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Consequence analysis in LPG installation using an integrated computer package

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Abstract

This paper presents the prototype of the computer code, Atlantide, developed to assess the consequences associated with accidental events that can occur in a LPG storage plant. The characteristic of Atlantide is to be simple enough but at the same time adequate to cope with consequence analysis as required by Italian legislation in fulfilling the Seveso Directive. The application of Atlantide is appropriate for LPG storage/transferring installations. The models and correlations implemented in the code are relevant to flashing liquid releases, heavy gas dispersion and other typical phenomena such as BLEVE/Fireball. The computer code allows, on the basis of the operating/design characteristics, the study of the relevant accidental events from the evaluation of the release rate (liquid, gaseous and two-phase) in the unit involved, to the analysis of the subsequent evaporation and dispersion, up to the assessment of the final phenomena of fire and explosion. This is done taking as reference simplified Event Trees which describe the evolution of accidental scenarios, taking into account the most likely meteorological conditions, the different release situations and other features typical of a LPG installation. The limited input data required and the automatic linking between the single models, that are activated in a defined sequence, depending on the accidental event selected, minimize both the time required for the risk analysis and the possibility of errors. Models and equations implemented in Atlantide have been selected from public literature or in-house developed software and tailored with the aim to be easy to use and fast to run but, nevertheless, able to provide realistic simulation of the accidental event as well as reliable results, in terms of physical effects and hazardous areas. The results have been compared with those of other internationally recognized codes and with the criteria adopted by

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Italian authorities to verify the Safety Reports for LPG installations. A brief of the theoretical basis of each model implemented in Atlantide and an example of application are included in the paper.

Keywords: LPG; Consequences analysis; Software package; Quantified risk analysis

1. Introduction

Hazards associated with the storage, handling and use of LPG are well known and the Italian authorities, during the last years, promoted a series of legislative modifications to improve the design and inspection of LPG installations and to achieve a better control of their risks.

In addition, some accidents recently occurred in Italy have highlighted the hazards posed by such installations, often located nearby populated areas and, consequently, the need to assess their compatibility with the territory and to plan the emergencies.

The risk analysis of LPG installations, that, integrated with other information, shall be included in the Safety Reports, allows to reach these objectives, provided that the analysis is complete and based on recognized standards and criteria. In order to give guidance how to comply with legislation, the Italian authorities have proposed a minimum set of accidental events, depending on the typology of the LPG installation, that should be considered and have represented the magnitude of the consequences that are expected by means of nomographs.

The analyst shall analyze these accidental events and assess their likelihood and consequences, or demonstrate the reasons for inapplicability on the basis of specific design features (i.e. for mounded storage vessels the Hot-BLEVE is not credible).

To assist the user in selecting the accidental events and in assessing their consequences an integrated package can be useful to ensure completeness and correctness of the analysis. With this purpose, the integrated software code Atlantide has been developed.

This code has been already utilized in some projects. So, its ability to fulfill the legislative requirements and to reduce the time required for the analysis has been demonstrated.

The bases, the structure, the models and the procedures implemented in the code are presented in this paper.

2. Quantified risk analysis in LPG installation

The Quantified Risk Analysis (QRA) represents a well defined procedure to be applied in order to both assess the degree of safety of a petrochemical plant and evaluate the risks associated with the installation itself.

The main steps of evaluations to be performed in order to reach these objectives are described below.

2.1. Hazard identification

The knowledge of what can go wrong is the first stage of the risk assessment process. Hazard identification involves the investigation of all the situations that may cause a potential accident, followed by an analysis of the combinations or sequences of events which could produce this. Typical hazard identification techniques are:

- check lists
- statistical analysis
- FMEA
- HAZOP

Among these, the Hazard and Operability analysis (HAZOP) is the technique most frequently used for considering, systematically, deviations from the design intent by the application of a series of guide words to process parameters, in order to identify possible problems [1]. This technique is completely general and can be applied to processes of any type or complexity.

In LPG installations no process operations are performed; therefore the expected accidental events can be attributed to random causes (i.e. failure due to material defects, wrong assembly/maintenance), external causes (collisions, fire) and misoperation during transferring operations (incorrect coupling of loading/unloading arms).

2.2. Probability evaluation

The probability evaluation requires the determination of the circumstances and conditions which the occurrence of a hazardous events are depending on and how those are interrelated. It allows to estimate the expected frequency of occurrence of an accidental event.

This is frequently performed by Fault Tree analysis, i.e. a logic combination of causes which may induce a specific undesired event (top event) coupled with event tree analysis, to identify the scenarios associated with the top event [2].

For loss of containment events, statistical data from data bank [3] are usually used.

2.3. Consequence analysis

The scope of this analysis is to evaluate the physical effects of the release of hazardous substances or energy following the accidental event.

Subsequently, based on the intensity of these effects, it is possible to assess the damage to the people and/or property (vulnerability).

To perform the consequences analysis it is necessary to characterize the evolution of the accidental event; the complete assessment is generally structured as follow.

(1) *Source term characterization* which is strictly related to the typology of accidental event and allows to identify the characteristics of the release (flow-rate, quantity, physical conditions, etc.).

The substances present in bulk in LPG installations are C3–C4 mixtures ranging from propane to butane which behave as a gas liquefied by pressure (i.e. flashes at atmospheric pressure producing a dense heavy flammable cloud).

Table 1
Threshold values for injuries/damage (translated from Italian regulation [6])

Physical phenomena	Effects				
	High lethality level	Start of lethality	Irreversible injuries	Reversible injuries	Structural damage
Pool/Jet-fire (stationary heat radiation, kW/m^2)	12.5	7	5	3	12.5
BLEVE/Fireball (transient heat radiation, kJ/m^2)	fireball radius	350	200	125	100 m (from Bottling); 600 m (from Spheres); 800 m (from Bullets)
Flash-fire (concentration limit)	LFL	1/2 LFL			
Explosion (Side-on overpressure bar)	0.6 −(0.3)[a]	0.14	0.07	0.03	0.3

[a] Value to be considered in presence of buildings/structures which collapse can cause indirect fatality.

(2) *Identification and study of physical phenomena involved* which, based on the source term characteristics and external conditions (i.e. meteorological conditions, presence and type of ignition, etc.) allows to identify the intermediate (e.g. Dispersion) and final phenomena (Fire and Explosion). Subsequently, by using mathematical models it is possible to evaluate the effects of thermal radiation, overpressure and missile generation.

The main consequences expected in LPG installations are associated with the effects of a catastrophic release (i.e. BLEVE) or to the combustion of the products released (either in liquid and/or vapor form) following an accidental event.

(3) *Damage assessment*, this step of the analysis allows to determine the damage produced by thermal radiation as well as by the overpressure effects on the population and property. Vulnerability models that rely on Probit equations [4] or simple effects → damage correlations can be used. For LPG installations toxic effects are not of concern and the Italian regulation [6] recommends the use of the threshold values given in Table 1 for the other effects.

2.4. Risk assessment

The combination of the probability of the accident with the damage allows the definition of the individual and social risk posed by the installation. This step is not required by the Italian regulations; the local authorities perform their judgment on the plant acceptability on the basis of both the probability of the accident and the magnitude of the consequences, without considering the combination of the two aspects.

Also for LPG installations, the Italian regulations [5,6], which implement the Seveso Directive on Major Hazards [7], prescribe to develop a Safety Report which shall include the description of accidental scenarios with a synthesis of the main results of the analyses performed according to the previous steps.

In addition a ranking of the plant based on the application of an Hazard Index method shall be provided [6].

The above information is used by authorities for land-use planning, in the vicinity of the installation, for defining emergency/intervention procedures and for imposing plant improvements in case of high risk to personnel and population.

The computer code Atlantide aims essentially at carrying out the consequence analysis in a risk assessment.

3. Description of the procedure and approach used

3.1. Event identification

An LPG storage installation can be subdivided, according to the Italian regulation [6], in some units, depending on the typology of the operations performed (storage, loading/unloading, bottling, pumping/compressing and associated piping).

The Atlantide software package starts from the definition of the substance involved, area of interest and main operating conditions.

For each of these areas appropriate accidental events, based on historical experience and statistical analysis, are automatically identified. The applicability of all the proposed accidental events and/or the necessity of integration should always be verified by the analyst on the basis of an Hazard and Operability analysis and specific Design Reviews. An example with the list of accidental events for the storage area is given in Fig. 3 (on Section 5); between these the analyst will select the ones he is interested to examine.

Given the characteristics and the conditions of the substances handled or stored, the releases originated in the LPG units can be assimilated either to a vapour or to a flashing liquid outflow which, hence, groups part of the accidental events pertinent to each area. In such a way, the characterization of each accidental event is drastically simplified because it can be done only by knowing the design features, the process conditions, the applicable failure case and then selecting an initial release size and orientation.

3.2. Scenarios evolution

The evolution of each release is represented using cause–consequence diagrams (Event Tree) that, starting from the initial accidental event, allow to build all the plausible scenarios. The influence of the different external conditions, such as presence of obstacles, ignition sources/delay, etc. are identified by ‘‘yes’’ or ‘‘no’’ at each branch of the Event Tree diagram, depending upon their possibility to occur. This representation identifies the intermediate analyses at each branch to arrive to the final event characterization.

The Atlantide code includes four Event Trees describing a continuous vapor release, an instantaneous release (following a vessel catastrophic failure), a continuous two-phase release with and without liquid rainout (accumulation) onto the ground. Fig. 1 shows the evolution of a flashing liquid release with possibility of rain out as in case of a jet flow that impacts onto the ground.

The four scenarios analyzed represent the set of all the phenomena that can derive from a loss of containment event or an emergency situation in a LPG installation; the final events studied are: Jet-fire, Pool-fire, Fireball/BLEVE, Flash-fire and Explosion (UVCE).

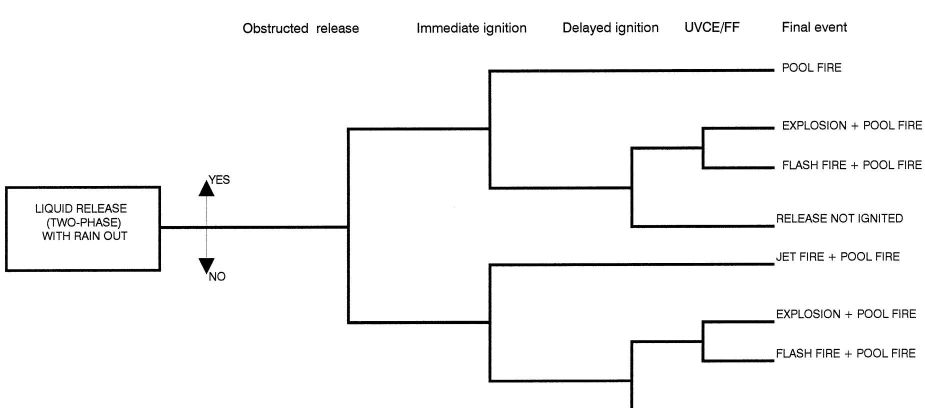

Fig. 1. Typical Event Tree for a flashing liquid continuous release.

Depending on the layout of typical LPG installations, UVCE analysis is performed only if the quantity of flammable gas in the cloud is greater than 100 kg [8], where damaging overpressure are expected. Otherwise, only the Flash-fire phenomenon is considered.

The presence of safety measures, like containment bunds, has been considered during the liquid spreading/evaporation analysis and in the calculation of thermal effects from pool fire.

The domino effect related to a flame impingement on a mobile tank in the loading area that can generate a Fireball is also taken into account.

3.3. Consequences modeling

From the sequence of events defined by the Event Trees it is possible to perform a series of calculations that, starting from the evaluation of mass flow rate or released quantity, cover the analysis of spreading and evaporation of the liquid onto the ground and the dispersion in the atmosphere of the released gas or evaporated liquid.

This allows to obtain the input data for the simulation of the relevant final phenomena and consequently to determine the physical effects originated from the release of energy (thermal radiation load and overpressure intensity) as well as to estimate the area where damage are expected. Missiles effects from vessel fragmentation are not analysed but information such as number of fragments generated or maximum range can be obtained from statistical data published in literature [11].

The relations implemented in the code to perform the analysis of an accidental release, from source term evaluation to the final phenomena simulation, are given in Appendix A. A series of comparisons with the results given by more sophisticated programs and/or experimental data has been performed during the implementation of

Table 2
Comparison between Thermal Radiation distances (m) calculated with Atlantide (Code 1) and FRED (Code 2) for an horizontal jet-fire of propane

Mass flow rate (kg/s)	Thermal radiation level (kW/m^2)							
	12.5		7		5		3	
	Code 1	Code 2	Code 1	Code 2	Code 1	Code 2	Code 1	Code 2
1	15.5	15	16.8	16.3	17.7	17.2	19.5	19.5
2	21	20.8	22.2	23	24.21	24.5	26.7	27
3	25.2	25.5	27.5	27.8	29	29.5	32.2	34
4	28.7	27	31.4	32.5	33.3	34.5	37	39
5	31.6	32	34.6	35	36.7	37.5	40.7	43.5
6	34.5	34	37.8	38	40.2	41.2	44.6	46
7	37	37.2	40.6	41	43	44.5	48	50
8	39.3	39	43	44	45.9	47.5	51	53.5
9	41.5	41	45.6	45.8	48.5	50	54	58
10	43	43.5	48	48.5	51	52.5	57	60
20	59	58	65	66	70	71	78	81.5
30	70.5	70	78	79.5	83.6	85.5	94	99
40	79.5	79	88.3	89	94.7	98	106.7	115

the models and relations. In general the agreement is good and acceptable for the purpose of the code; the details of the validation executed are described in Ref. [12].

An abstract of these results is given in Table 2, shown are the thermal radiation distances from an horizontal jet-fire calculated with Atlantide vs. the ones obtained with a confidential effects calculation program [23] developed by an international oil company. The excellent agreement demonstrates the correct implementation of the model used [19].

A specific Flash-fire model is not included in this release because it is assumed, as generally recognized [9], that the hazardous area extends up to the LFL/2 boundary of the dispersed cloud. This is also confirmed from preliminary comparisons with the results obtained using an accurate program based on a revision of Raj and Emmonds model [10].

Neither the effects of cold BLEVE (overpressure generation, missile propagation) associated with the violent flash-evaporation in case of rapid depressurizing due to a catastrophic rupture are included in this preliminary release of the program. An additional model simulating this effect could be easily added. However, it has to be verified, according to some theories, that the conditions necessary so that the phenomenon happens are met at the instant of failure [11].

4. Program structure

The software package ATLANTIDE has been developed to implement the models and correlations summarized in Appendix A and to perform the analysis as described in Section 3.

Atlantide runs in MS-Windows™ environment; the program uses applications of Delphi 1.02 (by Borland) which is a Object Oriented Program in Object Pascal language.

A flow diagram representing the structure of Atlantide is given Fig. 2. A full description of the code is given in Ref. [12].

The substances treated by the code are:

-LPG

-Butane

-Propane

The chemical and physical properties (densities, heat capacities, vapor pressure, flammable limits, etc.) of these substances are stored in a database which can be easily retrieved once the substance is selected; the user can insert the operating pressure and temperature to obtain the values of the properties of interest.

Once the substance and relevant operating conditions have been chosen, meteorological conditions (ambient temperature, wind velocity and humidity relative) must be introduced to start the analysis.

Then, according to Section 3.1 the unit of concern has to be selected and one of the relevant accidental event to be analyzed has to be chosen from the proposed list (see Fig. 3 in Section 5).

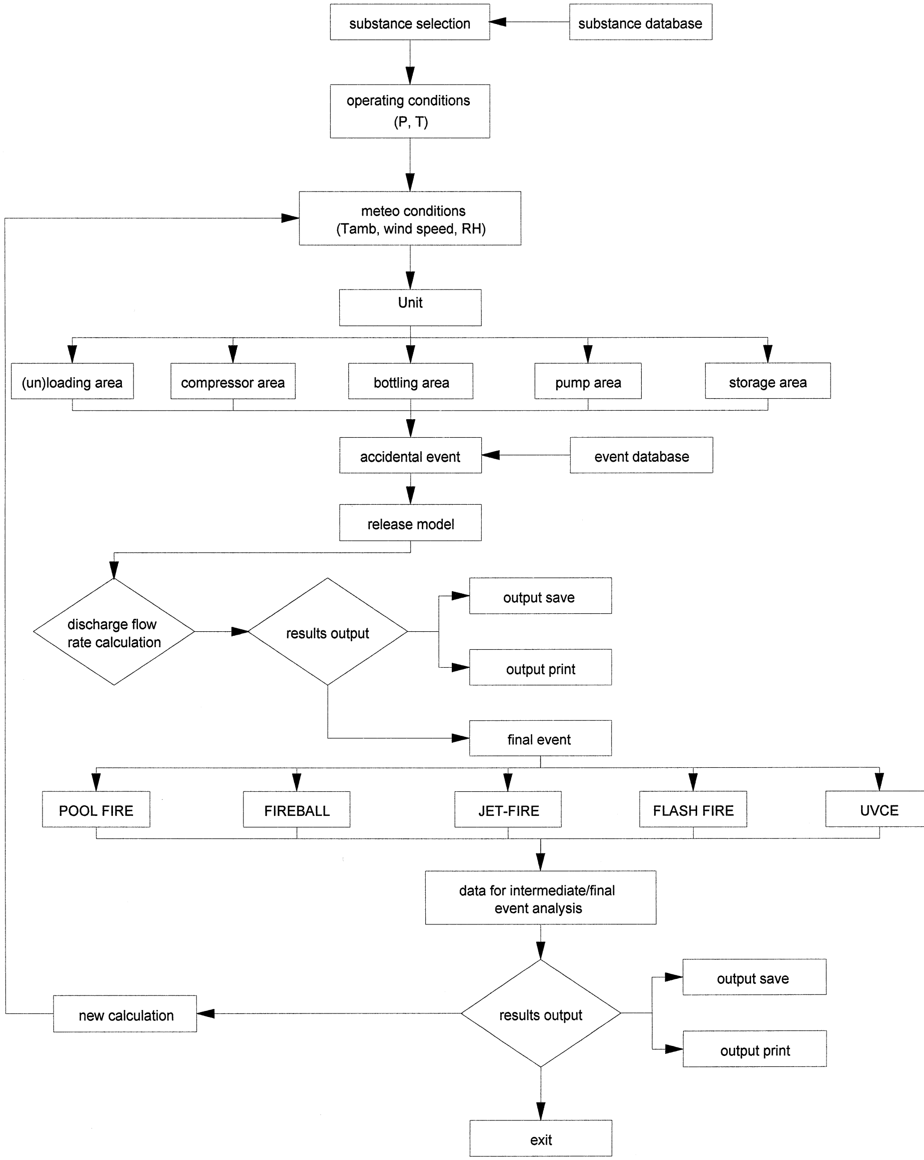

Fig. 2. Flow diagram of Atlantide code.

The first step of calculation in Atlantide is the evaluation of the release flow rate on the basis of the input data (rupture size); this gives output data which are used as input for the subsequent calculations, according to the branch of the sequence. As described in Section 3.2, the analysis is strictly related to the final events which are activated depending upon the applicable scenario.

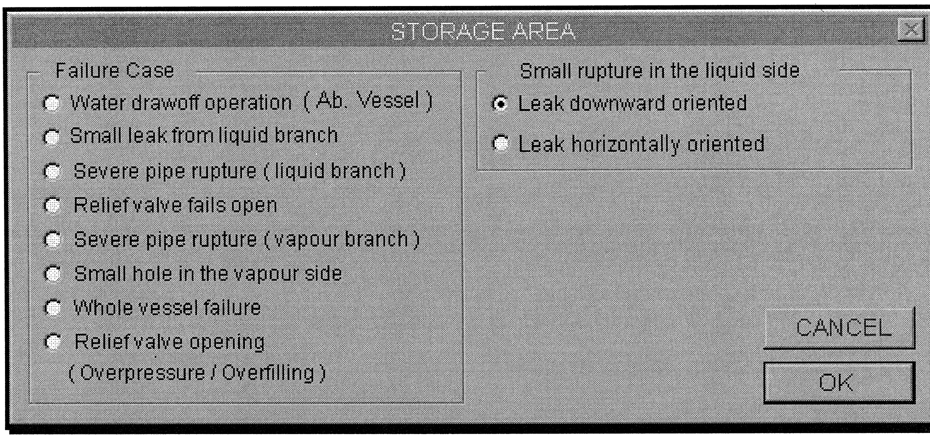

Fig. 3. Atlantide screen output with accidental events relevant to the storage area.

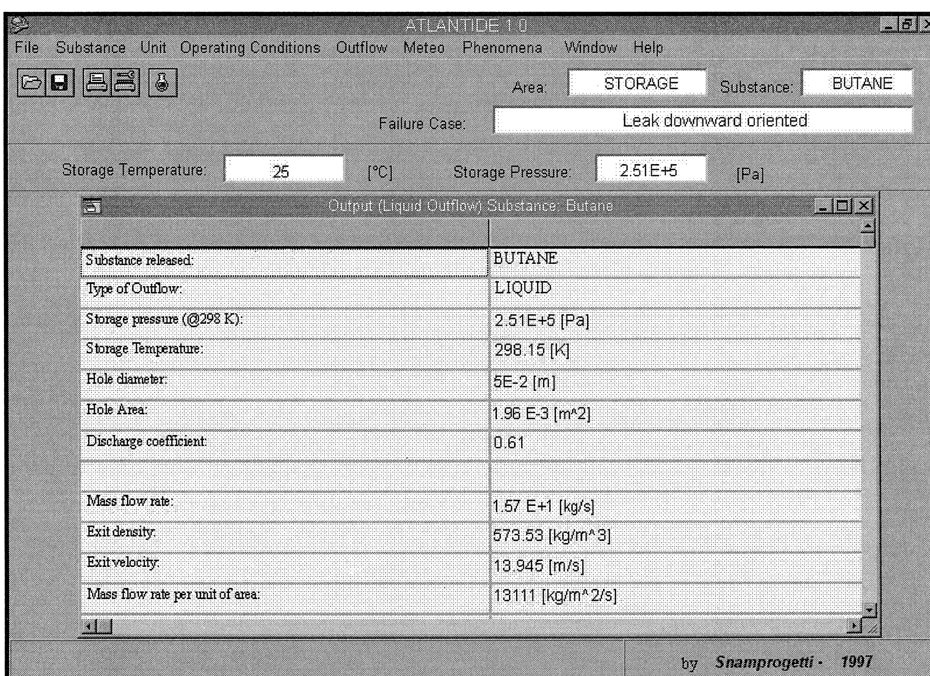

Fig. 4. Atlantide screen output with outflow results for the sample case.

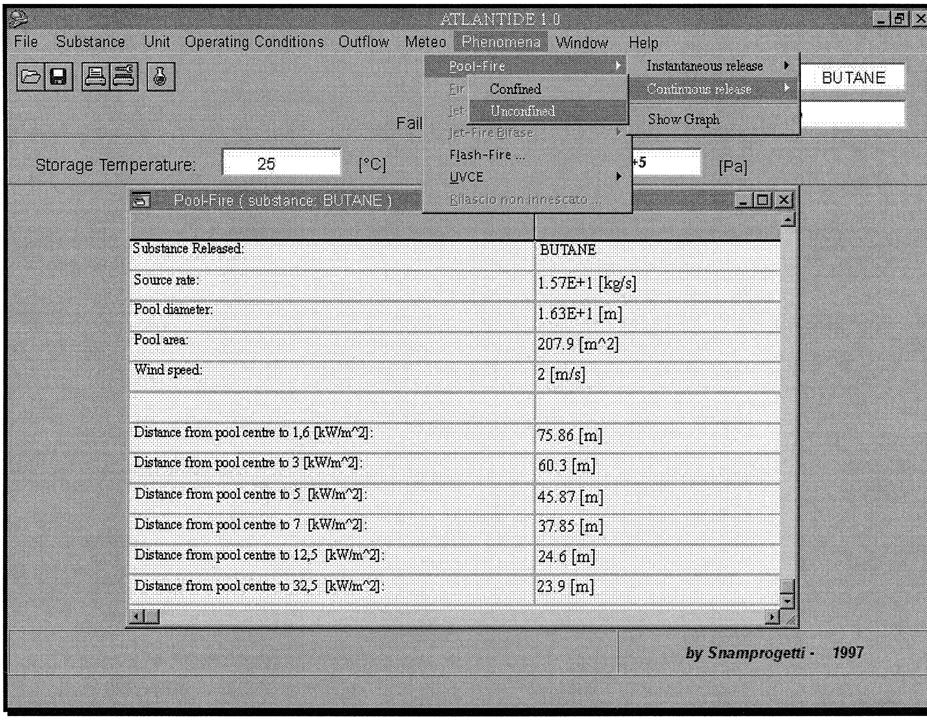

Fig. 5. Atlantide screen output with thermal radiation distances for the sample case.

At prefixed steps of calculation, the check of the intermediate output/input data may be requested. Some data can be modified to perform comparative analysis without the necessity to restart the whole study.

The second step of calculation gives the magnitude of the associated consequences, as result of the analysis of the final events (phenomena), in terms of hazardous distances and related damage; both in tabular and graphical format/output (see Fig. 5 in Section 5).

Default threshold limit values for effects are adopted according to the Italian regulation [6]; however, other values can be chosen for the main phenomena (e.g. Jet-fire, UVCE). For thermal radiation and for overpressure effects, the following results are given:

- distance where the threshold limit values are reached;
- magnitude of the consequences at user defined distances.

5. Example of application

An example of application of Atlantide is described below.

It refers to a liquid release, downward oriented, from the bottom of a storage vessel with the formation of a pool-fire (in case of immediate ignition).

Table 3
Differences between Atlantide and D.M. 15/05/96 [6] for the sample case

Thermal radiation (kW/m^2)	Distance (m) from pool edge calculated with Atlantide	Distance (m) from pool edge (according to Fig. III/1 of Ref. [6])
12.5	16	15
7	29	28
5	37	41
3	52	56

Using the tool bar it is possible to select, in the existing database, the substance of interest (in this case *butane*); in the same input screen the operating (pressure and temperature) conditions have to be introduced.

As described in Fig. 2, the selection of the initial event is done by choosing the part of the plant ''*Unit*'' of interest, which activates the list of the failure cases applicable according to Ref. [6]. All the accidental events relevant to the storage area, including the selected one ''*Small rupture in the liquid side*'', are shown in Fig. 3.

The subsequent scenario implies a (initially) liquid release directed towards the ground; this will lead to a pool formation and, in case immediate of ignition, to a Pool-fire. Otherwise, in case of flammable cloud dispersion and delayed ignition, to a Flash-fire or an UVCE.

Atlantide calculates, automatically, the mass flow rate, the mixture density and exit velocity just selecting the outflow calculation option. Some results and the main input data are shown on Fig. 4.

Following this calculation the meteorological conditions must be introduced and the ''*Phenomena*'' (final events) window is highlighted; it can be noticed, on Fig. 5, that only the final events foreseen in the correspondent Event Tree branches are activated. As an example, the pool-fire calculation following the unconfined spreading of the liquid onto the ground is performed.

Fig. 5 shows the results of the analysis in terms of flame characteristics and distances where the reference thermal radiation levels are reached.

These distances have been compared with values given in the Italian guideline [6], where nomographs for similar conditions are presented; as shown in Table 3 the agreement is very good.

6. Conclusions

A integrated computer code, named Atlantide, has been developed to perform the consequence analysis in LPG installation; it allows to analyze the main accidental scenarios originated from typical accidental events occurring in such plants, according to the Italian regulation [6].

The models implemented for the simulation of physical phenomena are based on published literature and internal developed codes.

Some applications to risk analysis studies have been performed demonstrating the ability of this preliminary version of the software to fulfill with legislative requirements and to save time respect to a standard analysis performed using simplified relations or more sophisticated computer packages. In particular, the use of the nomographs included in the Italian guideline [6], does not allow to analyze automatically linked events nor to consider specific aspects which depend on the behavior of the substances released in a LPG installation. In fact, the main scope of these nomographs, as declared in Ref. [6], is only to provide a uniform means of comparison for the authorities.

On the other hand the use of more sophisticated programs often requires to adapt the overall scenarios in relation to the events/phenomena characteristic of these installations.

The next phase of the development of the code will be the inclusion of other models, for Flash fire and cold BLEVE simulation, and a post-elaboration of the output.

Acknowledgements

This work is based on the master degree thesis [12] developed by M. Molinari and G. Moreschini during a stage in Snamprogetti. Special thanks is due to Prof. G. Biardi, the tutor of the graduates at Politecnico di Milano, for the helpful suggestions he formulated. The authors are grateful to all the colleagues that contributed to the development and the review of this paper. In particular, to Dr. G. Uguccioni and Dr. R. Fiore of Safety and Reliability Dept. of Snamprogetti.

Appendix A. Description of models / relations implemented in Atlantide

A.1. Source Term

For the substances implemented in the code Atlantide the release rate from a break/rupture occurring in the vapor phase of a vessel or along a pipe connected to it, is calculated using the following relations.

A.1.1. Gas outflow

The value of mass flow rate, Q (kg/s), from an orifice is given by [13]:

$$Q = C_D A_u \psi_0 \left[P_0 \rho_0 \gamma \left(\frac{2}{\gamma + 1} \right)^{(\gamma+1)/(\gamma-1)} \right]^{1/2}$$

where: P_0 = Upstream pressure (N/m^2); $\gamma = C_p/C_v$ is the specific heatsratio; C_D = Discharge coefficient (= 0.61); A_u = opening area (m^2); ρ_0 = gas density (kg/m^3) at internal conditions.

The parameter $\psi_0 = 1$, if critical (choked) conditions occur at the orifice and flow velocity is sonic; while, in case of unchoked flow conditions, it is given by the following relation:

$$\psi_0 = \left\{ \frac{2}{\gamma - 1} \left(\frac{\gamma + 1}{2} \right)^{(\gamma+1)/(\gamma-1)} \left(\frac{P_a}{P_0} \right)^{2/\gamma} \left[1 - \left(\frac{P_a}{P_0} \right)^{(\gamma-1)/\gamma} \right] \right\}^{1/2}$$

where P_a is the atmospheric pressure (N/m^2).

According to Ref. [13] a slightly different equation is used if a short pipe is connected to the vessel.

A.1.2. Liquid / two-phase outflow

The liquid and/or two-phase release rates are calculated using the relations proposed by Fauske [14] which deal with the following release situations:

- saturated or subcooled outflow from a hole on the vessel;
- saturated or subcooled outflow from a pipe connected to the vessel (with or without friction).

In the first case the Bernoulli equation is used for the mass flow rate Q (kg/s); neglecting the liquid head it assumes the following form:

$$Q = C_D A \sqrt{2(P_{st} - P_{atm}) \rho_l}$$

where: p_{st} = saturated or subcooled pressure (N/m^2), depending on the storage conditions, ρ_l = liquid density (kg/m^3) and the other symbols have the same meaning as above.

In case of subcooled outflow from pipe, no friction, a similar relation is used for the mass release rate, Q (kg/s), assuming that the Saturation pressure P_{sat} — at the internal temperature — is a good approximation for expansion at the throat exit:

$$Q = C_D A \sqrt{2(P_{st} - P_{sat}) \rho_l}$$

In the case saturated outflow from pipe, no friction, the mass flow rate per unit of area, G_{sat} (kg/m^2 s), is calculated according to the following equation [14]:

$$G_{sat} = \frac{h_{fg}}{v_{fg}} \sqrt{\frac{1}{T_{st} c_f}}$$

where: h_{fg} = latent heat of vaporization (J/kg); v_{fg} = change in specific volume from liquid to vapor (m^3/kg); T_{st} = storage temperature (K); c_f = liquid specific heat (J/kg K).

If the friction is considered, the above equations are multiplied by a reduction factor depending on the ratio of the length (L) to the diameter (D) of pipe:

$$0 < F = f(L/D) \leq 1$$

The flash fraction and mixture characteristics (density, velocity, rain-out fraction) after the downstream expansion at the atmospheric pressure are given in Ref. [14].

A.2. Spreading / evaporation

In order to analyze the vapor dispersion in case of liquid release with pool formation (due for example to liquid Rain Out) it is necessary to model before the phenomenon of spreading and evaporation. This problem is defined by determining at any time the radius, thickness and evaporation mass flow-rate.

The situations to be modeled are:

- continuous or instantaneous releases;
- confined/unconfined spreading.

A.2.1. Liquid spreading

The characteristic dimensions of the liquid pool, assuming that at any instant its shape is cylindrical, can be calculated using the following equation:

$$\frac{\mathrm{d}r}{\mathrm{d}t} = \left[2g(h - h_{\min})\right]^{1/2}$$

where: r = pool radius (m), t = time (s), g = gravity constant (m/s^2); h = liquid thickness (m), $h_{\min}$ = minimum liquid thickness (m) that depends on the type of substrate [15].

In case of instantaneous release the maximum radius (m) is given by Mecklenburgh [15]:

$$r = \frac{1}{2}\sqrt{\frac{4W_0}{\pi \rho_{\mathrm{L}} h_{\min}}}$$

where: W_0 = released mass (kg), ρ_1 = liquid density (kg/m^3) and the other symbols have the same meaning as above.

For a continuous releases, the maximum diameter, in case of unconfined pool, is reached when the equilibrium between the discharging liquid flow-rate and the evaporating rate occurs. Neglecting the quantity evaporated during the spreading and assuming a very small minimum liquid thickness, the following relation is obtained for diameter vs. time:

$$D = \left(\frac{512\, gGt^3}{9\pi\rho_{\mathrm{L}}}\right)^{1/4}$$

where: D = pool diameter (m), G = liquid release rate (kg/s) and t = time from release (m)

A.2.2. Liquid evaporation

For boiling pools having a temperature below the ambient one, as is LPG after the flash at atmospheric pressure, the evaporation is governed by the heat conduction with the substrate. By solving the Fourier equation, with proper boundary conditions, the following relation for the evaporating mass, m_{vap} (kg/s), is obtained [16]:

$$m_{\mathrm{vap}} = \frac{Q_{\mathrm{cond}}}{\lambda} = \frac{1.77 \dfrac{D^2}{4} \chi_{\mathrm{s}} k_{\mathrm{s}} (T_0 - T_{\mathrm{p}})}{\lambda \sqrt{\alpha t}}$$

where: Q_{cond} = heat conduction flow rate (kW); λ = heat of vaporization (kJ/kg); χ_{s} = ground roughness factor, k_{s} = ground thermal conductivity (kW/m K); α = thermal diffusivity (m^2/s); T_0, T_{p} = substance, ground temperature (K), respectively.

A.3. Dispersion

Atlantide has two different dispersion models that allows to treat vapor or two phase jet releases and heavy gas dispersion from evaporating pools.

A.3.1. Turbulent free jet

The relations implemented in Atlantide are based on the turbulent free jet theory. These derive from the momentum and mass conservation equations between the exit nozzle and a downstream plane where air is entrained, so jet diameter increases and its velocity decreases. The concentration profile across the jet is fixed (i.e., Gaussian or Exponential) and the angle of divergence of the jet is constant.

For vapor jet release (critical or subcritical), the relations given in the Yellow Book by TNO [13] allow to calculate the concentration and velocity along the jet axis and the distance where a fixed concentration is reached.

An analogous relation is given by Fauske [14] for horizontal two-phase jet dispersion, assuming a constant air entrainment coefficient.

By integrating the proposed equations, with simplified hypotheses, over the extension of flammable region (between UFL and LFL), the explosive mass is calculated.

A.3.2. Heavy gas dispersion

For heavy gas produced by pool evaporation the model proposed by Britter–McQuaid [17] has been implemented in Atlantide. According to this model the first step is to calculate the downwind distance, x (m), where the prefixed gas concentration (i.e., UFL or LFL) is reached. The following relation [17] gives this distance:

$$x = 22.6 \cdot \left[\frac{C_{\mathrm{m}}}{C_0} \right]^{-1/2} \left(g_0^2 \frac{Q_{\mathrm{m}}}{\rho_2} \right)^{-1/10} \sqrt{\frac{Q_{\mathrm{m}}}{\rho_2}}$$

where: $\frac{C_{\mathrm{m}}}{C_0}$ is the degree of dilution respect to the initial concentration; $g_0 = g\left(\frac{\rho_2 - \rho_{\mathrm{a}}}{\rho_{\mathrm{a}}}\right)$ is the gravitational constant multiplied the relative density; ρ_2, ρ_{a} = gas, air density (kg/m^3), respectively; Q_{m} is the gas release rate (kg/s).

The second step is to calculate the area which represents the boundary of the cloud during the dispersion. This is well approximated by a parabola with a defined initial extension (upwind and crosswind) around the origin of release and a lateral width varying with the downwind distance. Considering only the 2/3 of the distance up to the lower flammable limit x_{LFL}, the area this parabola can be calculated using the relations given in Ref. [17].

Then, using the cloud maximum height at this distance, L_v (m), that depends on the volumetric gas rate and wind speed [17], the volume of the flammable cloud can be obtained [12].

A similar procedure, based on Britter–McQuaid [17], is implemented to analyze the dispersion and to calculate the flammable mass in case of instantaneous heavy gas release [12].

A.4. Final Phenomena

A.4.1. Jet-Fire

For the jet-fire simulation the Thornton model [18] is implemented in the code. The relevant relations are based on ignition of pressurized gaseous jets that expands to 0.006–1.53 Mach No. The flame geometry is assumed to be a cone frustum whose characteristic dimensions (inclination, lift-off, bases diameter, and length) are calculated by means of relations that include the expanded jet diameter and velocity and wind speed.

Two different models are used for crosswind jet fire and horizontal jet fires; these are fully described and validated, respectively in Refs. [18,19].

Once the flame geometry has been defined the following experimental relation is used to calculate the flame surface emissive power E_S (kW/m^2):

$$E_S = \frac{F_S Q \Delta H_C \times 10^{-3}}{A}$$

where: $F_S = [0.21e^{-0.00323 u_j} + 0.11] f(\mathrm{MW})$ is the fraction of heat radiated as function of fuel molecular weight, MW (kg/kmol.), and u_j (m/s) the jet velocity; A is the flame area (m^2), Q is the gas release rate (kg/s) and ΔH_C is the lower calorific value (kJ/kg).

Then by using the following relation it is possible to calculate the thermal radiation q (kW/m^2) from flame to on observer located outside the flame:

$$q = \tau F E_S$$

where: τ = atmospheric transmittance and F = view factor. In the code only the expressions of F for two preferential locations, on the side and along the flame axis, are implemented.

A.4.2. Pool-Fire

For the analysis of pool fires a series of simplified relations, that provide the thermal radiation, are used. These have been obtained by interpolating the results of simulations performed with the code HCFire [20], fixing the weather conditions (wind speed, relative humidity and ambient temperature) and varying the pool diameter. For example, the general relation obtained for the defined thermal radiation levels has the following form with low wind speed (0–2 m/s):

$$Y = a + bX + \frac{c}{X}$$

where: Y (m) is the distance to the fixed thermal radiation level and X (m^2) is the pool area.

The coefficients a, b and c assume different values depending on the level of thermal radiation of interest, as given in Ref. [12].

A.4.3. Fireball

For the analysis of fireball the model presented in Ref. [21] is chosen. This reference proposes experimental correlations for the fireball diameter, height and duration.

By combining these, the following relation for the surface emissive power P_s (kW/m^2), when the sphere is at its maximum diameter, is obtained:

$$P_s = 0.0092\,\phi H_c M^{0.09}$$

where: ϕ is a coefficient (0.25–0.4); H_c (kJ/kg) is the calorific value and M (kg) is the released fluid mass.

Introducing the factors that take into account of the transmissivity of radiation and of the geometrical configuration, the following relation is obtained for the thermal radiation on an observer P_R (kW/m^2):

$$P_R = P_S F \tau$$

where: F = geometric view factor for an elevated sphere [13] and τ = atmospheric transmissivity coefficient.

A.4.4. Vapour Cloud Explosion (UVCE)

For the simulation of UVCE, the Multi-Energy method proposed by Van den Berg [22] is used. This method is based on experimental evidence that only the parts of cloud partially confined and obstacled are able to produce significant overpressures.

A series of parametric curves, 10, numerically generated in function of the initial strength of explosion, were produced and allowed to obtain the characteristics (peak value and duration) of the overpressure during the propagation outside the flammable cloud.

An interpolating relation that fits the curve of blast strength no. 6, that represents the situation of congestement found in an LPG installation, is implemented in the code.

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