H13-89

DISPERSION MODELING OF ACCIDENTAL TOXIC GAS RELEASES – A MODEL COMPARISON STUDY.

Sirma Stenzel[1], Kathrin Baumann-Stanzer[1]

[1]Central Institute for Meteorology and Geodynamics (ZAMG), Vienna, Austria

Abstract: Several air dispersion models are available for the prediction and simulation of hazard areas associated with accidental releases of toxic gases. The model packages (commercial or free of charge) include a chemical database, an intuitive graphical user interface (GUI) and automated graphical output. They are easy to use and can operate fast and effectively during stress situations. The models assist the emergency responders or decision makers through the 3 stages of the emergency management: preparedness, response and recovery (analysis) stage. Some models are furthermore used to prepare emergency response plans (intern or extern) meeting regulatory requirements such as the EEC Seveso Directive. Each model was developed with its strength and limitations and the choice of the proper model approach depends on the particulate demands.

For the purpose of the study the following models were tested and compared: ALOHA (EPA), MEMPLEX (Keudel av-Technik GmbH), Breeze (Trinity Consulting), Trace (SAFER System) and SAMs (Lohmeyer). The models are applied for a set of reference scenarios and the resulting hazard areas are compared. Key problems in coping with accidental toxic release are discussed.

Since the input requirements differ from model to model, and the outputs are based on unequal criteria for toxic area and exposure, a high degree of caution in the interpretation of the model results is required.

Key words: *hazardous gas releases, dispersion modelling, meteorological analysis.*

INTRODUCTION

In case of accidental release of hazardous gases in the atmosphere, the emergency responders need fast information about: the direction and the dimension of the gas dispersion and the area in which the optimal countermeasures should be taken. For assessing possible consequences (damages) and applying optimal countermeasures, calculations done with dispersion models can be used. The models are suited to modeling safety, accidents and emergency response scenarios.Models can be also used for the task to carrying out risk management, especially to prepare emergency plans and meeting regulatory requirements such as the EEC Seveso Directive. The plans are prepared by assessing a range of reference scenarios and estimating the final effects and damages taking into account typical weather conditions (worst weather scenarios), the chemical properties of the release substance and the sensitivity of a potentially exposed population.

The **research project RETOMOD** (reference scenarios calculations for toxic gas releases – model systems and their utility for the fire brigade) was conducted at the ZAMG in cooperation with the Vienna fire brigade, OMV Refining & Marketing GmbH and SyneX GmbH. RETOMOD was funded by the KIRAS safety research program at the Austrian Ministry of Transport, Innovation and Technology (www.kiras.at). The main tasks of the project were

- Sensitivity study and optimization of the meteorological input for modelling of the hazard areas (human exposure) during the accidental toxic releases
- Comparison of several model packages in respect to the utility for the fire brigades

Threshold values for toxic level of concern

A basic problem in coping with accidental toxic release is the relative width spectrum of values for toxic level of concern, like IDLH, ERPG, AEGL, MAK etc. and the different criteria for their application by the particulate emergency responders and organizations - Table 1 gives an example of the width spectrum of toxic level of concern values (threshold values) for ammoniac and chlorine. There is a number of research studies focusing on this problem, anyway the end decision is up to the authorities. The practical experience in disaster operations and exercises has shown that fire brigades and authorities prefer different assessment values. To improve the communication and cooperation between them therefore converting between the different values on hand will be helpful and on the other hand, standardization of the assessment values will be highly desirable.

Table 1. An example of the width spectrum of threshold values for ammoniac and chlorine:

Substance	IDLH (30min)	ERPG-1 (60min)	ERPG-2 (60min)	ERPG-3 (60min)	AEGL-1 (30min)	AEGL-2 (30min)	AEGL-3 (30min)	MAK TmW	MAK Kzw
Ammoniac [ppm]	300	*25*	150	750	30	160	1 600	20	50
Chlorine [ppm]	10	1	3	20	0,5	2,8	28	2	4
Conversion factor to IDLH		10-12	2 – 3,5	0,4–0,5					

Comparison of dispersion models for hazardous gas releases

For the optimization of the input data for simulating the dispersion of accidental released toxic substances is of essential interest to figure out, which input data have a crucial influence on the calculation result. The calculation of the chemical release and the dispersion of the released toxic gases are very complex because of the large number of unknown variables that influence the output. Each model requires a number of input parameters, some of them are relatively easy to identify (e.g. wind, roughness), others can be determined in a real case using only assumptions, and therefore with large uncertainties (e.g. released mass or size of a leak). When interpreting the model results these uncertainties must be taken into account.

For the purpose of this study the following models were tested and compared: ALOHA (Areal Location of Hazardous atmosphere, EPA), MEMPLEX (Keudel av-Technik GmbH), Breeze (Trinity Consulting), SAFER System, SAM (Engineering office Lohmeyer). The following software packages descriptions are based on the information provided by the manufacturer as well as personal experience with the program implementation in the frame of the project. For each model a table with the subjective estimations of the model (for better visualization of the model features for the firefighters) is included in the figures below. For the detailed investigation and comparison of software packages demo versions have been requested from the companies (in the case of commercial software).

MEMPLEX MET is distributed form the Switzerland firm Keudel av-Technik GmbH (http://www.memplex.com) and contains a detailed substance data base (inclusive first aid help) with several modules for estimation the hazard zones. The program was validated, based on several real accident cases (ISi Technologie GmbH, 2006). The model is easy to operate, robust and in operational use by many fire brigades as emergency response tool (inclusive Vienna Fire Brigade).

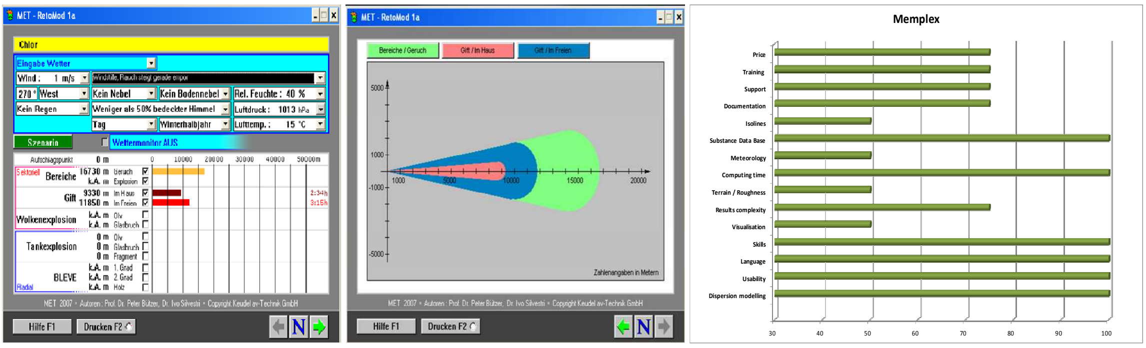

Figure 9.Example of Memplex input and result window and table with subjective estimations of the model (the estimations are given in percentage, where 50% means: satisfactory-, 75%: good- and 100%: very good represented from the model)

ALOHA (Areal Location of Hazardous Atmospheres) was designed in cooperation between the US National Oceanic and Atmospheric Administration (NOAA) and the US Environmental Protection Agency (EPA and NOAA, 2007, www.epa.gov). ALOHA is applied by first responders, fire fighters as well as for emergency planning and training. ALOHA is free of charge together with the chemical data base ***CAMEO*** and the visualization software ***MARPLOT*** (CAMEO's mapping program).

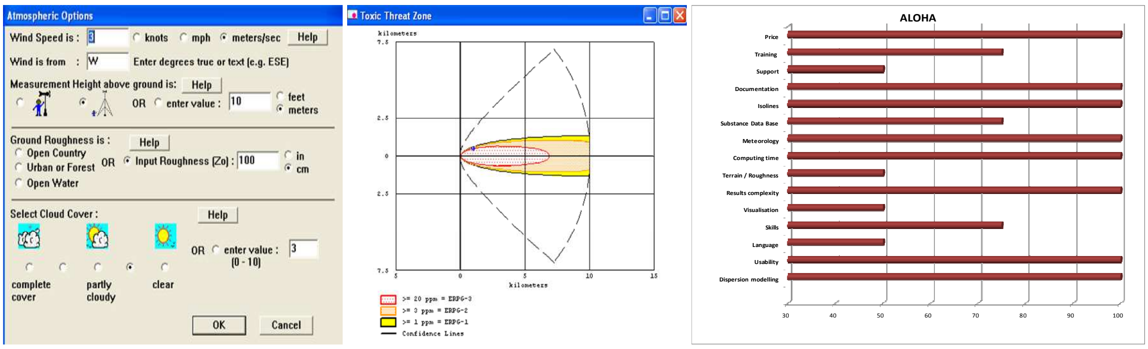

Figure 2. Example of ALOHA input and result window and table with subjective estimations of the model.

TRACE / Hazmat Responder: commercial software products from the American firm SAFER STAR ("System for transportation accident response"/ www.safersystem.com) with a full suite of product for planning and especially for real-time response to chemical emergency. TRACE (**T**oxic **R**elease **A**nalysis of **C**hemical **E**missions) is used for facility studies, emergency preparedness planning, meeting regulatory requirements and quantitative risk analysis studies. The model offers in addition a variety of applications such as: risk management planning, human response management, quantitative risk- and population exposure assessment. The model contains a consequence analyses enhancement, which allows to define the air changes per hour, population distribution and evacuation time and to evaluate the consequences of an accidental release on the surrounding community. HAZMAT Responder is the product for emergency response by dealing with place specific hazard accidents.

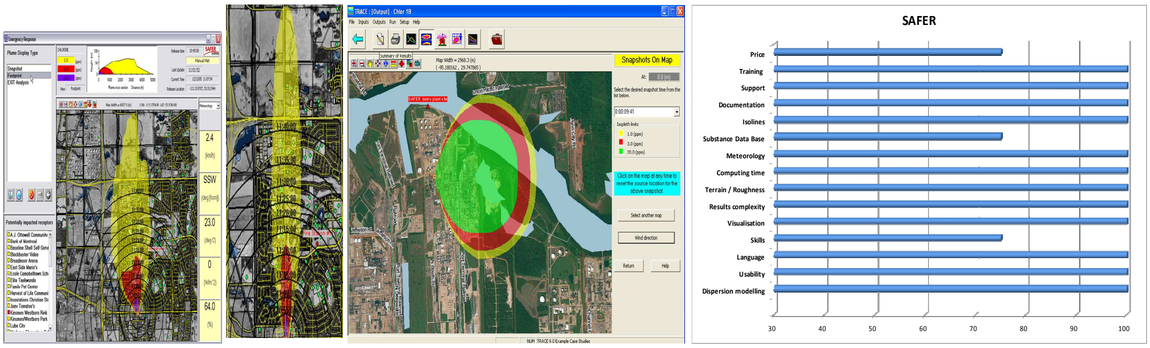

Figure 3 Example of TRACE/Hazmat Responder input and result window and table with subjective estimations of the model.

BREEZE HA is a commercial software package distributed by the environmental consulting firm Trinity Consulting (www.breeze-software.com). The products are used by environmental professionals to analyze the effects of air pollutant emissions and explosions. These models include all industry-standard dispersion models, developed or recognized by the U.S.EPA and many other environmental authorities (Trinity Consultants, 2004).

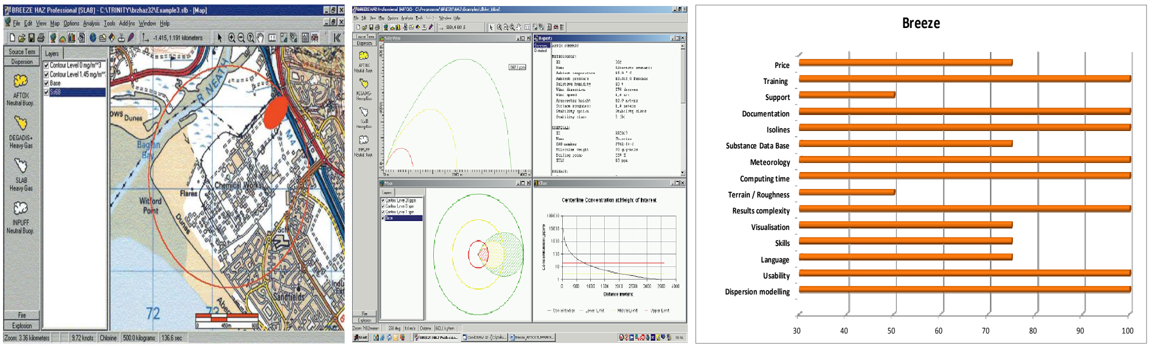

Figure 4 Example of Breeze input and result window and table with subjective estimations of the model.

SAM-S is commercial software from the German engineering firm Lohmeyer GmbH (www.lohmeyer.de) for real time simulations of the dispersion from the hazard substances after release from chemical plants or by transport accidents (Flassak T., W. Bächlin, H. Frantz, A. Lohmeyer, 2004). In the offered demo version the results are presented within Google Earth.

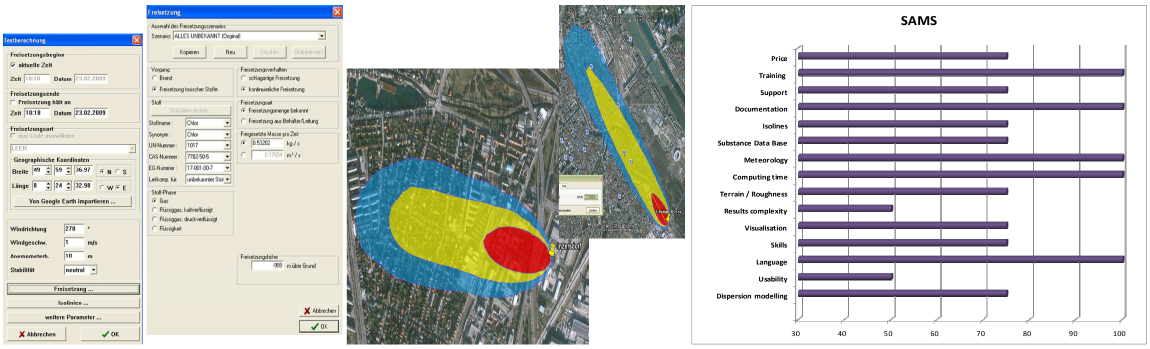

Figure 5. Example of SAM-S input and result window and table with subjective estimations of the model.

A reference scenario is defined as a scenario which is supposed reasonably likely to occur, and whose effects reflect the actual protection system implemented (Koining H., 1999). A set of reference scenarios for chlorine, ammoniac, butane and petrol were proceeded with the models above in order to predict and estimate the human exposure during the event. The models simulate the accidental release of the gases above and estimate the potential toxic areas and the calculated hazard distances are compared. The variations of the model results are measures for uncertainties in source estimation and dispersion calculation. Case 1 describes a train accident with wagon with chlorine, while in case 1A a wagon is accidently totally destroyed and the complete wagon volume evaporated from the built pool. In case 1B a continuous release from a leak takes place. Release scenarios: A= Puddle (instantaneous release), B= Leak (continuous release). By the selection of the scenarios a focus on the chemical agents of interest and input from the fire brigade practice was considered.

Table 2. A short overview of the reference scenarios for model comparison.

Scenario	Substance	Wagon	Volume [m^3]	Filling level [%]	Mass [t]
1	Chlorine	Railway car	30	90	40
2	Ammoniac	Railway car	95	90	55
3	Butane	Truck	17	70	7
4	Petrol	-	-	-	1

The model outputs, presented in the following figures, show that the dependence of the hazard distance on the atmospheric stability, wind speed and the roughness is mostly simulated from the models in the expected way. The calculated hazard distances differ partly to some orders of magnitude due to different input requirements as well as due to different internal model assumptions. None of the models is found to be ‘more conservative’ than the others in all scenarios. Not in all cases, the same models shows, the largest to, respectively the smallest hazard areas. Based on the individual case studies it cannot be generalized that a particular model is more "conservative" in contrast to the other models. Since the input requirements differ from model to model, and the outputs are based on unequal criteria for toxic area and exposure, a high degree of caution in the interpretation of the results is needed. More details can be seen at Baumann-Stanzer, K., Stenzel, S. (2010).

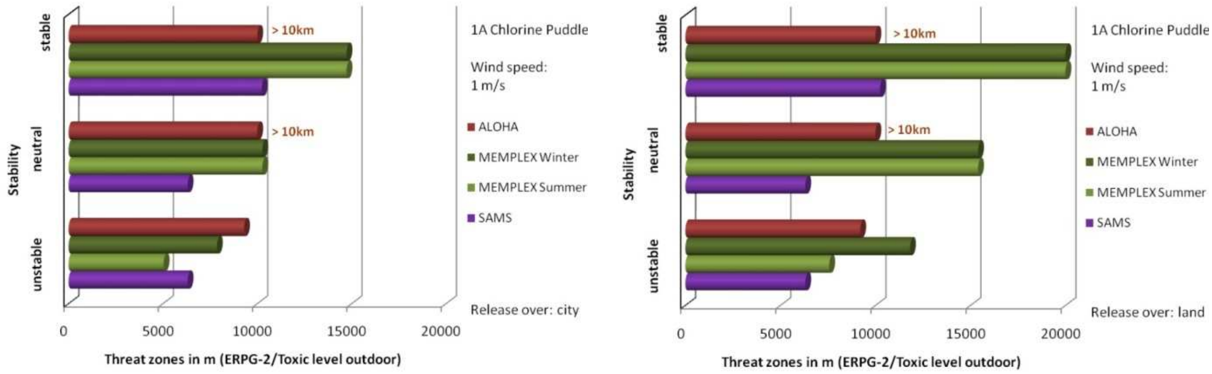

Figure 6. Comparison of the hazard distances for scenario 1A (release over city/land).

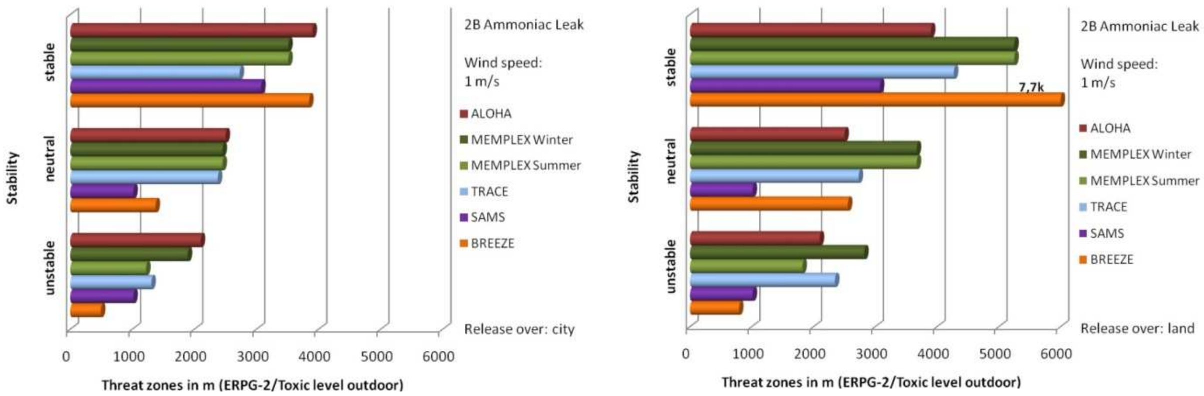

Figure 7. Comparison of the hazard distances for scenario 2B (release over city/land).

CONCLUSIONS

Modeling the release and dispersion of toxic gases requires a large number of input parameters. Some of these parameters are easy to identify. Others, in particular, information for determining the source, are subject of great uncertainty. Therefore (conservative) assumptions often have to be made, which tend to over-estimate the hazard zones. Since the input requirements differ from model to model, and the outputs are based on unequal criteria for toxic area and exposure, a high degree of caution in the interpretation of the model results is required - especially in the case of slow wind speeds, stable atmospheric condition, and flow deflection by buildings in an urban area or by complex topography.

The comparison of the calculated different models hazard distances for selected reference scenarios shows partly a relatively large variability. The differences in the model results are mainly due to different requirements on the input parameters but also on different internal model assumptions. The comparisons show that none of the models tend to more conservative results than the others. Based on the individual case studies, it cannot be generalized that a particular model is more "conservative" in contrast to the other models.

The five tested models offer a very clear user interface, but differ significantly in the demands on the user expertise and in particular regarding the outcome. With correspondingly higher complexity of the model calculations, the many uncertainties in the model outputs, resulting from inaccurate input parameters can be to some extent reduced. For this reason, for fixed industrial plants the application of complex model systems is recommended, which can consider environmental effects. In mobile applications, however, complex calculations that take into account terrain, buildings, etc. are not possible in the current state of technology. The use of a relatively simple and robust program, which deliberately requires only few input parameters, appears to be more useful in respect to the application by the firefighters in this case.

REFERENCES

Baumann-Stanzer, K., Stenzel, S., 2010: Uncertainties in modelling hazardous gas releases for emergency response. Meteorologische Zeitschrift, accepted.

EPA and NOAA, 2007: The CAMEO Software System ALOHA, User's Manual.

Flassak T., W. Bächlin, H. Frantz, A. Lohmeyer, 2004: Dokumentation SAM-S.

ISi Technologie GmbH, 2006: Modelle für Effekte mit toxischen und brennbaren Gasen (MET)

Koining H., 1999: Referenzszenarien zur Richtlinie 96/82/EG. Bericht im Auftrag des Bundesministeriums für Umwelt, Jugend und Familie, Wien.

Trinity Consultants, 2004: User's Guide for the BREEZE HAZ AFTOX, DEGADIS, SLAB, DISPERSION, FIRE/ EXPLOSION and PROFESSIONAL software packages.