s; class D
VT2	B 3	LNG	88.0	167.0	Pool	T_a = 33.8 ºC; P=0.94 bar; u_{ref} = 5.4 m/s; class B
VT3	DT 3	Ammonia	133.0	166.0	Jet	T_a = 17.2 ºC; P=1 bar; u_{ref} = 2.4 m/s; class D

Concentration fields were predicted at the lowest level of measurements (between 0.4 and 1.5 m high from the ground level) to maintain a somewhat consistency in the analysis, but also, corresponding to ‘normal heights of exposure to hazmat gases’. To demonstrate the overall findings, time evolution and quantile-quantile plots, in addition to quality metrics estimated using the statistical BOOT Software (Chang J.C. and Hanna S.R., 2005) were analysed, based on direct comparisons of modelled against measured peak concentrations at the sensors locations. Figure 2 presents time evolution plots of modelled and measured peak concentrations during the initial 500 s after the release start.

Overall, modelled peak concentrations follow the behaviour and ranges of measured values. VT1 and VT2 simulated results tend to substantially approximate to, and in some instants nearly overlap, observations during the analysed period of time, despite the overestimation tendency in a large fraction of the simulation periods, excepting in VT3 plot. Notwithstanding the deviations, modelled outputs highlight EFRHAs capability to predict different release and dispersion conditions in a reasonable way. VT1 modelled peak concentrations overestimation tendency in the initial 30 s is mainly due to the implemented modelling approach for the definition of hazmat gas instantaneous releases, in which it is assumed that a nearly cylindrical cloud is already formed in the initial instant. This will result in the direct estimation of the ‘overlapping’ initial peak concentration, even if in reality did not reached the measurement sensor. Nonetheless, simulated values clearly approximate to measurements during a large fraction of time. VT2 outputs evidence the overestimation of peak concentrations decay, showing that the assumption of a continuous release may not be the most correct for further estimation of evaporation rate, even so, the lack of precise information of evaporation rate, duration and other relevant information disables the evaluation of accuracy and consistency of modelled outflow results. When analysed a vapour jet release (VT3), simulated concentrations tend to underestimate measures after 250 s. Still, it is evident that initial increase of peak concentration values shows a substantial closeness to measured data. The analysis of VT test cases time evolution plots shows the reasonable agreement between simulated and measured peak concentrations for various typifying conditions.

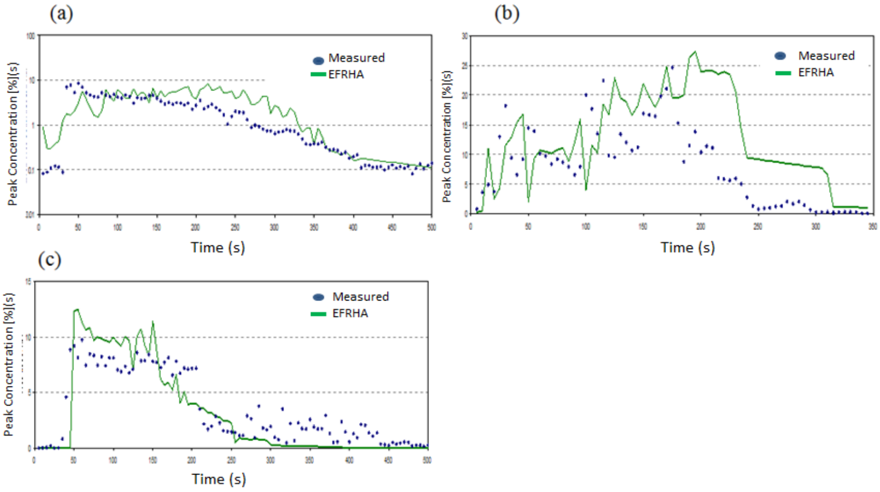

Figure 2. Comparison of measured and modelled peak concentrations [%vol/vol] time evolution at plume centreline for (a) VT1, (b) VT2 and (c) VT3 test cases runs during the initial instants after the release.

A more detailed evaluation of the level of correlation between measured and modelled ranges of values was performed through the analysis of the unpaired point-by-point quantile-quantile plots (see Figure 3).

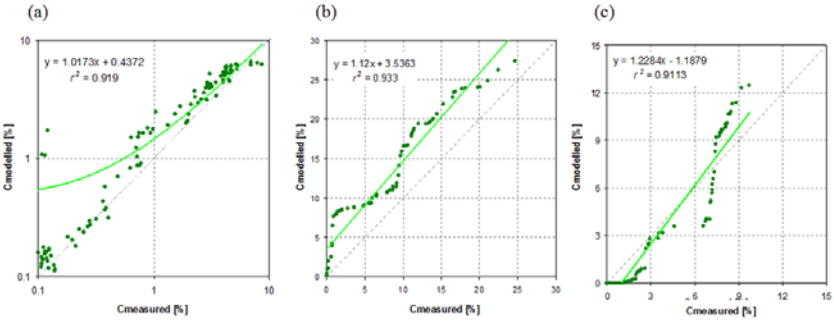

Figure 3. Quantile-quantile plots of modelled results against measurements concentrations [% vol/vol] for set of (a) VT1, (b) VT2 and(c) VT test cases.

Figure 3 highlights the relatively good correlation with experimental observations, demonstrating the capability to estimate the ranges of measured concentration values, despite the general overestimation (VT1 and VT2) and underestimation (VT3) tendencies. As evidenced by the estimate linear trend lines r^2, the analysed test cases present a reasonable correlation degree with measured observations. The punctual strong underestimation of some lower concentration measurements in VT1 reflects the strong influence of the cylindrical hazmat gas cloud shape at the initial instants. In VT2 it is noticeable a larger overestimation for lower and higher concentration values, whereas it is noted the underestimation of VT3 medium concentration values, caused by reaching null values before measurements records.

Paired and unpaired point-by-point quality metrics were estimated and the results (see Table 2) analysed. In general quality metrics satisfy or are close to the acceptance criteria; demonstrating EFRHA’s reliability to provide acceptable results when applied to set of VT test cases. FB results clearly demonstrate and corroborate previously observed overestimation tendencies, particularly in VT1. The positive FB value of VT3 reflects the underestimation trend, influenced by the negative deviations of lower and intermediate concentrations. FAC2, acceptance criteria is satisfied, except for VT3 that presents a value relatively close. NMSE acceptance limits are satisfied, and if combining with FB, NMSE, MG and VG values it is possible to say that, observed deviations are mainly caused by systematic errors. As regards to the unpaired quality metrics it is also possible to observe relatively small values, evidencing the previously good correlation between ranges of modelled and measured values.

Table 2. Summary of quality metrics for the set of DGD test cases

Run ID	FB	FAC2	NMSE	r	MG	VG	SB	SDSD
VT1	-1. 340	0.570	0.95	0.57	0.70	2.03	0.592	0.130
VT3	-0.240	0.506	0.66	0.56	0.43	8.71	0.170	0.100
VT5	0.121	0.450	0.36	0.84	1.95	2.72	0.160	0.810

Overall, qualitative and quantitative analysis of VT test cases quality metrics quantitatively shows EFRHA's reasonable capability to numerically reproduce the various phases of release and dispersion of hazmat gases. Moreover, despite some noticeable deviations, it is demonstrated the reliability to account different and typifying release conditions commonly analysed in the frame of CA studies.

MAIN CONCLUSIONS

Overall the work shows that EFRHA model can be used as a straightforward tool to support CA in the scope of training and planning, in addition to support decision and emergency response in case of hazmat gases accidental release in industrial and built-up areas. It also demonstrates the applicability of shallow layer as a plausible alternative to integral or complex CFD dispersion modelling approaches. From the performance validation exercise, acceptable agreement was obtained, showing the reasonable numerical representation of measured features. In general, quality metrics are within or close to the acceptance limits recommended for 'non-Computational Fluid Dynamics (CFD) models', demonstrating its capability to reasonably predict hazmat gas accidental release and dispersion in industrial and urban areas.

AKNOWLEDGEMENTS

The authors thank the financial support of Portuguese Ministry of Science, Technology and Higher Education, through the Foundation for Science and Technology, for the PhD grant of R. Tavares (SFRH/BD/22742/2005), and for the financial support of project INSPIRAR (PTDC/AAC-AMB/103895/2008), supported in the scope of the Competitiveness Factors Thematic Operational Programme (COMPETE) of the Community Support Framework III and by the European Community Fund FEDER. The authors also acknowledge the support of the European Science Foundation under the COST Actions 732 and ES1006.

REFERENCES

Britter R. and Schatzmann M., 2007: Model evaluation guidance and protocol. COST, Brussels.

Chang J.C., Hanna S.R., 2005: Technical descriptions and user's guide for the BOOT statistical model evaluation software package, version 2.0. 66 pp.

Douglas S. and Kessler R., 1990. User's Manual for the Diagnostic Wind Model. Eed. Carr, L. Volume III, EPA-450/4-90-007C, San Rafael, CA.

Folch A., Costa A., Hankin R., 2009: TWODEE-2: A shallow layer model for dense gas dispersion on complex topography, *Computer and Geosciences*, **35**(3), 667-674.

Hankin R. and Britter R.E., 1999: TWODEE: the health and safety laboratory's shallow layer model for dense gas dispersion. Part 1. Mathematical basis and physical assumptions, *J. Hazard. Mater*. **66** (3), 211–226.

Hanna S.R., Dharmavaram S., Zhang J., Sykes I., Witlox H., Khajehnajafi S., Koslan K., 2008: Comparison of six widely-used dense gas dispersion models for three recent chlorine railcar accidents, *Process Safety Prog*. **27**, 248–259.

Mannan S. (Ed.), 2005: Lees' Loss Prevention in the Process Industries. Hazard Identification, Assessment and Control, 3rd Edition, Vol. 1 - 3, Elsevier Butterworth-Heinemann, Oxford.

Tavares R., 2011: Accidental release of hazardous gases: modelling and assessing risk. PhD Thesis, University of Aveiro, Portugal.