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THE SEVEX PROJECT : An integrated numerical model for the dispersion of gas in a complex terrain

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Abstract

An interdisciplinary numerical model to investigate different potential accidental scenarios on chemical plants is presented.

The characteristics of storage and data concerning accidental releases are taken into account to calculate the source terms.

As some major chemical industries are located in valleys and/or on irregular sites, the topography plays a role in the deformation of wind and turbulent fields. The mesoscale meteorological model with a vertical transformation determines the three dimensional wind and turbulent fields around the chemical plant.

The lagrangian particle diffusion model in the new system of coordinates evaluates the dispersion of the gas. Different simulations are presented to demonstrate the ability of the model to investigate the impacts of potential releases of gas from chemical plants in a complex terrain.

1. INTRODUCTION

According to the European Directive 82/501 "SEVESO Directive", the Ministry of the Walloon Region is responsible for the external safety around areas of high risk activities in its region of competence. It is in charge for the delimitation of high risk zones where emergency planning must be prepared.

The SEVEX Project involves three Universities (University of Liège, Catholic University of Louvain and the Polytechnic Faculty of Mons) and financially supported by the Walloon Region. An important logistic (computers and software) was provided by IBM.

The SEVEX Project is developed to provide scientific methods to evaluate the risks of major accidental releases of contaminants in the atmosphere.

The methodology to determine risk areas for emergency planning is explained by G.Van Malder of the Ministry of the Walloon Region in the context of the 8th International Symposium of Loss Prevention and Safety in the Process Industries (Van Malder, 1994, to be published).

The philosophy of the SEVEX Project is the following. From a risk and safety analysis, different scenarios of major accidents are defined and provide scientific and technical information to a numerical interdisciplinary model integrating three kernels or modules.

i) Source term module
ii) Meso-meteorological module
iii) Meso-scale dispersion module

The source module solves the BLEVE-fireball, the UVCE and the dispersion of a dense toxic gas. The two first phenomena are local. Details about the BLEVE-fireball and UVCE are given in other publications.

More details about the dispersion of a toxic gas will be given. The source term module examines the different steps of the releases at the local scale. The transport of contaminants at the meso-scale is calculated by means of a three-dimensional lagrangian module taking into account the actual topography, the wind and turbulent fields of the site.

In the past (5 years ago), the numerical solution of the problem required high performance computers. With the evolution of the technology, a standard work station is able to resolve the three modules of the SEVEX Project.

The simulations are not carried out on real time, not because the resolution of the modules require a too long time but, because the safety personnel (in the industry and in emergency headquarters) are busy with other essential tasks. It could be done anyway.

For each scenario of accident, sets of simulations are prepared corresponding to different meteorological conditions. The associated results (concentration, dose levels, wind fields, stability of the air, ...) are stored on magnetic or paper supports. With the cooperation of responsibles of the security at different levels, geographical zones of risks are prepared. Copies of these maps would be ready to use by safety teams in care of emergency.

2. SOURCE TERM MODULE

Starting from a safety analysis of a chemical plant several scenarios of potential accidents are considered.

The source module has also the possibility to examine two sub-scenarios the BLEVE (Boiling Liquid Expanding Vapor Explosion) fireball and the UVCE (Unconfined Vapor Cloud Explosion). They are not described in this contribution.

The complete description of the characteristics of the storage is introduced in the module: chemical compounds, capacity and geometry of the vessel, temperature and pressure (inside and outside the reservoir). Data concerning the accidental releases must be given :

i) instantaneous or continuous release, duration,
ii) size of a hole in the storage wall or length of a broken pipe,
iii) parameters of the jet (liquid, gaseous or biphasic) and of the cloud,
iv) size of a possible retaining dike,
v) meteorological data,
vi) characteristics of the site (mainly the roughness length).

After the initial computation stages (namely the release flow rate), the dynamical behaviour of the cloud at the local scale is considered (dense gas or aerosol dispersion). The cloud dispersion is studied by means of an integral model, the Box Model. The simplicity of this model and the quality of the results (comparison with observation) justify its use for the initial phases of the dispersion. The Box Model will provide the initial conditions for the three dimensional passive dispersion models which take into account the topography, in conjonction with a realistic wind and turbulent fields.

The Box Model is a generalization of other models found in the literature (Fryer and Kaiser, 1979 and Jagger, 1983) by the incorporation of the dispersion of vapor and aerosol.

The dispersion follows four sequences: formation, gravity phase, entrainment of air and cloud heating and finally the transition to a passive diffusion phase.

According to the type of releases two main scenarios are considered.

i) Instantaneous release

The source term module considers the gas as denser (or not) than the air. Due to the impossibility to take into account the real shape of the environment the gas is assumed to be confined in a cylinder with a uniform concentration and temperature. The dispersion follows the four sequences :

-) *Formation phase*

In this phase, the cold cloud is assumed to be a cylinder with a height h and a radius R. The initial height is supposed to be equal to the radius. The initial temperature is the pollutant normal boiling point and the vapor fraction is computed on the basis of an adiabatic flash at atmospheric pressure.

-) *Gravity phase*

Due to the gravity the walls of the cylinder must slump on the ground. The rate of change in the radius follows the semi-emperical law:

$$\frac{dR}{dt} = K \sqrt{gh \frac{\rho_{cloud} - \rho_{air}}{\rho_{air}}} \qquad (1)$$

where K is an experimental coefficient (values between 1 and 1.44).

The concentration is uniform in the cylinder and directly related to the mass and the volume of the cloud. The gravity phase is responsible of an increase in the radius and a decrease in the height of the cloud.

-) *Entrainment phase*

The entrainment of air induces a heating of the cloud and an increase in its volume. Natural and forced convection may produce an additional heating of the cloud.

The rate of entrainment of air is given by

$$\frac{dm_a}{dt} = \rho_{air} (\pi R^2) U_{Top} + \rho_{air} (2\pi Rh) U_E \qquad (2)$$

where $U_E = \alpha_1 \frac{dR}{dt}$ entrainment velocity at the edges of the cylinder

$U_{Top} = \alpha_2 U_1 R_1^{-1}$ entrainment velocity at the top,

$$R_i = \frac{g l_s}{U_1^2} \frac{\rho_{cloud} - \rho_{air}}{\rho_{air}}$$

with U_1 the longitudinal turbulent velocity proportional to the friction velocity u_*. The coefficients of proportionality between U_1 and u_* and the characteristic turbulent length l_s are given in tables as function of Pasquill categories and heights above the ground. Calibration of the model gives the best results for $\alpha_1 = 0.5$ and $\alpha_2 = 0.05$ values.

When there is a difference of temperature between the ground and the cloud the natural and forced convections and (solar and earth) radiation heating must be incorporated.

The cloud is advected downwind at the wind velocity at mid-cloud height. To correctly describe the evolution of the characteristics (temperature, water vapor and composition) of the cloud in the downwind direction the liquid droplet vaporization and the incorporation of moisture must be taken into account in the enthalpy balance.

-) *Transition to the passive phase*

Progressively the dilution of the gas increases and the diffusion becomes passive. Two tests are examined.

The first test is based on the comparison between the rate of increase in the radius due to the gravitational slumping of the edges of the cylinder and the one induced by the turbulence alone.

The dispersion becomes passive when :

$$\frac{dR}{dt} = K \sqrt{\frac{gh}{\rho_{air}} (\rho_{cloud} - \rho_{air})} \leq 2.14 \frac{d\sigma_y(x)}{dt} \qquad (3)$$

where $\frac{d\sigma_y(x)}{dt} = C^* u(t)$

with u(t) the wind speed at half cloud height. C^* is a constant depending on the Pasquill stability class and varying between 0.22 for a class A to 0.04 for a class F.

The second test is based on the difference between the actual specific masses of the cloud and of the air. A difference of 10^{-3} kg/m^3 is adopted as a criterion.

When one of theses criteria is satisfied the cloud is supposed to diffuse as a passive constituent.

At this step the user has the choice either to use a classical gaussian model in which the radial and vertical coefficient of dispersion are calculated according to Briggs (1973), or to switch to a 3-D dimensional passive dispersion model.

As the originality of the SEVEX Project is to calculate the dispersion in a complex terrain no details on the gaussian models will be given.

Data transferred from the source term module to the 3-D dispersion model are: meteorological data, geographical information (position of the release, time, date, topography, surface roughness, ...) and information about the cloud of the gaseous pollutant. The toxic is confined in a virtual cylinder source located at a downwind distance (x_v, y_v, z_v) and characterized by a radius R_i, a height h_i and a mean concentration C.

ii) Continuous release

The source term module calculates the release rate and its evolution. The modeling of the release is divided into three regions: jet region, dense cloud region and neutral cloud dispersion region. Different situations of releases are considered (liquid, gaseous and flashing liquid with and without friction through ducts).

The discharge rate and the other characteristics (pressure, temperature, vapor fraction, velocity, ...) essential for the computation of the releases in the three regions are determined by more or less classical formulas

- *Jet region*

  The model is based on the work of Iannello et al.(1989). The jet itself leaving the source expands and is computed by means of two sub-modules. This jet calculation is necessary for further phases of dispersion and also for the study of the UVCE.

  - Expansion Module

    The jet atomizes to droplets and flashes. 1-D equations of conservation for the momentum and the energy give the jet velocity after expansion and the partial vapor pressure in which the total pressure is assumed to be equal to the atmospheric pressure. The temperature is the normal boiling point of the chemical released. The fraction of unflashed liquid leaving the jet and forming the rain-out liquid is determined. The rain-out model is the model developed by Wheatley (1986).

  - Entrainment Module

    The jet at the ambient pressure is diluted by turbulent mixing with the atmosphere. A model based on the work of Ricou and Spalding (1961) evaluates the mixing process. The 1-D spatial evolution of the temperature, vapor fraction and composition is derived from rigorous applications of the energy balance. The jet structure and its modelization remains as long as the momentum dominates over buoyancy and atmospheric turbulence effects. The Richardson number is introduced as a criterion to decide if the jet structure is still on application.

  - Remark : the evaporation of the pool is also taken into account.

- *Dense cloud dispersion*

  The dissipation of the jet structure can generate a dense cloud. The gas cloud forms a steady plume with a rectangular cross section and studied by means of a Box Model. This model is very similar to the one described in the case of an instantaneous release.

  The parameters describing the evolution of the cloud are the height h, the half width L, u the velocity of the cloud and the concentration C, the volume flow rate of pollutant Q_v given by :

$$Q_v = 2\,L\,h\,u \quad \text{and} \quad C = \frac{Q}{Q_v} \tag{4}$$

  - Gravity phase

    The spatial evolution of the half width and the mass flow rate through a given cross section of the plume are:

$$\frac{dL}{dx} = \frac{K}{u}\sqrt{gh\frac{\rho_{cloud} - \rho_{air}}{\rho_{air}}} \tag{5}$$

- Entrainment phase

$$\frac{dQ_a}{dx} = 2\rho_{air} L U_{Top} + 2\rho_{air} h U_E \qquad (6)$$

with the edge entrainment $U_E = \alpha_1 u \frac{dL}{dx}$ and the top entrainment $U_{Top} = \alpha_2 U_l Ri^{-1}$ velocities.

As in the case of an instantaneous release the downwind evolution of the characteristics (temperature, water vapor and composition) of the cloud is deduced from the enthalpy balance taking into account the liquid droplet vaporization and the incorporation of moisture.

- Transition to passive diffusion

The criteria of transition from a dense to a passive dispersion are the same as in the case of an instantaneous release. Once neutral, the dispersion ant the transport are driven by the 3D-particule model.

The source term module has been calibrated with data from the RISO National Laboratory (Experiments EEC55 and 57 in 1989 for example) and from experiments in the Tortoise Desert. A good agreement (Levert et al., 1992) with observations is found for the envelope curves describing the evolution of the half-width and for the height of the cloud.

3. MESO-METEOROLOGICAL MODULE

The meso-meteorological module calculates the 3-D fields of wind and of turbulence around a chemical plant. The ground can be flat or hilly. This module is a 3-D Planetary Boundary Layer Model (Schayes and Moyaux, 1992) originating from the URBMET model (Bornstein,1987), in which the topography treatment and a more refined surface influence have been introduced in order to be adapted for our applications. The model is governed by boussinesq flow equations and written using the vorticity formulation. The main advantage of the vorticity formulation is the elimination of the density and pressure terms in the equations of motion.

The coefficients of horizontal turbulent viscosity and diffusivity have the same numeric values (10^3 m^2/sec). The coefficients of vertical turbulent viscosity λ_m and diffusivity λ_θ are related to the mean turbulent kinetic energy defined by $\varepsilon = \frac{1}{2}(u'^2 + v'^2 + w'^2)$ and to the mixing length l_k :

$$\lambda_m = C_m l_k \varepsilon^{0.5}$$

$$\lambda_\theta = \alpha_\theta \lambda_m \qquad (7)$$

with $\alpha_\theta = 1.35$

The mixing length takes into account the stability of the layer by a Monin Obukov length.

As the turbulence is not isotropic energy Therry and Lacarrère (1983) suggested a correction to the experimental expression of the mixing length to l_k : $l_k = \left(\frac{w'^2}{\varepsilon}\right) l_\varepsilon$ where l_ε is given by:

$$\frac{1}{l_\varepsilon} = \frac{1}{\kappa} + \frac{C_1}{ZI} - \left[\frac{1}{\kappa} + \frac{C_2}{ZI}\right] m_1 m_2 + \frac{C_5}{l_s} \qquad (8)$$

with $m_1 = \dfrac{1}{\left[1 + (C_3 . ZI)/\kappa\right]}$

$$m_2 \begin{cases} = 0 & \text{if } L \geq 0 \\ = \dfrac{1}{\left[1 - (C_4 . L)/ZI\right]} & \text{if } L < 0 \end{cases}$$

$$\frac{1}{l_s} \begin{cases} = 0 & \text{if } \dfrac{\partial\theta}{\partial z} \leq 0 \\ = \left[\dfrac{g\beta \dfrac{\partial\theta}{\partial z}}{\varepsilon}\right]^2 & \text{if } \dfrac{\partial\theta}{\partial z} > 0 \end{cases}$$

C_i are experimental constants , L the Monin-Obukov length and Zi the height of the atmospheric boundary layer. κ and θ are respectively the Von Karman constant and the potential temperature.

Geographical maps provide altimetrical and roughness data of the surrounding region. A transformation for the vertical coordinate is introduced given by

$$z \rightarrow \eta \qquad \text{where} \qquad \eta = s\frac{z - z_g}{s - z_g} \qquad (9)$$

with s, z and z_g are respectively the altitude of the top of the model, z the altitude and z_g the altitude of the ground. It has the advantage to modify the irregular topography into a simpler one. Unfortunately extra terms are generated in the equations of motion, temperature and humidity and mean turbulent kinetic energy. Very close to the ground, the surface layer with constant fluxes is treated analyticaly: modified logarithmic profiles (Louis, 1979) give the vertical distributions as a function of the stability of the layer.

The model provides at each grid point the vorticity and the wind velocity, the potential temperature and the friction velocity u_*. The model is solved with a grid of 1 km in the horizontal direction and from 10 m to several hundred meters (the top of the model is at 2000 m height) in the vertical direction. The number of vertical grid points is 12. The horizontal extension of the numerical model is (29 km x 29 km). The source of pollution is located not far from a boundary in order to maximize the downwind dimension of the numerical grid.

For the determination of geographical delimitation of risk areas it is extremely important to consider not only the most frequent situations but also the worst conditions. A set of typical meteorological scenarios is chosen: geostrophic wind of 4, 8, 12 m/sec for 12 or 16 directions and 2 stability classes (one corresponding to a covered sky during the day and the second a to a clear night).

The meso meteorological module transfers not only the roughness of the ground and the velocity field but also all the data required to calculate the turbulent effects and the stability of the atmospheric layer.

4. LAGRANGIAN PASSIVE DISPERSION MODULE

A good model must fulfill several conditions. The computation process must be accurate and take into account the topography and its characteristics. To satisfy these requirements a lagrangian particule diffusion method based on the scheme of Yamada and Bunker (1988) is used to calculate the transport and the dispersion of the released pollutant.

The principles of the method are the following:

-) The mass of toxic gas is divided into a great number of elements or "particules",
-) Each particule has a finite size with its own characteristics (velocity, temperature, pressure, concentration, ...),
-) Each puff particule is advected by the velocity of the air $\mathbf{u}_p$,
-) The positions of particules are updated at each time step (order of 10 sec)
-) The concentration at every point (x, y, z) is calculated as the contribution of all the particules present over the terrain. The concentration following Yamada and Bunker (1988) is:

$$C(x,y,\eta,t) = \frac{1}{(2\pi)^{1.5}} \sum_{p=1}^{N} \frac{M_p}{\sigma_{x_p}\,\sigma_{y_p}\,\sigma_{\eta_p}} \exp\left(-\frac{1}{2}\frac{(x_p - x)^2}{\sigma_{x_p}^2}\right) \cdot \exp\left(-\frac{1}{2}\frac{(y_p - y)^2}{\sigma_{y_p}^2}\right) \left\{\exp\left(\frac{1}{2}\frac{(\eta_p - \eta)^2}{\sigma_{\eta_p}^2}\right) + \exp\left(-\frac{1}{2}\frac{(\eta_p + \eta)^2}{\sigma_{\eta_p}^2}\right)\right\} \quad (10)$$

where M_p is the mass of the particule, N the number of particules, (x_p, y_p, η_p) and $(\sigma_{x_p}, \sigma_{y_p}, \sigma_{\eta_p})$ the coordinates and the geometrical characteristics of the particule p.

4.1. Model equations

i) Velocity distribution

The position of each particule at each time step δt is calculated by the following equation :

$$\mathbf{x}(t_{new}) = \mathbf{x}(t_{old}) + \int_{t_{old}}^{t_{new}} \mathbf{u}_p(\mathbf{x}(t), t)\, dt \approx \mathbf{x}(t_{old}) + \mathbf{u}_p(t_{old})\,\delta t \qquad (11)$$

The velocity is divided in two parts : $\mathbf{u}_p = \mathbf{u}_m + \mathbf{u}_t$ with $\mathbf{u}_m$ the mean velocity deduced and interpolated from the meso-scale meteorological model and $\mathbf{u}_t$ a characteristic turbulent velocity calculated with turbulent data given by the same model.

If u' represents the downwind component of the velocity, v' the crosswind component and w' the vertical one, Yamada (1985) proposes the expressions :

$$\begin{aligned} u'(t+\delta t) &= a_u\, u'(t) + b_u \sigma_u\, \xi \\ v'(t+\delta t) &= a_v\, v'(t) + b_v \sigma_v\, \xi \\ w'(t+\delta t) &= a_w\, v'(t) + b_w \sigma_w\, \xi + (1-a_w)\, TL_w \frac{\partial}{\partial z}\sigma_w^2 \end{aligned} \qquad (12)$$

where

$$a_{u,v,w} = \exp\left(-\frac{\delta t}{TL_{u,v,w}}\right) \qquad (13)$$

$$b = \left(\sqrt{1-a^2}\right)$$

$\sigma_{u,v,w}$ the standard deviations of the wind velocity fluctuations,

$TL_{u,v,w}$ the lagrangian time scales for the components of the velocity (u,v,w),

ξ a random number from a gaussian distribution with a zero mean and a unit variance.

The first term of (12) is an autocorrelation component of the wind velocity fluctuations, the second directly associated to the turbulence in the planetary boundary layer and the last in the third relationship is introduced to avoid an accumalation of particules in regions of very weak turbulence.

The lagrangian time scales depend on the stability within the planetary boundary layer and on the height of inversion. They are estimated as follows (Hanna, 1982 and Zannetti, 1990).

Three situations can occur : stable, unstable and neutral. The worst for environnental consequences is the stable case. The lagrangian time scales and others characteristic of dispersion are :

$$\begin{aligned} TL_u &= 0.15\frac{h_i}{\sigma_u}\left(\frac{z-z_g}{h_i}\right)^{0.5} \approx 0.15\frac{h_i}{\sigma_u}\left(\frac{\eta}{h_i}\right)^{0.5} \\ TL_v &= 0.15\frac{h_i}{\sigma_v}\left(\frac{z-z_g}{h_i}\right)^{0.5} \approx 0.15\frac{h_i}{\sigma_v}\left(\frac{\eta}{h_i}\right)^{0.5} \\ TL_w &= 0.1\frac{h_i}{\sigma_w}\left(\frac{z-z_g}{h_i}\right)^{0.8} \approx 0.1\frac{h_i}{\sigma_w}\left(\frac{\eta}{h_i}\right)^{0.8} \end{aligned} \qquad (14)$$

with

$$\sigma_u = \sigma_v = 2u_* \left(1 - \frac{\eta}{h_i}\right)$$

$$\sigma_w = 1.3u_* \left(1 - \frac{\eta}{h_i}\right) \qquad (15)$$

u_* is the friction velocity and h_i the height of inversion
If $\eta > 0.9 h_i$ the computed values are those corresponding to $\eta = 0.9 h_i$.

ii) Particule distribution

Each particule represents the center of a puff. The distribution of mass around this center are assumed to be gaussian; the variances are determined as the integration of the velocity variances encountered over the history of the puff. According to the classsical theory of homogeneous turbulence the variances are :

$$\sigma_x^2 = 2\sigma_u^2 \int_0^t \int_0^z \exp\left(-\frac{\xi}{TL}\right) d\xi \, dz \qquad (16)$$

Approximatively this expression is simplified into :

$$\sigma_x = \sigma_u \, t \qquad \text{if} \quad t \leq 2TL_u \qquad (17)$$

$$\sigma_x^2 = 2\sigma_u^2 \, TL_u \, t \qquad \text{if} \quad t > 2TL_u \qquad (18)$$

Similar expressions are used for the variances in the other directions.

5. RESULTS OF A SIMULATION

To take into account the variation of the wind direction during the release, we calculate the envelope curves of isoconcentration associated to a direction of the wind and two adjacent directions (+ and - 22.5°).

The model has been tested and the results of simulations have been compared (Bourouag et al., 1992) with results of others models (gaussian models) and observations.

Fig.1 presents the topography of the site of Jemeppe-sur Sambre in Belgium and the envelope curves at 1 m above the ground relative to an instantaneous release of 55T of chlorine.

For safety purposes it is important to know the absolute maxima of concentration at any place; the indicated values are the maxima corresponding to three simulations involving geostophic winds of 4, 8 and 12 m/s and a stability of the air D.

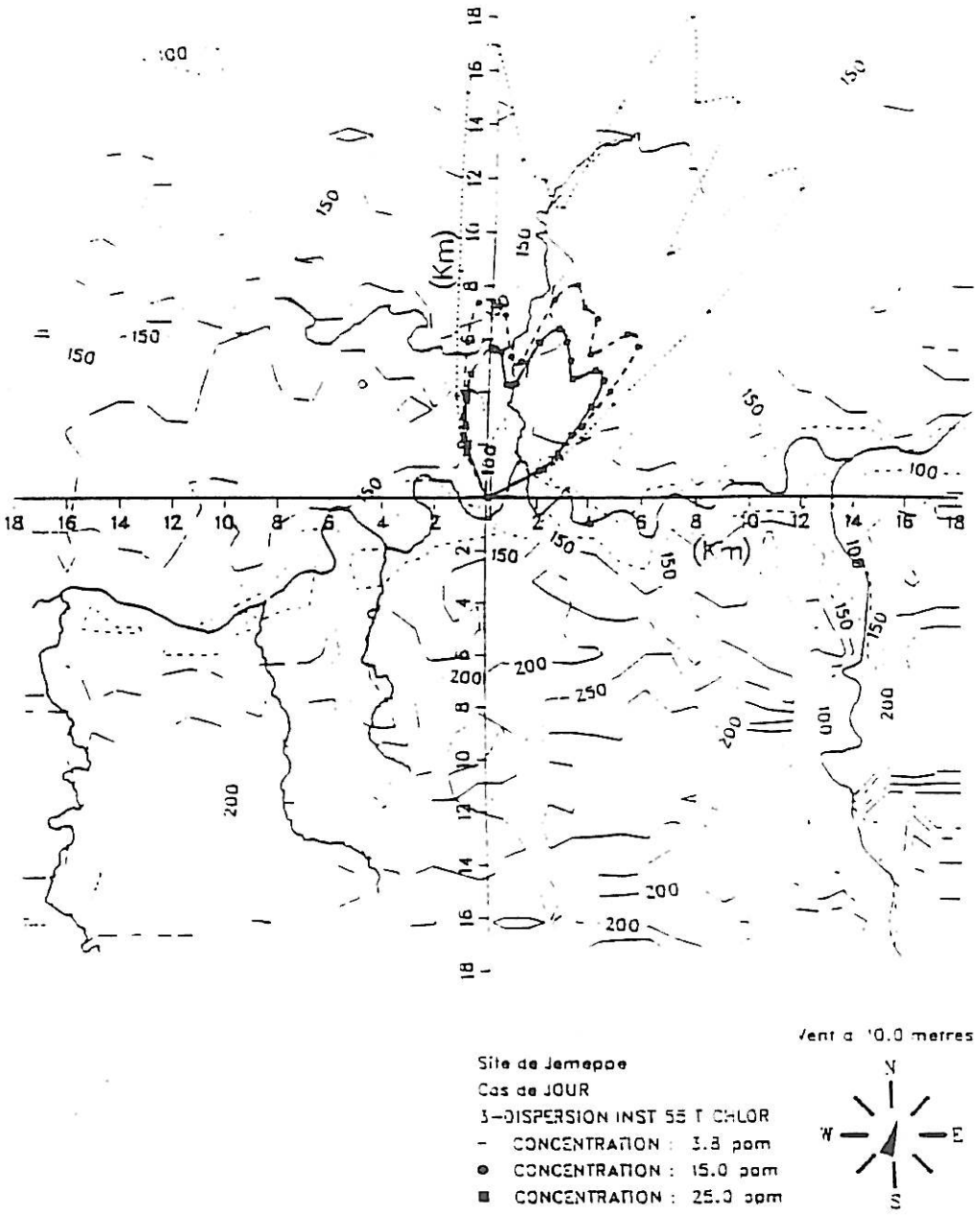

Fig. 1. Topography of Jemeppe sur-Sambre and curves of isoconcentration never exceeded for an instantaneous release of 55T of chlorine.

6. CONCLUSIONS

The major interest of the SEVEX Project is to compute all the aspects and consequences of accidental releases through a set of coherent models. The final product is maps showing the maximal concentrations never exceeded during an accident scenario. This information is of first importance for Public Authorities.

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