STRRAP

(STOCHASTIC TOXIC RELEASE RISK ASSESSMENT PACKAGE)

A SYSTEM FOR HAZARDOUS MATERIALS RISK ASSESSMENT

N.J. Scenna[1,2] , A.S.M. Santa Cruz[1], S.M. Godoy[1]

[1] *GIAIQ - Grupo de Investigación en Informática Aplicada a la Ingeniería Química*
Universidad Tecnológica Nacional - Facultad Regional Rosario
Zeballos 1341 - S2000 BQA Rosario (Santa Fe) - Fono Fax 54 341 4484909
República Argentina

[2] *INGAR - Instituto de Desarrollo y Diseño (Fundación ARCIEN – CONICET)*

Avellaneda 3657 – S3002GJC Santa Fe – Fax 54 342 4553439

República Argentina

Abstract

This work presents a methodology and a powerful computational tool, STRRAP (Stochastic Toxic Release Risk Assessment Package) useful in risk assessment and emergency planning related to a gas release of hazardous materials. It can be used in punctual releases or in truck- transportation accidents. Also, it can be extended to rail, maritime and pipeline transport involving other types of scenarios. The present methodology takes into account the random behaviour of meteorological conditions like wind intensity, wind direction, atmospheric stability and day/seasonal condition (diurnal or nightly/summer or winter) specific of the place under study. After a stochastic simulation based on a diffusion model for dense and light gases is done, the downwind concentrations are obtained, so distances of interest and/or individual and societal risk can be determined. For this application a procedure that reduces considerably the simulation time has been introduced. All the subroutines and procedures have been integrated in a computer program which makes the management of the information and results easy. Finally, test results are shown to underline the main contribution of the system.

Keywords: Emergency Planning, Transportation of Dangerous Substances, Consequence and Vulnerability Analysis, Risk Assessment.

1. Introduction

Circumstances that can endanger people's health, environment and goods have to be taken into account when dangerous substances are transported. Therefore, both public and private organisms must coordinate the use of means and resources to protect properties and people but also to mitigate negative effects at low cost. Consequently, hazardous-substance transportation is a subject of evaluation and planning. So, optimal computational tools must be designed to evaluate risk and provide useful information for emergency planning in optimal time.

Road-accident rates in hazardous material transportation have increased during the last decades. In fact, 95% of cases reported in the 20^{th} Century has occurred in the last 30 years [1]. Due to the consequences of these events, it is important to improve the available tool and develop new ones. Here, an algorithm that reduces the computational time is presented.

Experts in *reliability engineering* know that zero risk does not exist, even if investments in prevention are made. Only increasing investments can substantially minimize risks. Consequently, contingency plans considering evacuation and pollutant isolation/confinement must be carefully prepared. Any attempt to design or plan beforehand or even upgrade logistics, necessary elements, schedules and so on, implies the need of defining and evaluating risk scenarios that take into account both stochastic and state-of-knowledge uncertainties. Hence, decision-making and emergency planning arrangement require to be based on computing procedures considering the presence of these two uncertainties in transport accident scenarios.

Stochastic uncertainty is due to the inherent natural variability of parameters in the involved physical process. For instance, the natural variability of the weather affects pollutant diffusion processes. Although additional data cannot reduce the stochastic uncertainty, they can provide information about its probability distribution.

The problem of computing physical consequences produced by the spill or release of a dangerous substance implies the development of various incidental scenarios. Consequently, all of them must be evaluated. The stochastic nature of meteorological parameters will be here considered in order to go deeper in the calculus of pollutant diffusion consequences. In fact, different release scenarios during a period of time in which all atmospheric parameters vary randomly should be studied. Besides, this should be done considering variable discharge rates as function of the hole size distribution. A release of a liquid or a gaseous substance generates different qualitative effects like a pool and/or a cloud formation, an explosion, a jet, a BLEVE and so on.

Here, results only for hazardous pollutant diffusion events in road transportation will be shown (Figure 1). Therefore, concentrations of a toxic gas which reach the established health criteria will be determined.

2. The Problem definition

STRRAP is based on a simple representation of emitters and receptors (grid). Figure 2 represents a transportation incident along a road where a dangerous substance release occurs. Multiple emitters can be represented given their coordinates (X,Y). An arrange of emitters can be part of a road, a pipeline or a maritime trajectory. Note that a fixed emitter point (stack, tank release, etc.) can be considered as a particular case with only one emitter.

The road is cut up into finite length portions and the surrounding area is divided into square sections as a grid.

Thus, the problem is defined considering each road portion ΔL_{Ri}, as a potential fixed emission point along the road. Then, the pollutant concentration can be calculated at each grid point (X_j, Y_k), with j = 1, … , M; k = 1, ... , N; on the area. So, the concentration distributions due to the emission of the potential accident occurring in ΔL_{Ri} are obtained.

Diffusion of a pre-established hazardous substance quantity results in different concentration distributions in each point of interest in a given area depending on the accident characteristics and release parameters. This is due to the random value of the meteorological parameters given a time horizon taken for the analysis. So, a stochastic atmospheric scenario is considered for each point source. Then, each stochastic atmospheric parameter within the model is represented by a probability density function. Therefore, considering an emission along the entire road, the expected concentration histograms will result just from adding all histograms at each point (X_j, Y_k) along a given time horizon. Once these histograms (which can be set according to seasonal, annual, or other bases) are created, the scheduler will have important data to compute the expected resource demands along the established time horizon for emergency planning or risk assessment.

The downwind concentration of the toxic gas decreases as distances increase. The most criteria used to divide the risk area into two sub-areas: a little one called the “red zone”, being the most dangerous, and a bigger one called the “yellow zone”, which is less dangerous. The 2000 ERG [2] define them as *Initial Isolation Distance* and *Protective Action Distance (PAD)*. We will use this definition in this work to determine safe distances.

The *Initial Isolation Distance* defines a circular area surrounding the place of the incident, where the downwind concentration of the toxic gas is such that could endanger people’s life. The *Protective Action Distance (PAD)* defines a square downwind region where people exposed to it can have irreversible health effects and/or be disabled to escape causing their death.

The two distance definitions are outlined according to Figure 3.

The health criteria used to determined the *PAD* and the *Initial Isolation Distance* are the American Industrial Hygiene Association’s Emergency Response Planning Guideline Level 2 and 3 (ERPG-2 and ERPG-3) respectively.

Summarizing, safe distances, a concentration distribution map of the hazardous substance and an associated risk map on the geographical zone of interest will be calculated considering the random weather characteristics.

If this procedure is repeated for more dangerous transported materials, a very good approximation of possible hazardous scenarios and a quantitative measure of their impact can be obtained.

In previous works [3], [4], the simulations were carried out considering all grid points and the contribution of all the emission points from the road. This methodology, although quite rigorous, demand a very high computation time. So a more effective calculation procedure, based on an adequate problem simplification is presented in this work.

3. Methodology and Computational System

3.1. Methodology - Gas-Diffusion Model

There are several very efficient gas-diffusion models being available the necessary data. The two kinds of models widely used for gas dispersion in the atmosphere are:

1. Gaussian models for light and neutral gases (its density is lower than or equal to the air density).
2. Heavy gases models.

STRRAP include both options. Option 2, which is the most complicated, will be described. For heavy gas diffusion calculation we use DEGADIS.

Aerosol presence inside the cloud, heat exchange between the cloud and the ground and other factors influence on the model characteristics.

DEGADIS[#] simulator, broadly recognized by the specialized literature, is a free disposal computation program for calculating dense gas dispersion. The DEGADIS model [5] was designed to model the atmospheric dispersion at ground level, area-source dense gas (or aerosol) clouds released with zero (initial) momentum into an atmospheric boundary layer over flat, level terrain. It describes the dispersion processes, which accompany the ensuing gravity-driven flow and entrainment of the gas into the atmospheric boundary layer. This has been verified by comparing a wide range of laboratory and field-scale heavy gas release/dispersion data.

As previously stated, each stochastic atmospheric parameter within the model is represented by a probability density function. The shape and size of these functions define the range of values that parameters may take and their relative probabilities.

So, given the input data distributions the approximation to the concentration distributions (probability density function) must be calculated at each given grid point, using a suitable model.

DEGADIS solves systems of equations in terms of meteorological data, surface roughness, substance physicochemical properties and accident scenario (type of diffusion, flowrate, etc.) given in the input vector. To consider random variables for certain inputs, we use the Monte Carlo method. Therefore, according to the stochastic approach and the distribution of each stochastic parameter, a quantity of random numbers will be given to each accident scenario (input trial) proportionally to the event occurrence likelihood. Thus, DEGADIS simulator solves the output vector corresponding for each generated input. If this procedure is repeated with each trial, an approximation to the output distribution may be obtained. Consequently, this methodology provides information about the probability density function of the pollutant concentration at a given point when taking into account the characteristics of the emitting source (road section) and random meteorological parameters. Wind velocity, wind direction and atmospheric stability are considered *stochastic parameters*. Besides, their probability distributions are conditioned following a causal dependence (Figure 4). Thus, both stability and wind velocity distributions are conditioned by the wind direction distribution probability, which, in turn, depends on whether it is day or night. Equal probability of accidents along the road is assumed. Also, equidistribution with respect to time (hour of the day or night) is adopted.

On the other hand, the considered *deterministic parameters* are gas properties and roughness surface. Also, atmospheric pressure, relative humidity and temperature are assumed deterministic adopting the most representative value along the time horizon to simplify the problem. Figure 5 shows the calculation methodology. First, the system verifies the input data: substance identification, and flow rate (that is, the accident scenario description). A complementary program generates the random input sets in which each variable vector corresponds to each DEGADIS run. Therefore, given the input distributions and the accident scenario, this interface generates the corresponding input files for the DEGADIS program to carry out each trial. According to Figure 5, another auxiliary program reads all the outputs files generated by DEGADIS and calculates all the parameters of interest (maximum and minimum concentration, concentration distributions, the

---

[#] See references.

number of trials in which the concentration is higher than the hazardous levels, etc.) for each grid point (j, k). Up to this point, the release characteristics were assumed to be known. Nevertheless, release flowrate (continuous release) or released quantity (discontinuous release) are also uncertain variables. In fact, it will depend on the accident characteristics (container breakage, relief valve failure, etc.). Indeed, release flowrate may be a function of each atmospheric condition (temperature, relative humidity and atmospheric pressure). Here, we will assume a given probability density function for release flowrate, independent of the other parameters. Also, only continuous releases will be considered. In this way, we can incorporate a second hierarchical level in which the release flowrate is given by a particular number of discretized values of the probability density function. So, for each given flow rate, all the previously described calculations are made. Figure 5 includes this step.

3.2. The Computational System

As shows Figure 6, STRRAP is comprised of three parts (See Scenna, et al [6]):

1. The pre-processor
2. The processor
3. The post-processor

The pre-processor is in charge of the input file generation. It reads accident data included within a pattern file. That is, it generates the random variable values that will be substituted in the pattern file before calling the calculus module. Since the values of the random variables (season, day-night condition, wind direction, wind velocity, and atmospheric stability) have been determined, the pre-processor writes a file (*inp* extension). It holds the variables specified for the user and those achieved by random generation.

The processor module, which keeps intact the DEGADIS calculus subroutine, calculates the downwind pollutant concentration in each grid-point according to the conditions previously settled by the pre-processor.

The DEGADIS code was translated into FORTRAN 90 to make program interactions active. In addition, all the results can be displayed in a graphical way to make the user's task easier. Several subroutines or auxiliary programs have been developed. For example, since DEGADIS outputs give the concentration profiles along the wind direction only, the concentration for all the other grid points must be calculated using a simple formula and a coordinate transformation. This part of the process was implemented in such a way so as to optimize the calculation speed.

The coordinate-change subroutine not only computes the concentration at the receptor points for every trial, but also writes all the generated cases in an output file, and creates another file to store all the cases in which the critical toxicity index stipulated by the user has been overcome (Figure 6).

In a previous version of our package, the cycle pre-processor – processor was repeated so many times as random trials were generated, for all point sources along the road. The simulations were carried out considering all receptors (grid points) and the contribution of all the emitters from the road, spending a lot of computational time.

It is easy to show that a specific grid point is affected by a small quantity of emitters (Scenna, et al [4]). In this version of STRRAP we use this fact to simplify the algorithm and the computational time. Only affected receptors and potential critical emitters are considered.

Indeed, a further simplification can be made. Actually, if we consider one emitter and localize all the receptors affected by it, we can determine a zone of impact which can be supposed invariant and be reproduced along the road. We call this the reference emitter (RE). Translating its results (concentration histograms) to the complete route, the new affected receptors keep a direct relationship with the reference one. The only assumption (added to the equidistribution of accident probability along the road) is that we use the same set of random values for all the emitters along the road in each trial. So, we only need to simulate one point source and translate its effects to the whole affected region surrounding the road. It reduces considerably the computing time (8 min. vs. 8 hrs.) without lost of accuracy.

So, using the “intelligent” translation algorithm, all grid points affected along the entire road and their histogram concentrations can be obtained.

Finally, the results are stored in a data base, and by means of suitable queries the information of interest is obtained. Iso-concentration areas can be traced over the maps. In addition, it is also possible to determine iso-probit and iso-risk areas and the frequencies wherewith the receptors have been affected by means of an ad-hoc software developed in Visual Basic (PLOT-DEGADIS software). Figure 7 shows a risk map built for a Risk analysis of a chlorine release in the circumvallation highway of Rosario city.

As we mentioned, the software stores only those values of concentration where the specified health criterion is overcome. So, in the calculus of safe distances, each receptor is linked up with each emitter by means of the data base. In this way, distance (receptor-emitter) distributions can be determined. We adopt the 90-percentile value of this distribution as the safe-distance. This was selected because is an equilibrate criteria that offers an adequate protection to people and reasonable planning and response emergency costs. The use of a greater percentile could unnecessarily increase the risk of the people exposure at the beginning of the accident. Figure 8 shows the 90-percentile (*PAD*) and the distance distribution of a chlorine release in the circumvallation highway of Rosario city.

4. Conclusions and future works

A software to be applied in Risk analysis and Emergency planning, STRRAP, is presented. This system can be used for static emission points (for example storage tanks, stacks, etc.) or for mobile sources, like the hazardous material transportation problem (road, rail, pipeline, etc.). The road is discretized in several sectors. Output histograms are calculated in short time covering all road sectors.

Our model considers variability of population density, meteorological variables and accident scenarios.

Although this prototype of STRRAP has only the possibility to simulate gas diffusion scenarios, other common types of accidents like fire or explosions (see the interesting work of Papazoglou et al. [7]) can be easily included. In future works, this procedure will be applied to the most representative scenarios in a general risk assessment context (for example fire, microorganism diffusion and particulate material diffusion, etc).

For graphical representation, STRRAP can interact with AUTOCAD. Currently, its interfacing with the GIS system (Geographical Information System) is being analyzed [8].

5. Acknowledgments

The authors thank to Universidad Tecnológica Nacional, CONICET and Agencia Nacional de Promoción Científica y Tecnológica for their financial support to carry out this work

6. References

[1] E. Planas-Cuchi, H. Montiel, and J. Casal, "A Survey of the Origin, Type and Consequences of Fire Accidents in Process Plants and in the Transportation of Hazardous Materials", *Trans. I.ChemE*, Vol. 75, part B, pp. 3-8, Feb. 1997.

[2] Brown, D.F.; Policastro A.J. et al: "Development of the Table of Initial and Protective Action Distances for the 2000 Emergency Response Guidebook. October 2000.

[3] A. Santa Cruz, N.J. Scenna, and M. Muñoz, "A Computational System for Risk Analysis of Incidental Toxic Gases Releases Considering Stochastic Variables", *JAIIO 2002*.

[4] N.J. Scenna, and A. Santa Cruz, "Chlorine transportation risk assessment in Rosario city", *sended to Reliability and System Safety for publication, 2004*.

[5] J. A. Havens, and T.O. Spicer, "Development of an Atmospheric Dispersion Model for Heavier-than-Air Gas Mixtures", *Final Report to U.S. Coast Guard*, CG-D-23-85, USCG HQ, Washington, DC, May, 1985.

[6] Scenna, N.J.; Santa Cruz, A. S. M.; Godoy, S. M.; Biscotti, P.S.: "STTRAP- A Software for Application in Risk Analysis and Emergency Planning", *AST 2004*.

[7] I. Papazoglou, Z. Nivolianitou, O. Aneziris, M.D. Christou, G. and Bonanos, "Risk-Informed Selection of a Highway Trajectory in the Neighborhood of an Oil-Refinery", *Journal of Hazardous Materials*, A 67, pp. 111-144, 1999.

[8] M.D. Abkowitz, P.D.M. Cheng, and M. LePofsky, "Use of Geographical Information System in Managing Hazardous Materials Shipments", *Transp. Res. Record*, 1261, pp. 35-39, 1990.

DEGADIS, EPA, United States Environmental Agency, Air Quality Models, http://www.epa.gov/scram001/t22.htm.

7. Figures

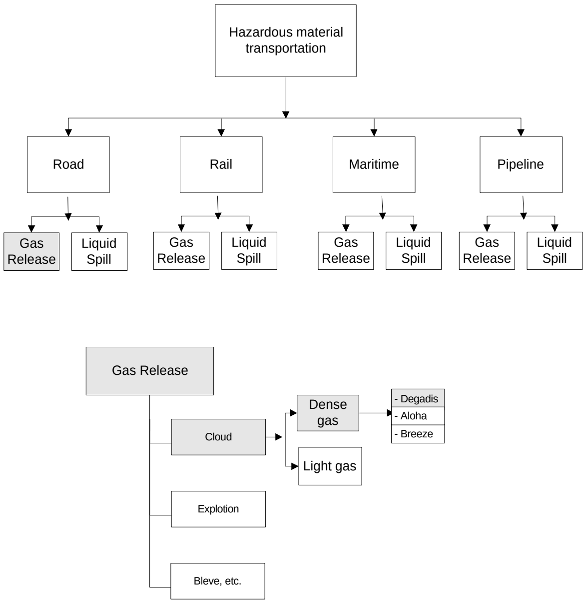


Figure 1. Event tree for evaluating transportation accidents

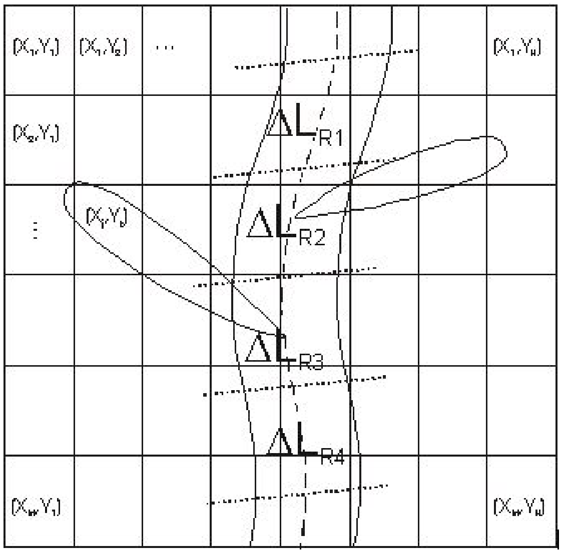


Figure 2. Discretization of the emission points and the receptor grid points.

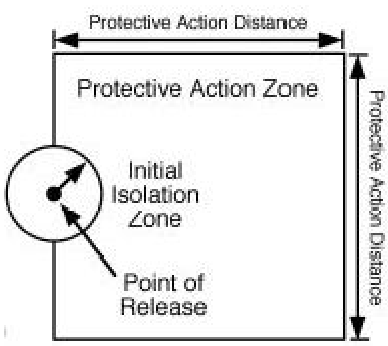


Figure 3. Representation of Initial isolation and Protective action zones.

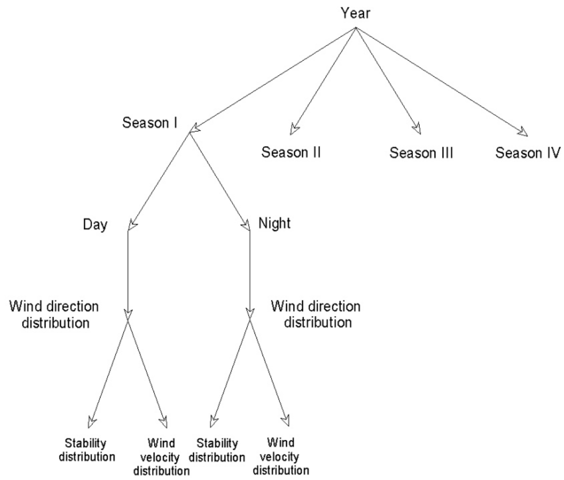


Figure 4. Hierarchical levels of probability density functions

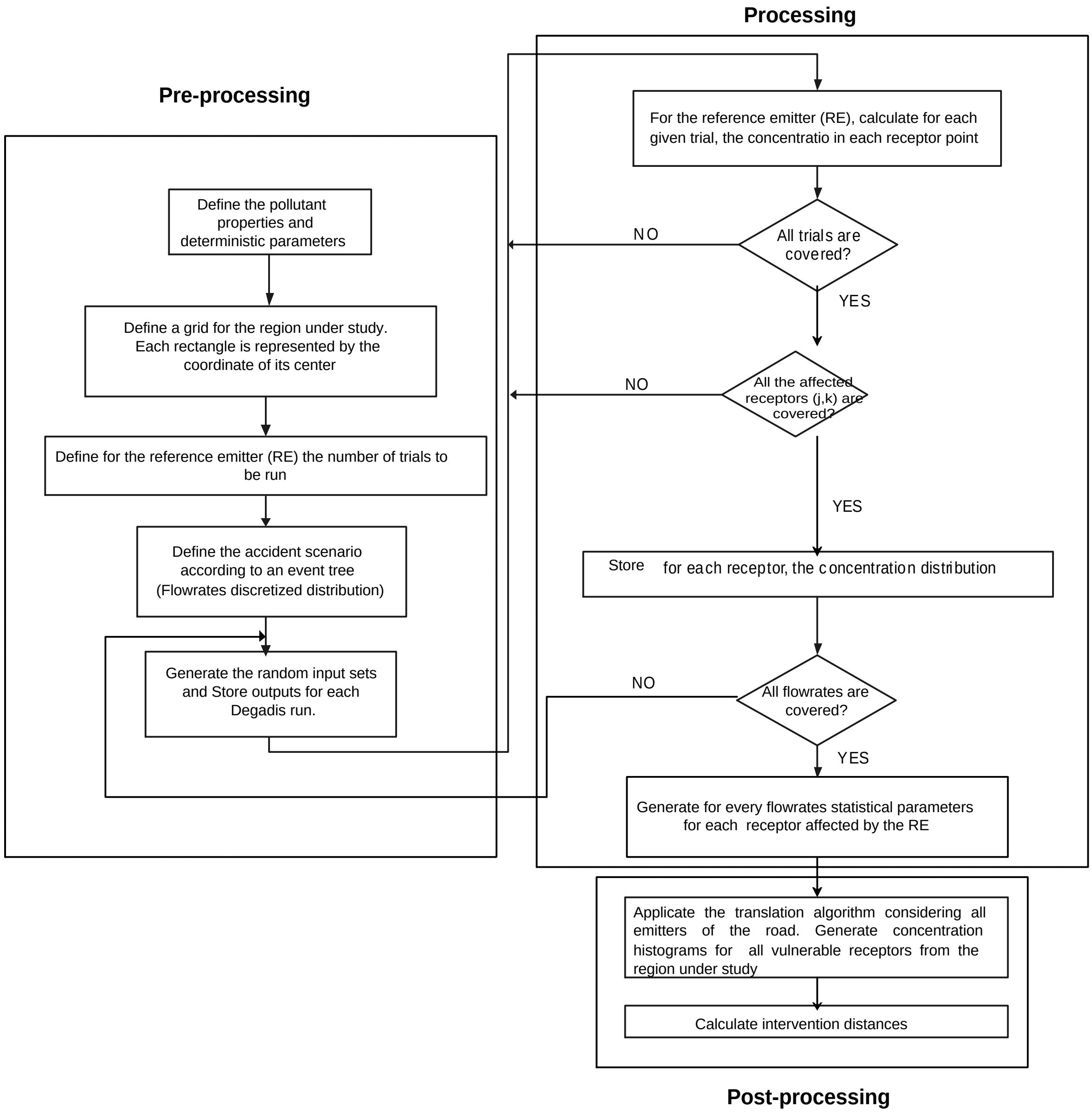
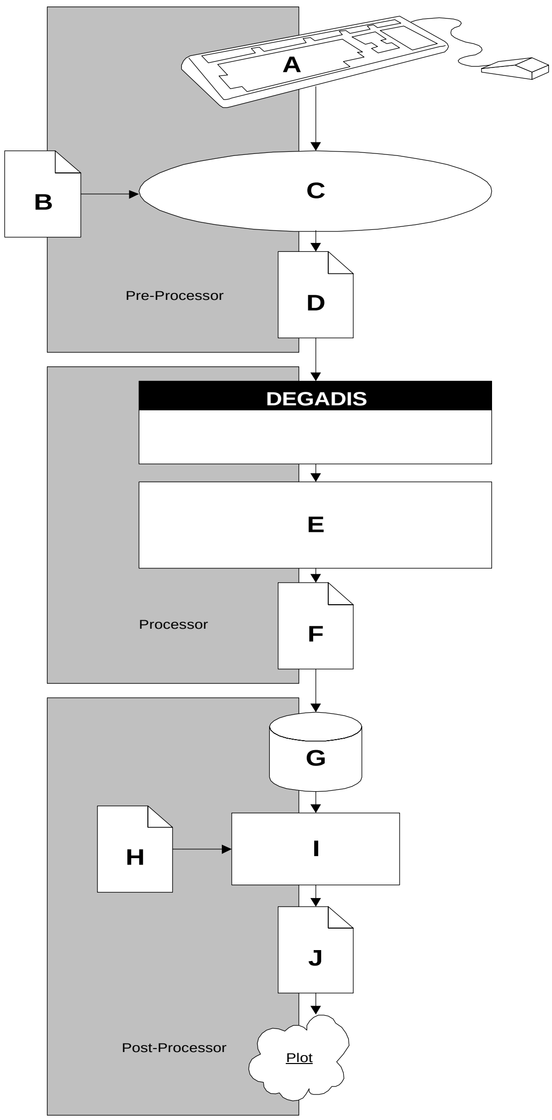


Figure 5. The Pre-processor - Processor - Post-processor cycle



A - Pollutant identification, flow rates, type of release, etc.

B - Probability distribution of meteorological variables

C - Random cases Subroutine

D - Input file for DEGADIS

DEGADIS: Diffusion Model

E - Coordinate-change Subroutine

F - Outputs of the modulus of calculus

G - Data Base

H - Emitter coordinates

I - Translation algorithm Subroutine

J - Concentration histograms for all receptors and distances distribution

Figure 6. Flow diagram of the computational system

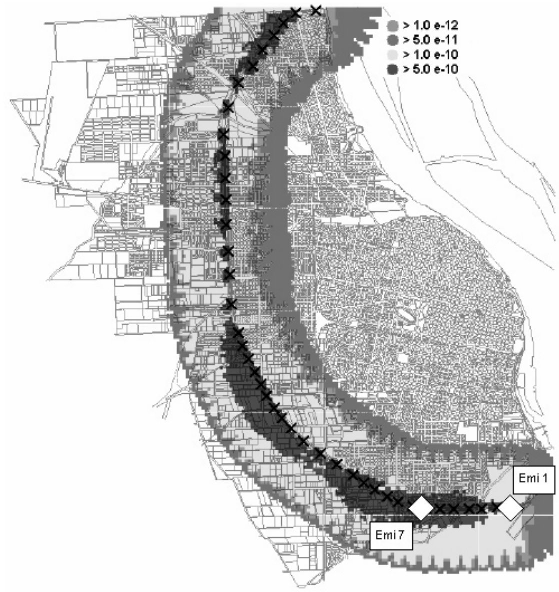


Figure 7. Iso-risk map. Rosario city circumvallation

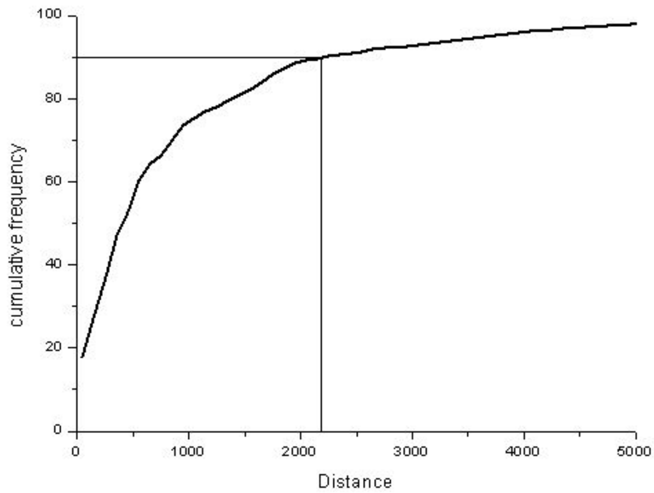


Figure 8. PAD and Distance distribution for a chlorine release