

## H13-81 DISPERSION MODELING OF ACCIDENTAL TOXIC GAS RELEASES – SENSITIVITY STUDIES AND OPTIMIZATION OF THE METEOROLOGICAL INPUT

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**Abstract:** Dispersion modelling of accidental toxic gas releases is needed to analyze release scenarios (“worst-case scenarios”) for the preparation of emergency response plans as well as for real-time risk assessment and management.

Most hazard response models nowadays can be coupled directly to automatic meteorological stations. Additionally, the use of the observation-based analysis and forecasting system INCA (Integrated Now-casting through Comprehensive Analysis) for this application is discussed. In the frame of the project INCA data were compared with additional measurements conducted at two near-traffic sites in Vienna. INCA analysis and very short term forecast fields (up to 6 hours) are found to be an advanced possibility to provide on-line meteorological input for the model package used by the fire brigade.

Uncertainties in the meteorological input together with incorrect estimates of the source play a critical role for the model result. Sensitivity studies with the models TRACE (SAFER Systems) and MET (Keudel av-Technik GmbH) are presented. The influence of the following meteorological parameters is discussed: wind speed, atmospheric stability, air temperature, air humidity, precipitation, roughness length. The influence of the meteorological input on the hazard distance calculation furthermore depends on the chemical characteristics of the toxic release. Worst case weather scenarios for emergency response planning therefore are not necessarily the same for different toxic substances.

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

### INTRODUCTION

Whenever hazardous gases are accidentally or deliberately released into the atmosphere the emergency responders need fast information about the area involved and the maximum impact to be expected. Dispersion models are used to assess possible consequences (damages) and to support the planning of the countermeasures (e.g. protective equipment for the firemen, evacuation of people).

The research project RETOMOD (reference scenarios calculations for toxic gas releases – model systems and their utility for the fire brigade) was conducted by 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](http://www.kiras.at)).

The main tasks of the project were

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

### Comparison of INCA data with measurements

INCA (Integrated Now-casting through Comprehensive Analysis) is an observation-based analysis and forecasting system, created to complement classical NWP forecasts by providing improved forecasts at short lead times (very-short-range up to +12 hours). INCA is operationally computed with 1km spatial and 15 min (precipitation) to 1 hour temporal resolution (Haider *et al.*, 2007). INCA takes into account, as far as possible, all available data sources (ALADIN model results, station data, radar and satellite data, radio-soundings, AMDAR, etc) and uses them to construct physically consistent analyses of atmospheric fields.

The meteorological fields analyzed with INCA are:

- 3D: temperature, humidity, wind
- 2D: precipitation, cloudiness, global radiation

In the frame of the project INCA data are compared with measurements, conducted at two near-traffic sites in Vienna. INCA analysis is found to be an advanced possibility to provide on-line meteorological input for the model package used by the fire brigade.

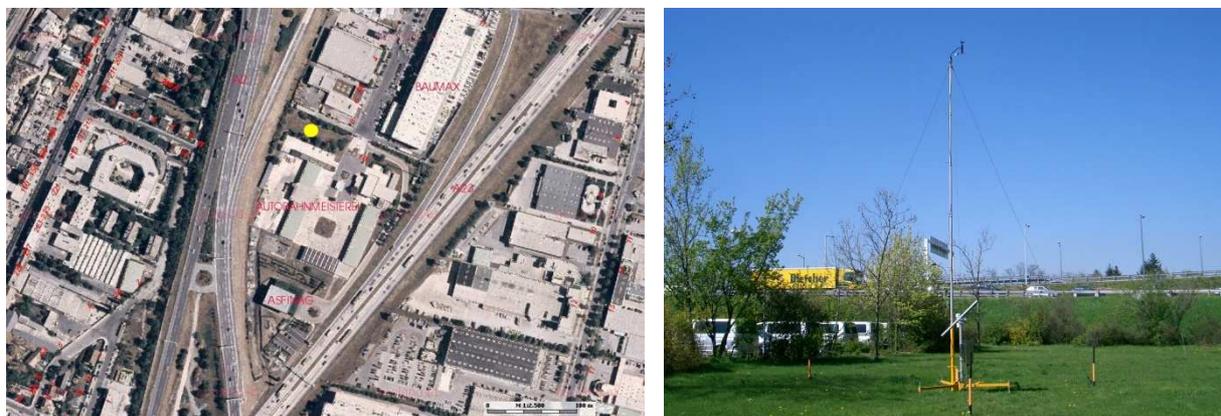


Figure 1. Site for the meteorological measurements within the RetoMod project at Vienna / Inzersdorf.

At both sites, INCA wind speeds are on average 1 to 1.5m/s higher than observed (see Figure for the measured and analysed average wind speeds at Inzersdorf). Modelled and observed wind-speeds are correlated with a factor of 0.8 at both sites. The main wind directions at Inzersdorf are well reproduced by INCA (Figure 11), south-westerly winds are deflected by a station-near building. Less agreement is found at Erdberger Brücke (not shown).

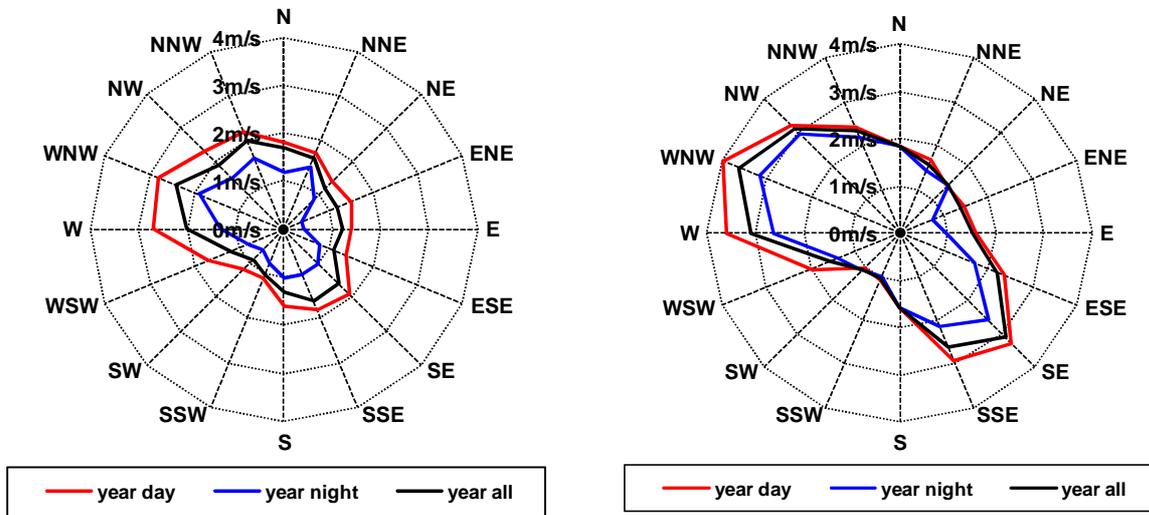


Figure 2. Mean wind speeds averaged for wind direction sectors from the measurements (left) and INCA analysis (right) for the Inzersdorf station in Vienna.

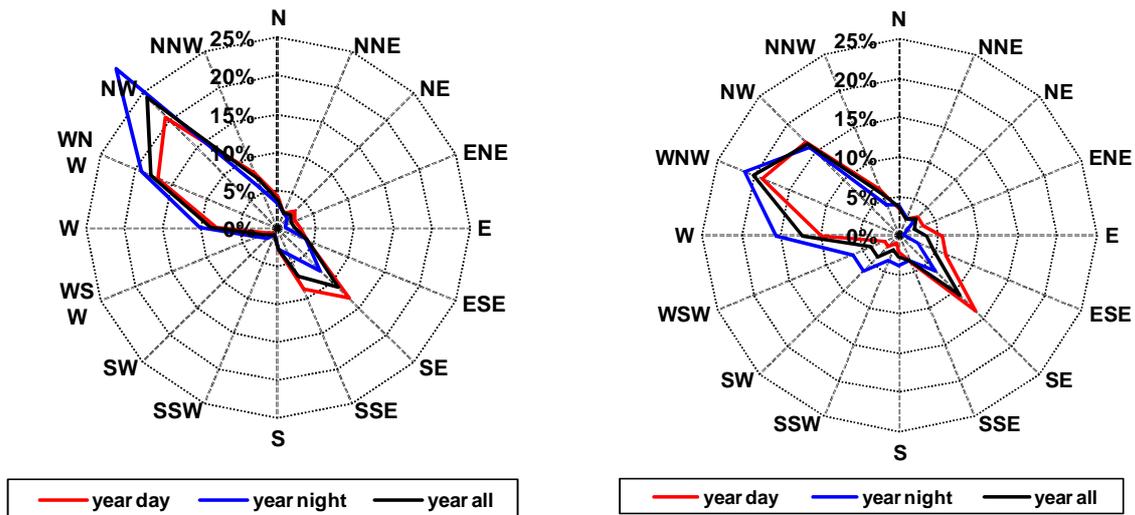


Figure 11. Wind direction frequency observed (left) and analysed (right) for the Inzersdorf station in Vienna.

**Influence of the meteorological input data – worst case weather scenarios**

In order to interpret model results and assess the consequences, a quantification of the influence of input parameters on the computational results is essential. The influence of the meteorological input on the results of the hazard distance calculations strongly depends on the chemical characteristics of the toxic release. Worst case weather scenarios therefore are not necessarily the same for different toxic substances e.g. the boiling point of the substance in relation to the ambient temperature can play an important role for the size of the toxic distances. Sensitivity studies were conducted for four chemicals (chlorine, ammoniac, butane and petrol) in order to assess the effect of the variability in the meteorological input parameter (wind speed, atmospheric stability, air temperature and surface roughness) on the magnitude of the impact zones.

**Sensitivity to wind speed**

The distances for the toxic areas computed by the models typically decrease with increasing wind speed. The wind speed determines the transport speed of the toxic cloud, the dispersion of the cloud and the mass transfer (evaporation from a puddle). The wind speed furthermore influences indirectly the exposure period of the affected persons in the area of concern (dose). As presented in Figure , the width, height and length of the toxic plume vary with wind speed for chlorine and ammoniac. Under calm wind conditions, heavy gases (e.g. chlorine) tend to form a compact, not very high, shallow plume (“pancake-shaped”) around the source. With increasing wind speeds the width of the plume decreases. The model

calculations for ammoniac reveal a general decrease of plume range with increasing wind speeds. For response analysis it is suggested that the wind speed and direction should be estimated from on-site or nearby measurements. For planning analyses, it is reasonable to consider worst case wind directions and wind speeds in order to estimate the maximum potential impacts.

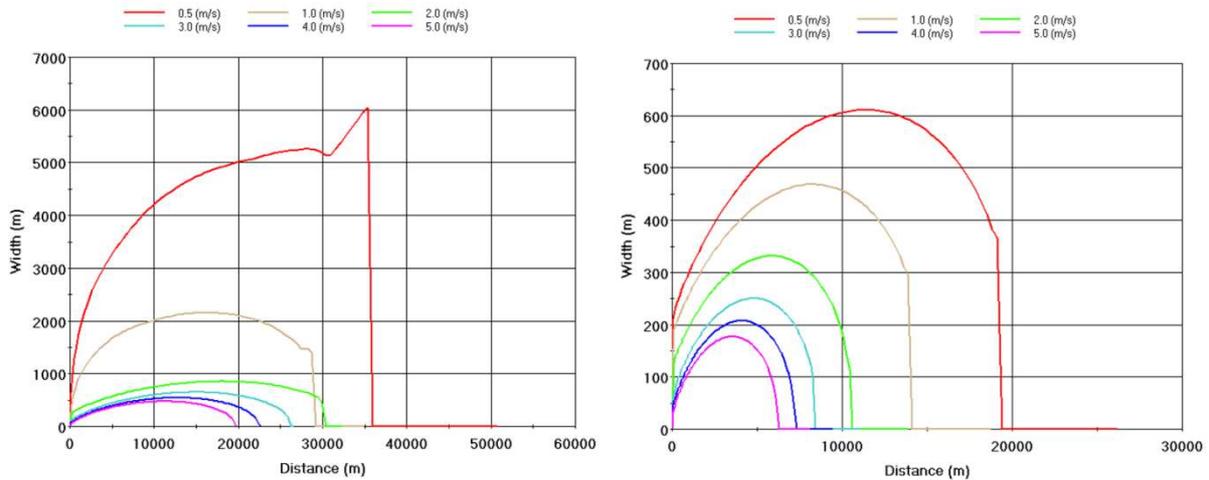


Figure 4. Sensitivity of the toxic distances to wind speed (left: chlorine, right: ammoniac). The calculations are conducted with the model TRACE for stable atmospheric conditions (class F) and release over city (100 cm roughness length).

**Sensitivity to atmospheric stability**

The stability categories are usually derived internally in the model depending on the sky cover, the wind speed and the roughness parameter. In the heavy gas scenario (Figure , left), the maximum plume width decreases and the maximum horizontal range increases with increasing stability.

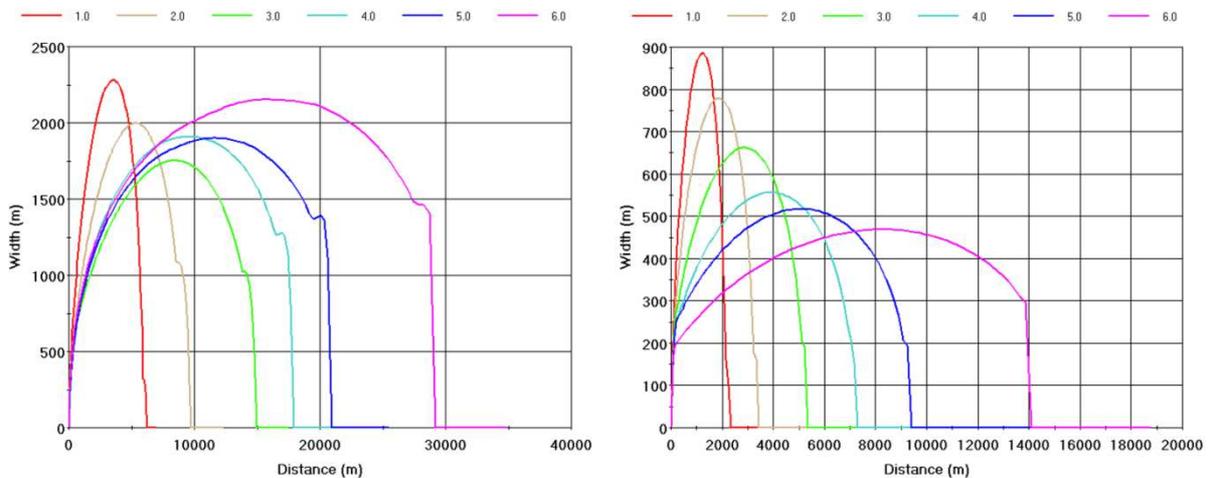


Figure 5. Sensitivity of the toxic distances to atmospheric stability (left: chlorine, right: ammoniac). The calculations are conducted with the model TRACE for 1 m/s wind speed, release over city (100 cm roughness length).

For near field impacts, dense gas may be only weakly sensitive to the stability. In the ammoniac scenario (Figure , right), maximum plume width and height are more or less independent from stability. The maximum horizontal range is largest under very stable conditions and smallest under unstable conditions.

**Sensitivity to air temperature**

The ambient temperature in connection to the boiling point of the substance determines whether the liquid flashes, boils or evaporates. As shown in Figure (left), the maximum hazard distance for chlorine (heavy gas) is almost not sensitive to the temperature changes up to 15 °C, after that the distance increases rapidly with temperature.

For ammoniac (Figure , right) the influence of the temperature is more complex as discussed by Bubico and Mazzarotta (2008). The vapor mass fraction in the released gas is decreasing with increasing temperature below 10 °C and increasing with temperature above. A maximum of 70% vapor mass fraction is reached at 25 °C.

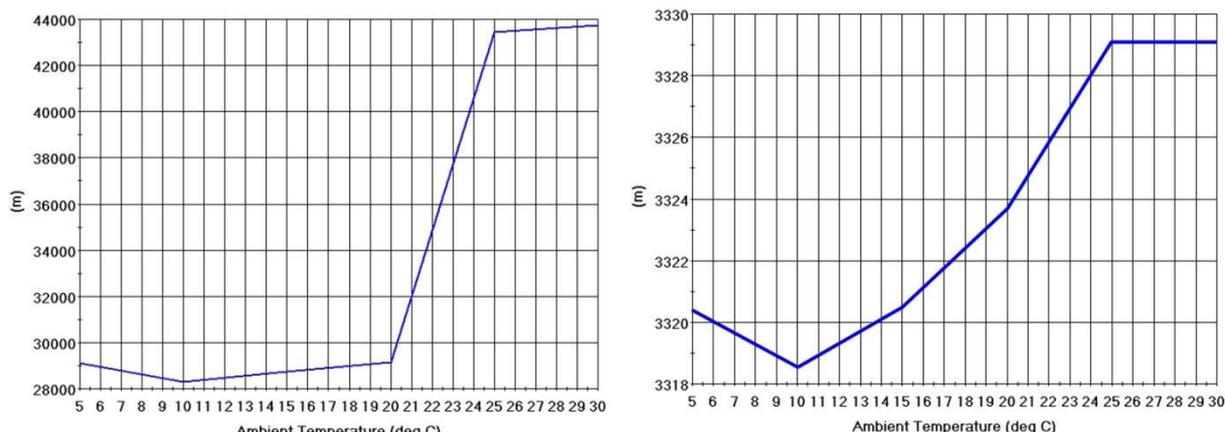


Figure 6. Sensitivity of the maximum toxic distance to air temperature (left: chlorine, right: ammoniac). The calculations are conducted with the model TRACE for release over city (100 cm roughness length), 1m/s wind speed and stable conditions (class F) for chlorine release and unstable conditions (class B) for ammoniac release.

**Sensitivity to roughness length and precipitation**

Roughness length is required as input parameter by most models and influences the hazard distances e.g. increasing the surface roughness by a factor of 10 may result in concentration reductions by a factor of 2. For planning purposes, where more conservative results are needed, it is probably more appropriate to use a smaller roughness height. Figure (left) illustrates the expected increase of the hazard distance with decreasing the roughness length (neutral stability).

It should be noted that only few models (such as MET) consider the impact of rain and fog (Figure , right). None of the tested models is sensitive to changes in the parameters: pressure or humidity.

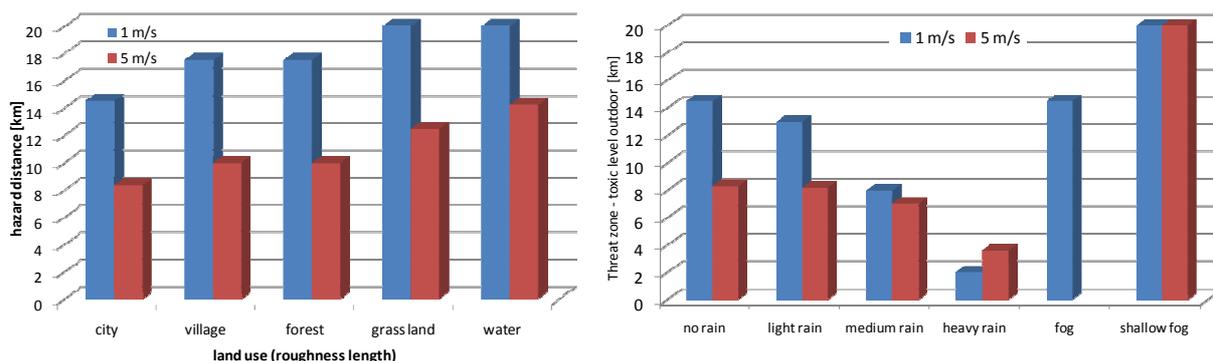


Figure 7. Sensitivity of the maximum hazard distance to roughness length (left) and precipitation (right). The calculations of a chlorine release are conducted with the model MET.

**CONCLUSIONS**

Modeling hazardous releases 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 to a large uncertainty. Therefore conservative assumptions often have to be taken 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.

In mobile applications, such as a traffic accident with a hazardous material transportation, the availability of a representative meteorological station cannot be assumed. In this case, it is recommended to use meteorological analysis data to take advantage of the better spatial coverage. INCA is found to give a good representation of wind direction as well as air temperature and humidity (not presented here) for near-traffic sites in Vienna, but tends to analyze on average 1 to 1.5 m/s higher wind speed than observed.

Besides the use of real-time analytical values, it is suggested to consider INCA-short range forecast (for the following hours) as, for example, an expected wind rotation or precipitation are crucial for the dispersion of the toxic gas and therefore the information can be quite helpful for the emergency responders or decision-makers.

In deciding which sources of information should be used to describe the meteorological conditions for a model run in real case application, it must be noted that the required meteorological parameters for the calculation results are differently relevant: for most substances, such as chlorine and ammonia, the wind speed is of major importance, together with information for the atmospheric stability. Stable, low wind conditions result in the largest toxic areas for the release of these toxic substances. Depending on the chemical characteristic of the released chemical, the ambient temperature may also be relevant in relation to the temperature of the released gas or liquid.

The results are discussed in detail in Baumann-Stanzer and Stenzel (2010).

#### REFERENCES

- Baumann-Stanzer, K., S. Stenzel (2010). Uncertainties in modeling hazardous gas releases for emergency response. *Meteorologische Zeitschrift*, accepted.
- Bubbico R., B. Mazzarotta (2008). Accidental release of toxic chemicals: Influence of the main input parameters on consequence calculation. *Journal of Hazardous Materials*, Vol. 151, 394-406.
- Haiden, T., A. Kann, K. Stadlbacher, M. Steinheimer, and C. Wittmann (2007): Integrated Nowcasting through Comprehensive Analysis (INCA) - System overview. ZAMG Documentation, 49p. [http://www.zamg.ac.at/fix/INCA\\_system.doc](http://www.zamg.ac.at/fix/INCA_system.doc)