# DEVELOPMENT OF A SIMULATION TOOL FOR CONSECUENCE ANALYSIS IN INDUSTRIAL INSTALATIONS

Pérez V. (a), García G. (b), Ávila M.G. (c), Castellanos F. (d), Wellens A. (e)

Facultad de Ingeniería, UNAM-MEXICO

(a) victorphz@comunidad.unam.com.mx, (b) gamarzaid@hotmail.com, (c) gavila@hotmail.com, (d) ing.fcastellanos@gmail.com, (e) wann@unam.mx

### **ABSTRACT**

At present, a variety of models exist to estimate the magnitude of the consequences of different types of accidents, most of them having an empirical basis. These models aren't for exclusive use in industrial facilities and can also be used for consequence analysis in for example chemical or petroleum industries or in environmental impact studies. Although a wide variety of mathematical expressions are available for events as unconfined or confined explosions, liquid spills or gas leaks, releases of hazardous materials, BLEVES or fires, few simulation packages exist that can assist a non-specialist in decision making related consequence analysis. In general, existing simulation packages are not freely available for undergraduate students due to their costs, accessibility or required knowledge.

This paper describes the development of a didactic tool for the simulation of accident consequences, for academic and free use in the Departamento de Ingeniería Mecánica e Industrial of the Universidad Nacional Autónoma de México. The software is being developed using Visual Basic, as this is a widespread developing platform, easily accessible and quick to assimilate among the students of the different disciplinary areas of the engineering faculty.

Keywords: Consequence Analysis, Dispersion Modeling, CALPUFF, AERMOD.

## 1. INTRODUCTION

Currently, due to the large amount of consumer goods that are required to meet the needs of human beings, is process-intensive industrials as well as more raw materials in most cases are classified high risk by flammability and instability of these (usually fuel).

No wonder that major recorded accidents occur:

- Chemical industry
- Oil industry
- Transportation of materials
- Accidents industrials within plants (mainly boilers and leakage of materials).

Predicting this type of accident is difficult especially if there is not a vitacor maintenance or there is no process for responding to incidents of any kind.

For this reason, it is important to keep in mind that while an incident is not present, does not mean it can not happen.

To estimate consequences of the eventualities of this nature has been developed simulation models are empirically based and that the occurrence and some kind of accident will always occur in an unpredictable manner so that the models allow an estimate of the magnitude of the consequences that could trigger an unwanted event before.

Based on historically recorded events such methods have been tested and types of incidents that are triggering the methods of these have been classified into the following groups:

- BLEVE
- Leaks
- Fires
- UVCE
- Explosions
- Detonations
- Implosions

In this work has been developed a computational tool (software) that grouped the different types of incidents for which has developed a simulation model in order to provide a tool to determine the main variables considered to estimate the magnitude of the consequences that may occur in the event of the event (accident).

In these models, use is made of physical parameters to estimate the conditions that affect the severity of the event (usually environmental conditions) as well as being specific to each type of incident.

Later succinctly addresses each of these events and shows the implementation within the computational tool presented here.

### 2. PROPOSED METHODOLOGY

The implementation of the models related to the analysis of consequences in case of accidents industrials described here, has developed a computational tool (software) in order to make a contribution to the academic faculty for teachers to students in different disciplinary fields in the Faculty of Engineering, UNAM, although initially considered as a support to those related to Industrial Engineering.

In this first version of the tool has been considered as a development platform to Visual Basic as the language of simplicity, versatility, syntax and semantics digestible and available to students without further delay.

It is considering the software is enriched in the near future in order that it can be a powerful tool strong and competitive open source and freely distributed through information technologies, including Web.

Overall, the development of the tool and its expected evolution is intended to have a robust tool for analysis of impact and implications for coping with the lack of resources needed for the acquisition of commercial tools such as the CALPUFF or AERMOD (although their focus is oriented towards the analysis of dispersion).

### 3. DEVELOPMENT

### 3.1. BLEVE

The BLEVEs (Boiling liquid expanding vapor explosion) is a type of mechanical explosion which corresponds to a special case of catastrophic explosion of a pressure vessel in which it occurs a sudden escape to the atmosphere of a large mass of fluid (gas or liquefied pressure) overheated.

The main feature is that the explosive expansion of the entire mass of liquid evaporates suddenly, increasing its volume 200 times.

The variables that most interest for this type of incident are:

- Critical temperature and pressure (thermodynamics).
- Fragments of materials.
- Number of fragments.
- Initial speed.
- Average speed.
- Overpressure.
- Speed of fragments in function away.
- Maximum distance range of the fragments.
- Thermal radiation.
- Diameter of the fireball.

- Initial diameter at ground level Hemisphere.
- Height of the fireball.
- Duration of the fireball.
- Thermal radiation received.

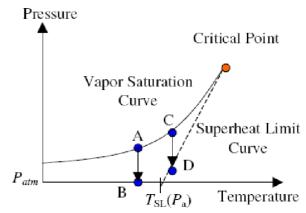


Figure 1. : Reid's 'Superheat Limit Temperature' theory for BLEVE formation.

### 3.2. FIRES

Due to the nature of the different materials used in industry and the environmental conditions that combine at some point, the fires have originated in material spills and from this state branches into evaporator, scattering clouds flammable pool fire, flash fire type, dispersions with concentration and toxic clouds depending on the case (see Figure 3).

To analyze the effects that are of interest to such incidents, the main variables of interest are related to thermal phenomena: thermal radiation, atmospheric transmissivity (tau), burning rate, flame height and diameter of the fire.

When facilities are closed and contained, is formulated in a manner equivalent to the radius of the rectangle of a puddle.

In the case of fire in the form represented in the figure, comparable to a liquid fire poured into a bucket, pond or swimming pool angular.

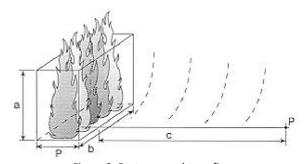


Figure 2. Features pool-type fire.

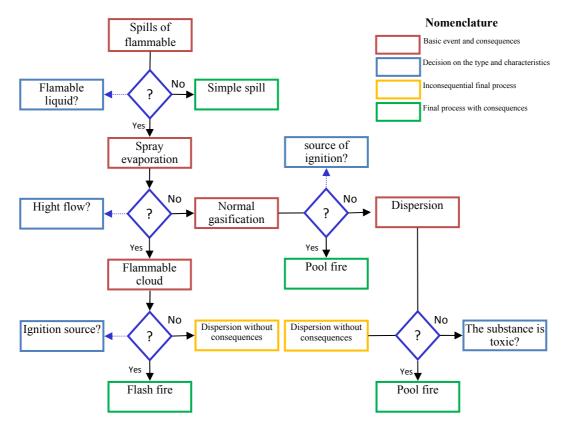


Figure 3. Classification of consequences

# 3.3. VAPOR CLOUD EXPLOSION NOT CONFINED (UVCE)

Such events can be defined as: Explosion explosive cloud of flammable gas which is in a large space, which pressure wave reaches a maximum pressure of about 1 bar in the ignition.

Unconfined explosions occur outdoors and are usually caused by a quick release of a flammable fluid with a moderate dispersion to form a large flammable cloud of air and hydrocarbon.

The parameter generally defined and measured is the pressure generated by the pressure wave as they propagate undisturbed through the air. Figure 4 shows graphically the value of the pressure versus time.

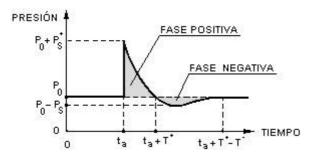


Figure 4. Variation of the pressure wave of an explosion.

In general, the vapor cloud explosions are not confined explosions and rarely have become detonations.

In the case where an explosion is not reached, there would be a quick way to fire blaze that could be defined as a fire called progressive diffusion or premixed flame at low speeds without causing pressure wave. Its most important effect would be the thermal radiation.

The parameter that most interested in this type of event corresponds to the pressure as shown in the figure 4, the pressure can be determined is maximum incident overpressure, maximum lateral pressure, dynamic pressure and overpressure reflected.

### **TNT Assessment Model**

It is based on the hypothesis of equivalence in blast effects from a given mass of inflammable material and a TNT.

In the explosion of a vapor cloud the shape of the initial wave of the explosion is different than an explosion of TNT, but from a distance both can be considered equal to that shown in Figure 4. The model establishes the following relationship:

$$W = \frac{\eta M - E_c}{E_c T N T}$$

W = TNT equivalent mass (kg)

M = Mass of flammable substance released (kg)

η = Performance (effectiveness) of the explosion empirical (0.01 to a 0.10).

 $E_c = Lower heat of combustion of flamable gas or vapor <math>\binom{kj}{kg}$ .

 $E_cTNT = Heat of combustion (detonation)$ of TNT (4437 A 4765  $\frac{kj}{ka}$ )

Once you calculate the TNT equivalent mass is used in Figure 5 for the most important parameters in terms of climbing distance Z.

$$z = \frac{R}{\sqrt[3]{W}}$$

 $R = Real \ distance \ in \ meters \ (m)$ 

W = Equivalent mass in kg.

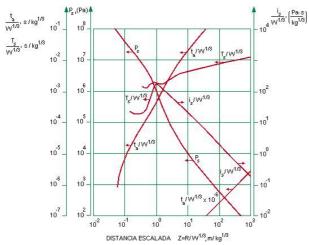


Figure 5. Parameters of the explosion based on the distance climbing.

 $P_3 = Maximum incident pressure in Pascals (Pa)$ 

 $is = Specific impulse in Pascal \cdot Second (Pa \cdot s)$ 

ta = Arrival time of the shock wave in seconds (s)

Ts = Duration of the overpressure positive phase of the shock wave in seconds (s)

### 4. RESULTS

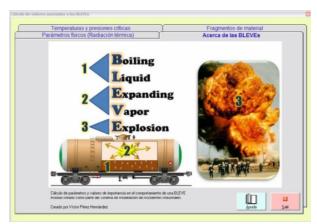


Figura 6. BLEVE Module

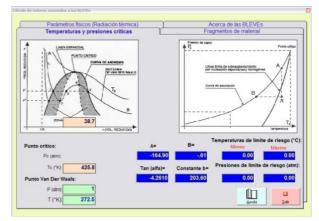


Figura 7. BLEVE - Determination of F and T.

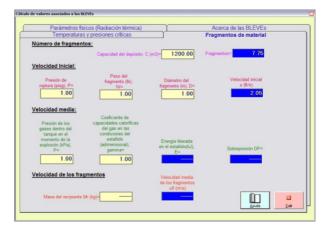


Figura 8. BLEVE - Determination of fragments



Figura 9. Liquid discharges

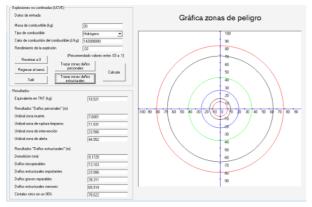


Figura 10. TNT equivalent explosion model

### 5. CONCLUSIONS

A simulation model was developed in Visual Basic; it is able to determine the adverse consequences of dangerous physical phenomena in industrial accidents. At this stage, the tool determines typical values related with the occurrence of BLEVES, fireballs, fires, UVCE explosions and spills. Future work includes integration the different modules in an expert system, able to define which type of accident can occur depending on existing ambient conditions, migrate the system to a more powerful developing platform and publish the system in web

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### **BIOGRAPHICAL NOTES**

Ann Wellens is a chemical engineer with postgraduate studies in Industrial Administration (KUL, Belgium) and a master degree in Environmental Engineering (UNAM, Mexico). At the moment she is a full-time lecturer in the Systems Department of the Industrial and Mechanical Engineering Division of the National University of Mexico (UNAM). She has been working in air pollution issues for the last 15 years, dictating courses, collaborating in research projects and participating in conferences related with mathematical modeling of air pollution dispersion and statistics.

Francisco Castellanos D. obtained his bachelor degree in Industrial Engineering (ITESM Campus Central de Veracruz, México).

Gamar Castillo G. obtained his bachelor degree in Computation Engineering (UNAM, México).

María Guadalupe Ávila G. obtained his bachelor degree in Computation Engineering (UNAM, México).

Víctor Pérez H. obtained his bachelor degree in Computation Engineering (UNAM, México).