

ETH - CHEMRISK: A PILOT DECISION SUPPORT SYSTEM FOR INDUSTRIAL ACCIDENTS EMERGENCY PLANNING AND PREPAREDNESS

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Abstract

ETH-CHEMRISK is designed in accordance with the principles and methods of emergency planning and preparedness as applied to the case of industrial (chemical) accidents. The outline of this decision support system design follows from both the features that nuclear and chemical accident consequence analysis share, and those that make the two different from each other. It uses and integrates concepts such as: data base, geographical information system, risk assessment, graphic driven software environment.

BACKGROUND

ETH - CHEMRISK is an attempt to answer the challenge of having the principles and method of emergency planning and preparedness to the case of chemical accidents. Most of the approaches, models and indicators in ETH - CHEMRISK come from the existing literature. Having in the background the well-quantified accident consequence assessment techniques in the nuclear industry, ETH-CHEMRISK is strongly supportive to the notion of Chemical Process Quantitative Risk Analysis (CPQRA). It uses specific indicators such as chemical doses, or limiting levels including the Immediate Dangerous for Life and Health (IDLH) levels, the Threshold Limit Values (TLVs), and the Short Term Exposure Limits (STEL). Proper allowance is also made in ETH-CHEMRISK for a method that, while more speculative and difficult to establish, would however increasingly gain terrain, namely the probit functions risk / consequence evaluation, that links, in essence chemical doses to their health effects - in fact, to the lethality of an environmental spill of toxic / hazardous chemicals. Though various methods -including probits- are available for quantifying the fire-related hazards entailed by chemical spills, the rather local, close-range nature of such hazards has less to do with the vocation and potential of ETH-RISK (Gheorghe et al., 1994) to address wider spatial distribution of hazards. All thermal and explosion related effects were left aside in the current version of ETH-CHEMRISK. While the back-end issue on how to quantify chemical accident consequences relied on the pooled wisdom at AIChE, the front-end issues of i) primary data and ii) the chemical accident source term definition were steered by a combination of selected

sources and independently originated solutions. Sources of primary data were (Guidelines, 1989; Diamonds, 1989) for the chemical accident source term. ETH-CHEMRISK draws upon the concept and prototype software ETH-RISK, designed for nuclear Accident Consequence Assessment (ACA). This stands true, in particular, for the dispersion model employed, which is an adapted version of the short range, complex terrain-sensitive model used with the module EXPOSURE.CH in ETH-RISK. The most radical adaptation of the latter to the chemistry's terms of reference include: augmenting the plume rise routines to the effect of covering non-bouyant (ground hugging) heavy gas flows; elimination of the deposition-related components of the models and software; generally, the replacement of dry-wet, and radioactive depletion mechanisms by a single, decay-like mechanism controlled by an user-estimated "chemical lifetime" - a technique also used with other software packages (TNO, 1989). Adequate procedures to account for i) instantaneous concentrations of released chemicals in air (chemical cloud position monitoring); ii) chemical doses, defined following AIChE's CPQRA methodology, as time-integrated powers of airborne concentrations of released chemicals; iii) probits and related lethality percentages. Three new software modules had to fill in. These are: NEEWMAP.WRK, DISPERS.CON, AND DISPERS. TIC. Consequent changes were made in the management of the GIS base, which is now controlled by a distinct module - NEWMAP.WRK. Moreover, given the far lower ranges in the distances to release sources that usually are of interest in a chemical accident, a new facility was added, namely to zoom over restricted zones on the 21 maps of the Swiss territory currently available with ETH-RISK, while preserving the grid resolution of 64 x 64 knots over whatever viewfield chosen.

ETH-CHEMRISK STRATEGY

The outline of the ETH-CHEMRISK design follows naturally from both the features that nuclear ACA and chemical ACA share, and those that make the two different from each other.

A Database Environment:

The fact that several hundred or more chemicals may each become the subject of an industrial / chemical

accident, has as a consequence the need to endow the DSS for chemical ACA with a rather well-developed database of chemicals that may be of interest. Such a facility should be instrumental not only in listing out its members, but also in providing selection and comparison mechanisms. Listing together all chemicals of a toxicity larger than (IDLH lower than) a given limit, or sharing the same fire hazards, or having well-defined probit function coefficients are, e.g. important assets, the need of which one cannot fail to perceive. With ETH-CHEMRISK one faces a two-fold environment, created by both the GIS base and the chemical data base. In case of emergency planning, while in a nuclear accident several dozen nuclides are of concomitant interest, and on several pathways (cloudshine, groundshine, inhalation, skin deposition, ingestion, etc.), in a chemical accident a single substance is, most usually, the subject of a hazardous release. The recently enhanced interest in "domino effects" in chemical accidents, cannot change this essential difference, that is bound to appear in the software's structure of the ETH - CHEMRISK. The emphasis on a single chemical and its physico-chemical characteristics is expressed, in the case in question, in the module CHEMDATA.WRK-an independent data base manager- handling 25 sequential files each holding a physico-chemical parameter, or feature of interest, for several hundred chemicals and their synonyms totalling 701 entries. Once a chemical is pointed at as the subject of an accident, all the other code modules would work on it, and only on it.

A Complex, Fluent Source Term Facility:

The present software includes a complex module that would be able to simulate a chemical release that may start as a liquid, continue with vapours, and end up as a gas outflow. The module SOURCE.WRK identifies the quantities of evacuated chemical that become airborne; this is to be further used with the dispersion models. Since the notion of chemical risks in chemical accidents would relate to rather short term exposures, the information that dispersion models are expected to provide should basically answer the following questions:

- i) where is the chemical cloud at a given time, and how intense the chemical concentration in the cloud is ?; and
- ii) what is the effect of the cloud passage, integrated over rather short times (15-30 minutes)?

Chemical Clouds and Their Time-Integrated Effects:

In ETH - CHEMRISK, answers to the first question are provided by module DISPERS.CON, whereas for answering the second question the module DISPERS.TIC was developed. Both modules would basically rely on the trajectory-puff model. The output of these models is given in a GIS style. However, it must be stressed that a full development of this DSS instrument would require detailed, close adaptation of the flow-cum-dispersion models in ETH-CHEMRISK to the topography of urban areas, perhaps beyond the model's current potential to account for these.

Impact Evaluation:

The GIS grid style is used to hold the information that is relevant for the impact of chemical accidents. Grids may hold airborne concentrations at a given time (mg/m^3 or ppm) when one runs DISPERS.CON, and time-integrals over determined, user-chosen durations, of certain chemical-specific powers ($0.653...2.5$) of the airborne concentrations, known as "chemical doses". Once concentrations or doses are grid - mapped by using a GIS environment, several possibilities are open (one may compare concentrations in a cloud at a given time). The technique of paths of minimum exposure developed in a nuclear emergency planning environment is fully functional also with ETH - CHEMRISK. Such paths can be easily mapped either with respect to the instantaneous positions of the travelling chemical cloud, or to its time-integrated effect (chemical dose).

ETH-CHEMRISK MODELS

There was a need in ETH - CHEMRISK for a variety of models to cover the varied phenomenology involved in a chemical accident with "off site" consequences. A tractable model was designed to determine the physical state of chemicals in their storage containments. A many-faceted outflow model had to take care of the transition from liquid discharges to vapours, and then to gases- the distinction between the last two varieties following from the assumption that vapours are ejected from punctured vessels containing liquids at a constant (vapour) pressure required by the vessel temperature, while gases are evacuated adiabatically, at decreasing pressures (and temperatures) as liquids were exhausted, till the vessel pressure equals ambient pressure. Dispersion models adopted for chemical accidents were generated from the original close-range dispersion model in ETH-RISK. And a **dose-effect relationship** had also to be adopted, from the referenced literature, to fit the case in point. The main aspect to be solved was to find a workable way to determine what mass and volume fraction from a given mass of chemical, squeezed into a storage vessel of given shape and volume, is in liquid state- the remaining space being assumed as occupied by saturated vapours at equilibrium with the liquid. Physical state models were used as a substitute to more accurate knowledge of the relationship of vapour pressure to temperature. Six outflow modes were assumed as possible, for a chemical in a vessel to escape into the environment. The chemical may emerge as: liquid, two-phase mixture, vapours (critical or subcritical outflow), gas (critical or subsonic outflow). Module SOURCE.WRK is able to monitor in a fluent manner the entire process described above, starting from the determination of the liquid fraction in vessel and continuing with a sequence of outflows as appropriate.

Takeoff Models:

It is important to note that what matters is the accident's source term in not only how much substance gets per time unit, but also, how much substance gets airborne (and thereby available for atmospheric transport and dispersion). The following systematics was used: i) gas

outflows and vapours outflows would go directly airborne; ii) for the two phase outflows, a simplified, conservative approach was taken in the sense that all substance that come out two-phase is assumed to totally flash in gaseous form as ejected, and becomes airborne; iii) for the liquid outflow, several cases were considered (ambient temperature above liquid's boiling temperature, ground temperature is higher than liquid's boiling temperature, ambient temperature is below boiling temperature etc.).

Dispersion Models:

ETH - CHEMRISK features a combination of trajectory and puff models. The *trajectory component* is sensitive to a variety of circumstances such as topography, latitude, time of the year, time of the day, dominant winds, insolation, atmospheric stability and inversion regime etc. Trajectory model's basic control parameters are: source related (geographical coordinates, time of emission, height of emission), meteo related (stability category, wind speed at 10 m height, direction etc), model specific (reference gradient coefficient and barometric exponent, solar factor, inversion layer exponent, reference friction coefficient, geostrophic ratio, reference mass factor. The *diffusion component* of the model relied on the notion that, instead of displaying a purely "molecular - gaussian" structure, plumes of pollutants are rather fractal in nature. A note is in order about placing rainy areas on maps. The idea was to construct an irregularly-shaped rainy area from circular "primitives". By exercising some ingenuity in overlapping such "primitives" one may, in principle, simulate rains of an arbitrary coverage and timing.

Dose - Effect Models

The following chemical risk indicators are used in the present structure of the ETH-CHEMRISK: IDLH, TVL, STEL, Toxic Dose, Probit Functions. One can map the values of all these indicators. Modules in the ETH - CHEMRISK decision support system feature a viewing option. This is to be used to get a variety of viewing angles as well as to zoom on the maps at work. Under probabilistic or deterministic assumptions regarding various parameters in the models' structure, the ETH - CHEMRISK converts, if so deemed, toxic doses to probits, and the latter to likely lethality percentages, and has these mapped over the geographic base environment.

SOFTWARE STRUCTURE

ETH-CHEMRISK is built upon two intertwined platforms. One is ETH-RISK's geographical base, and the other is the chemical data base developed for this code package only. The following is an enumeration of the main operative components of ETH-CHEMRISK:

- CHEWMDATA.WRK - the data base manager;
- SOURCE.WRK - the chemical source term;
- NEWMAP.WERK - allows the selection of one out of a number of maps- relief and road network included, as well as the isolation of a restricted viewfield around the source of release;
- DISPERS.CON - under probabilistic or

deterministic assumptions regarding the wind regime, and considering time of the year and day, insolation, topography, atmospheric stability, plume rise etc. monitors the chemical cloud position as the cloud travels with the winds over the territory;

- DISPERS.TIC - under probabilistic or deterministic assumptions, monitors toxic doses as these accumulate during cloud's passage. Converts, if so deemed, toxic doses to probits, and the latter to likely lethality percentages, and has these mapped over the geographic base.

USING ETH-CHEMRISK

ETH - CHEMRISK was designed to assist the emergency planning preparedness and simulation process. It allows the simulation of various scenarios and saving these scenarios in an *ad-hoc* database which later can be recalled; the information should be used in emergency planning decisions and land use planning. Some caveats are in order:

- being computation and graphics-intensive, ETH-CHEMRISK would prefer machines as fast as available;

- colors are of consequence with ETH-CHEMRISK. Its thematic maps may indeed look senseless in a black and white environment. An archiving facility is available at runtime with the executive modules. The respective de-archiving facility known as ALBUM includes an option on color changes that may help in getting better contrasts on black and white printers. ETH-CHEMRISK was tested for a variety of unexpected interrupts. However, at this stage in the experiment one cannot guarantee that some, unthought of, manoeuvres cannot block the system.

CONCLUSIONS

ETH-CHEMRISK is an exercise in applying to the case of chemical accidents several assets perceived in the ETH-RISK approach and, in particular i) the notion of an extensively interactive and transparent input machinery to cover a variety of "what if.." type of problems warranted in an abnormal chemical event; and ii) the setting of the entire endeavour in an appropriate data base, and a GIS-oriented, graphics driven software environment.

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