METHODOLOGY

PHAST METHODOLOGY FOR PURPOSE OF APPLICATION TO RISK REGULATIONS IN FRANCE

DATE: December 2023

This DNV memo documents the Phast methodology for purpose of application to risk regulations in France and accounts for information from the French regulators (INERIS), consultants (Technip) and the French Chemical Industry (UIC).

Reference to part of this report which may lead to misinterpretation is not permissible.

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ABSTRACT

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1 INTRODUCTION

The French Government defines the parameters and context of risk assessments on French territory. Two types of study are required, i.e. “Etudes de dangers” relating to industrial risk, and “Etudes d’impact” relating to environmental issues. This document is concerned with the former.

The submission criteria for industrial risk studies are defined in a set of documents that cover the whole realm of risk studies. These are summarised in the document usually known as the “circulaire de 10 mai 2010”i. This document and other documents published by the French authorities in French are also available from the INERIS website http://www.ineris.fr/aida/liste_documents/1/19096/1. The official (legal reference portal) website for French regulation is www.legifrance.gouv.fr

Phast is widely used by customers in France for performing consequence analysis in a broad spectrum of industries. The current document provides practical advice on the use of Phast when working in the context of the French regulations. This advice has been derived with the aid of the above ‘circulaire’, a best-practice document for the use of Phast produced by the UIC[ii], discussions with INERIS, Technip and the French chemical industry. It must be emphasized that this advice is not fully prescriptive and as such not officially endorsed by the French regulators. Regarding further details of the toxics calculations in Phast also reference is made to the Phast toxics theory document[iii].

This document briefly summarise the overall Phast methodology for application to risk applications in France according French regulations.

Chapter 2 summarises the overall Phast consequence modelling methodology and Chapter 3 summarises the risk methodology as recommended for application to risk applications in France according to the current French regulations. Appendix A contains further detailed practical guidance to the user on actually applying this methodology in Phast 6.7[1] including a worked-out example.

[1] After endorsement of the Phast 6.7 methodology, DNV will further extend the current document to also account for Phast 7.05.

2 FRENCH METHODOLOGY – CONSEQUENCE CALCULATIONS

The current section summarises methodology as far as relevant for the calculation of the key hazard zones (for toxic and flammable materials) using Phast.

2.1 Weather and substrate data

The circulaire includes information about the selection of the weathers (stability class, wind speed, temperature, humidity and solar flux) and the surface roughness (supplemented with additional information from INERIS):

- Weathers (used for all over France, but one can deviate from this; Circulaire - Section 1.1.2D3);
  - Selection of weather categories [stability class and wind speed (m/s)]:
    - Horizontal ground-level releases:
      - Day: D5
      - Night: F3
    - Vertical or elevated or light-gas releases:
      - Day: A3,B3/5,C5/10,D5/10
      - Night: E3,F3
  - Selection of ambient data:
    - Day: temperature 20^{o}C , humidity 70%, radiation 0.5kW/m^2
    - Night: temperature 15^{o}C, humidity 70%, radiation 0 kW/m^2
    - Presume by default ambient pressure = 1atm

- Substrate data
  - Surface roughness (not prescribed, but values below indicative)
    - Industrial site, suburb, forest: 0.95m (default value; corresponds with surface roughness parameter SRP = 0.17)
    - Other terrain where roughness is clearly lower (low vegetation, sparse houses, …): 0.18m (corresponds with SRP=0.1)
    - Water: 0.2mm (Phast value for water)
  - Presume by default dispersion substrate temperature and pool substrate temperature both equal to the ambient temperature, unless it is relevant to use different values

The above data are specified in Phast 6.7 in the *Weather* and *Weather/Atmospheric constants* tabs.

2.2 Toxic releases

2.2.1 Toxicity levels and toxic material properties

The following three toxicity levels are specified in the regulations (Circulaire – Section 1.1.11B):

- *SEI = "Seuil d'effets irréversibles"*: The level of irreversible effects corresponds to the concentration for a given exposure duration, above which irreversible effects could appear among the exposed population.
- *SPEL = "Seuil des premiers effets létaux"*. The level of primary lethal effects corresponds to a concentration for a given exposure duration, above which more than 1% mortality can be observed in the exposed population. Also called SEL 1%.
- *SELS = "Seuil d'effets létaux significatifs"*. The level of significant lethal effects corresponds to a concentration for a given exposure duration, above which more than 5% mortality can be observed in the exposed population. Also called SEL 5%.

The above irreversible effects and lethal effects correspond to inhalation 'acute' effects, where the effects occur within a period of 14 days.

The above toxicity levels are prescribed by means of ppm levels for a range of subsequent exposure durations. Table 1 and Figure 1 include data published by INERIS for chlorine, sulphur dioxide and ammonia.

If the above toxicity values are available from the French government website http://www.developpement-durable.gouv.fr/Seuils-de-toxicite,12753.html, these data should be used. If they are not available, the best-practice guide by Tissot et al.[iv] should be followed (e.g. use AEGL or toxicological knowhow). Also reference is made to the INERIS best practice guide by Antoine et al.[v] [not yet available online; an older version of this report is available online; see Penelon[vi]]. Where 5% lethality (SELS) values are not available, the 1% lethality (SPEL) values may be used. Additionally, if the exposure duration is less than the lowest duration presented in the toxicity table, one should not attempt to extrapolate to the required values, but only use the values for which data is available.

For most chemicals (as for chlorine and sulphur dioxide), the critical ppm level C_{cr} versus exposure duration t_{exp} is a straight line on a log/log scale, corresponding with an equivalent critical dangerous dose (toxic load, using the so-called Haber law) $L_{toxic}^{cr} = C_{cr}{}^{N}t_{exp}$. Note that the values of the exponent N are not always the same for lethal and irreversible effects. The values of exponent N and the critical dangerous dose L_{toxic}^{cr} can currently both be directly specified in Phast as toxics material properties; see Table 1 for the Phast input values. These properties are used and the 'dangerous dose' method is specified instead of the default 'probit' method.

For some chemicals however, the above curve is not a straight line. For example, for ammonia it is a bilinear curve, and therefore corresponding to two different critical doses to be used for lower and larger exposure durations; see Table 1 and Figure 1c.

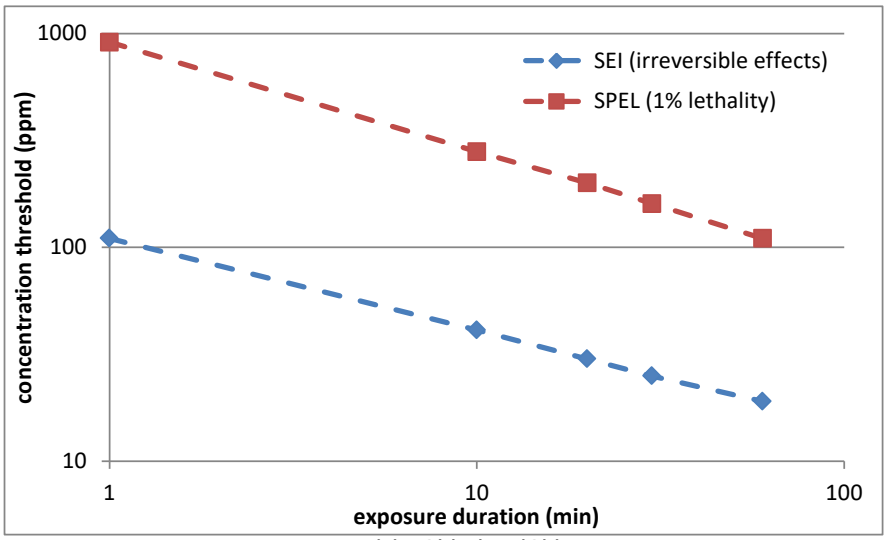
In addition INERIS advises in the calculation of the above effects not to extrapolate the threshold concentration below the minimum exposure durations at which data are not available. As shown in Figure 2, the threshold concentration for exposure durations below the minimum exposure duration should be taken equal to the threshold concentration at the minimum exposure duration. Thus this would mean that the Phast dangerous dose method would need to be adapted for durations less than the minimum exposure duration.

Chemical	Level	Concentration (ppm) at given exposure duration t_{exp} (min)					Toxic parameters (Phast input)		
		1min	10min	20min	30min	60min	DTL ($ppm^N min$)	N	range
Ammonia[vii]	SEI	1500	866	612	500	354	2.15E13 7.5E6	4.2 2.0	t_{exp} <10min t_{exp} >10min
	SPEL	25300	8200	5833	4767	3400	6.8E8	2.0	-
	SELS	28033	8833	6267	5133	3633	7.9E8	2.0	-
Chlorine[viii]	SEI	110	41	30	25	19	5.0E4	2.3	-
	SPEL	910	280	200	160	110	5.6E5	1.94	-

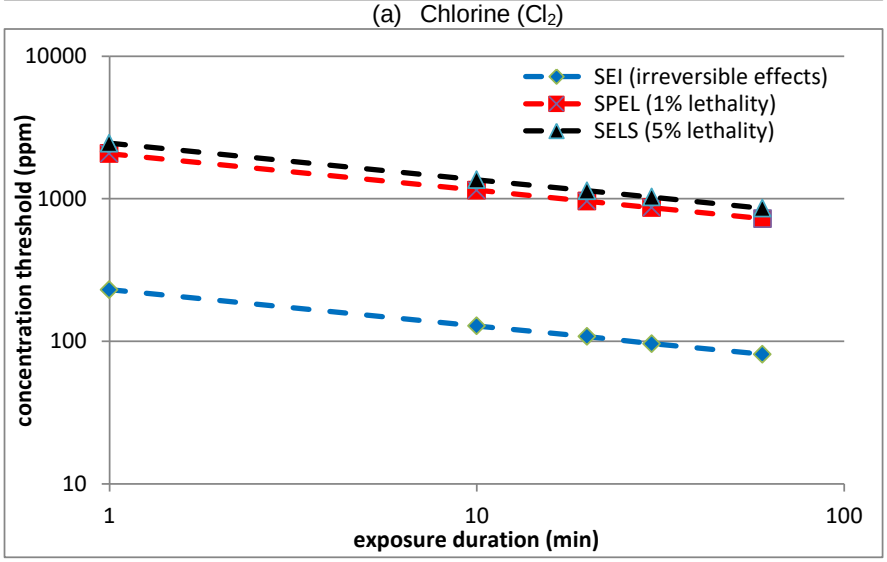
Sulphur dioxide[ix]	SEI	230	128	108	96	81	1.8E9	3.9	-
	SPEL	2071	1148	961	866	725	9E12	3.9	-
	SELS	2451	1358	1137	1025	858	1.7E13	3.9	-

Table 1. **French toxic threshold levels (SEI, SPEL, SELS) for list of chemicals[2]**
The table includes the prescribed concentration threshold levels at given exposure duration, as well as corresponding toxic parameters required as input for Phast simulation.

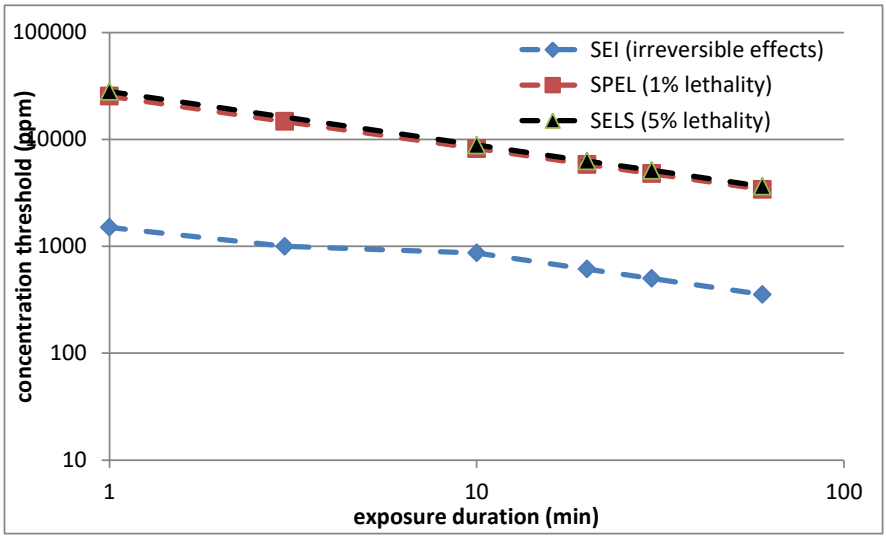
[2] This table is ideally to be further complimented with all known values. At present only the threshold concentrations are official values and not the (DLT,N) pairs. To this purpose they need to be approved by the French national expert group in Toxicology. Perhaps in the future thus a list of official values will be published, which could be subsequently integrated into a French version of the Phast material property database.



(a) Chlorine (Cl_2)



(b) Sulphur dioxide (SO_2)



(c) Ammonia (NH3)

Figure 1. **SEI, SPEL and SELS concentration versus exposure duration**

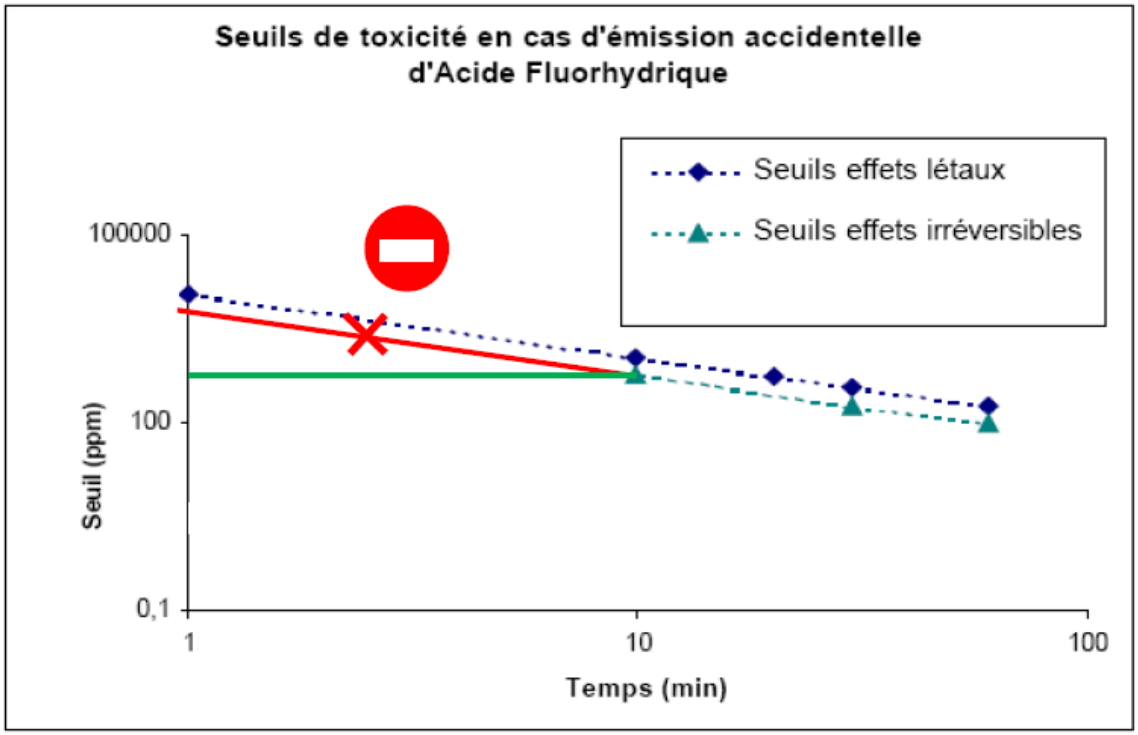


Figure 2. **Extrapolation of threshold concentration in case of missing information**
(Figure taken from INERIS slide; threshold concentration versus exposure duration)

2.2.2 Treatment of mixtures

Usually recommended method (outside France)

The probability of death, p_{death}^{i} for a given component i at a given position is calculated from the Probit Pr^i for each component i, as

$$p_{\text{death}}{}^{i} = \frac{1}{2}\left\{1 + erf\left[\frac{\text{Pr}^i - 5}{\sqrt{2}}\right]\right\} \quad (1)$$

Here *erf* is the mathematical 'error function', the probit Pr^i is set using the concentration c^i of the component in the overall mixture. If a mixture has been released, the overall probabilitity of death equals {1 – the product of surviving each material in turn}:

$$p_{\text{death}}{}^{mixture} = 1 - \prod_{\text{All components i}} \left(1 - p_{death}{}^{i}\right) \quad (2)$$

French method

Let $Seuil^i$ represent one of the critical ppm concentration levels SEI, SELS or SPEL for component i. Then the critical level $Seuil^{mixture}$ (ppm) for the mixture is calculated using Le Chatelier's mixing rule:

$$\frac{1}{Seuil^{mixture}} = \sum_{i=1}^{N} \frac{y_i}{Seuil^i} \quad (3)$$

Here y_i is the mole (volume) fraction of component i in the mixture, and where the summation is to be taken over all toxic components in the mixture.

For example consider a mixture of 0.1 mole fraction Cl_2, 0.1 mole fraction SO_2, and 0.8 mole fraction of inert N_2, than according to Equation (3) and Table 1, the toxicity level of irreversible effects for the mixture at an exposure duration of 1 minutes is given by

$$SEI^{mixture} = \left\{\frac{0.1}{SEI^{Cl2}} + \frac{0.1}{SEI^{SO2}}\right\}^{-1} = \left\{\frac{0.1}{110\,ppm} + \frac{0.1}{230\,ppm}\right\}^{-1} = 744\,ppm$$

In general the log ($Seuil^{mixture}$) versus log(t_{exp}) curve for the mixture will not be a straight curve, and therefore one may need to specify in Phast multiple doses to impose this methodology in Phast.

2.2.3 Phast effect calculations

For each hazardous release scenario, the analyst is required to determine the distance from the release point to the SEI, SPEL and SELS hazard distance given by the above ppm levels at the calculated exposure duration. The approach currently recommended by is as follows:

1. Establish material properties (from INERIS website; see Table 1):

   - 'Typical' toxic chemical:
     - minimum exposure time = 60s .
     - specify for each effect level i = SEI, SPEL, SELS) the critical dose DLT^i and the toxic exponent N^i (needs separate 'material' for each effect level)
   - *'General' toxic chemical:*
     - *different minimum exposure time (possibly larger than 60s, if missing value at 60s)*
     - *ppm levels for various exposure durations (for each effect level), resulting in different values for critical dose and/or toxic exponent N (needs separate runs for each set of different values)*

2. Phast calculations:

   2.1. Set averaging time t_{av}:

   - Using Phast averaging time equal to core averaging time t_{av}^{core}=600s:
     - Set downwind distance x^{SEI}, x^{SPEL}, x^{SELS} at which critical dose is reached for SEI, SPEL and SELS, respectively.
     - Use Phast concentration versus time graph[3] to determine exposure duration t_{exp}^{SEI}, t_{exp}^{SPEL}, t_{exp}^{SELS} at each of these distances;
     - Set averaging time[4,5] at each of these distances x^i (i = SEI, SPEL, SELS)
       - t_{av}^i = max[60s, min(t_{exp}^i, 600s)], recommendation by INERIS
         t_{av}^i = max[60s, min(t_{exp}^i, 3600s)], recommendation by TECHNIP and some of industry
     - In case of a 'general chemical' with multiple doses and multiple values of the exponent N, the above two steps may need to be repeated for each separate pair of values of dose and N. For example, for the bilinear curve of ammonia there may be a total of two series of runs, where those values should be selected corresponding to the calculated exposure duration.

     For a steady-state release, the exposure duration t_{exp}^i will be equal to the release duration if the hazard effect distance x^i is located upwind of the QI transition distance x_{QI} ($x^i \leq x_{QI}$), and will increase with increasing downwind distance downwind of the QI transition ($x^i > x_{QI}$). For an instantaneous release, the exposure duration will increase with increasing downwind distance. Because $x^{SEI} > x^{SPEL} > x^{SELS}$, we have $t_{exp}^{SEI} \geq t_{exp}^{SPEL} \geq t_{exp}^{SELS}$.

   - The above method is applicable for chemicals for which N is not too large. This is the case for most chemicals. In case N>>1, no time-averaging (averaging time = 18.75s) could be considered to be used, which is in line with DNV recommendations. Thus in this case the previous recommendation on minimum averaging time of 60 seconds does not apply.

   2.2. Redo Phast calculations using above averaging time t_{av}^i (for both actual and core averaging time) in order to reset distance x^i to critical dose for each of effect levels SEI, SPEL, SELS, etc.

   In case of a 'general' chemical where the minimum available exposure duration is larger than 60 seconds, extra caution needs to be applied in Phast in the dose calculation if the calculated exposure duration t_{exp}^i is less than

[3] For the current case (averaging time = core averaging time = 600s), the user needs to set the exposure duration from the concentration versus time graph. For the Phast option averaging time = exposure duration, the exposure duration is set automatically by default as 90% of the dose, i.e. the exposure duration is set as the duration between times at which 5% and 95% of the dose has been achieved.

[4] The minimum value of 60s is suggested so that it matches the minimum value of exposure time for which a threshold is defined in France. In parallel it is strongly recommended not to extrapolate at lower durations than 1 minute (sometimes 10 minutes), even if it can be very conservative.

[5] Full consensus has not yet been obtained in France between the two conflicting recommendations.

the minimum available exposure duration. In this case the user should specify the concentration of interest (see Figure 2) in order to determine the hazard distance x^i.

The above approach differs from the normal method of calculating toxicity in Phast, which is designed to generate lethality ellipses (for further use in a risk study) and for which a fixed averaging time of 600 seconds is recommended.

2.3 Additional recommendations for Phast model input

The recommendations below of Phast 6.7 input for flammable and toxic releases are in line with those given by the UIC[ii] and/or INERIS.

- *Models* tab (scenario definition)
    - (*Models/Location* tab) Elevation height of release (default 1m)
        - Use a minimum height of 1m for horizontal releases (except for pool evaporation).
        - For buried tanks/pipes, use elevation height of 0m with a positive release angle (non-horizontal inclined release).
    - *(Models/Scenario* tab) Consider to model pressurised catastrophic release which are expected to result in significant amount of rainout, as a horizontal release (at 1m height) with a very large orifice diameter. Note that in a future Phast version, the two-phase pressurised instantaneous dispersion model will be removed, after which DNV would recommend to use the latter model.
    - *(Models/Vessel* tab) Normally not tick 'Time-varying release', i.e. presume constant release rate based on initial pressure/temperature with entire vessel mass released. Use of 'time-varying release' requires currently advanced expertise by the user.[6]
    - *(Models/Flammable* tab) For flammable materials, select the 'TNO multi-energy model' (never tick 'TNT method')
- *Weathers* tab: see Section 2.1
- *Parameters* tab
    - (*Parameters/General parameters* tab)
        - Maximum release duration (default 1 hour) - can be reduced if can be justified with operator
        - Choose height for concentration output between 0m and 2m. Other heights can be used if there are sensitive targets at height.
    - (*Discharge parameters* / *Discharge* constants tab) Discharge parameters: increase maximum release velocity from 500m/s to 1500m/s.

      The default value of 500 m/s for the maximum release velocity (after expansion to atmospheric pressure) may not be appropriate.

      In case of choked flow at the orifice (e.g. leak scenario), the speed at the orifice (prior to expansion to atmospheric pressure) equals the sonic speed, and following the subsequent expansion supersonic flow occurs, which implies that the post-expansion velocity may be larger than the sonic velocity. Therefore the Phast option of sonic flow is not recommended. In addition, for chemicals with a small molecular weight (such as hydrogen) the speed of sound is larger than 500 m/s and therefore it is recommended to increase the above value (i.e. effectively no capping of the maximum release velocity).
    - *(Dispersion Parameters* / *Far field* tab) Use default of 'fixed averaging time' with always averaging time = core averaging time. Use default averaging time =18.75s for flammables, and select averaging time for toxics as described in Section 2.2.3
    - *(Toxics Parameters* / *Toxics* tab) For toxic materials, 'Use 'Use dangerous dose' method instead of 'Use probit' method
    - Case of flammable releases:
        - *(Flammable Parameters/ Flammables* tab*)*: use LFL instead of 0.5LFL (to evaluate the flash fire effects, to set the ignitable area, and to terminate the dispersion calculations)
        - *('Jet Fire Parameters* / *Jet Fire Radiation*', *Pool Fire Parameters* / '*Pool Fire Radiation*', '*Fireball and BLEVE Blast Parameters/ Fireball Radiation*' tabs) - radiation doses and radiation contours:
            - fire duration <2min: use radiation dose: 1800, 1000, 600 $(kW/m^2)^{4/3}s$ [use of N=4/3, as in Dutch BEVI Reference Assessment Manual]

[6] This recommendation is aligned with the general DNV recommendation as well as the recommendation adopted for risk calculations in the Netherlands. Future improvements on time-varying discharge and dispersion modelling are planned, following which modelling for time-varying releases is expected to be more accurate and more straightforward to apply.

- fire duration >2min: use radiation contours: 8, 5, 3 kW/m^2 [above levels relevant for humans, for structures relevant levels are 8, 16, 20 kW/m^2]

- *Explosion Parameters/ OverPressures* tab
  - apply as centre of explosion the 'Cloud centroid' instead of 'Cloud front'
  - apply as overpressure levels 0.05, 0.14, 0.2, 0.3 barg

- *Materials/Toxic* tab. For toxic materials specify toxic exponent N and dangerous toxic load (see Section 2.2.1 and Table 1 for details; may be different values depending on SEI, SPEL, SELS and possibly also depending on exposure duration).

3 FRENCH METHODOLOGY - RISK CALCULATIONS

This chapter provides a very brief outline of the risk-related calculations. No details are given relating to specification of population, ignition sources, scenario selection/frequencies, wind-direction probabilities etc.

Figure 2 figure 3 ? depicts the risk matrix applicable for land-use planning regulations (PPRT – Plans de prévention des risques technologiques) with along the horizontal axis the severity level ("niveau de gravité" 1-5: number of people affected) and along the vertical axis the frequency (A-E). The risk matrix is split up into an unacceptable zone (red and dark orange), an ALARP zone where mitigation measurements are to be taken (light orange and yellow), and an acceptable zone (white).

All hazardous phenomena with effects out of the industrial site should be positioned in the matrix. For each different accident/effect, the location is to be set in the risk matrix (from frequency, effect level, number of people). The risks from different accidents/effects need to be summed to arrive at an overall cumulative hazard level ("aléa") at each geographical location; see Figure 4 [like in Phast Risk (Safeti) for individual risk].

One map needs to be produced with the cumulative aléa (any kind of effect), while three separate maps need to be produced for recommending adequate safety measures for thermal, toxic and pressure effects, respectively; see Figure 5.

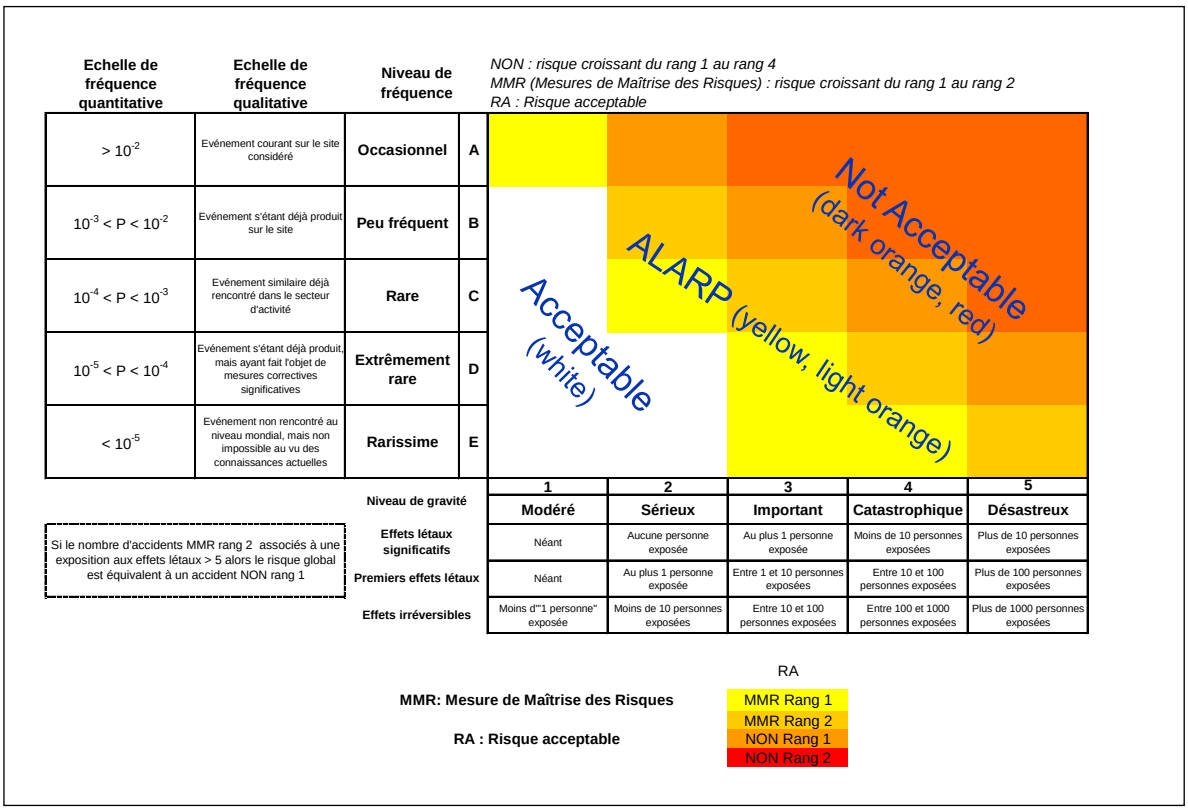


Figure 3. **Risk Matrix**
(Figure adapted from presentation by Yvon Mouilleau[x])

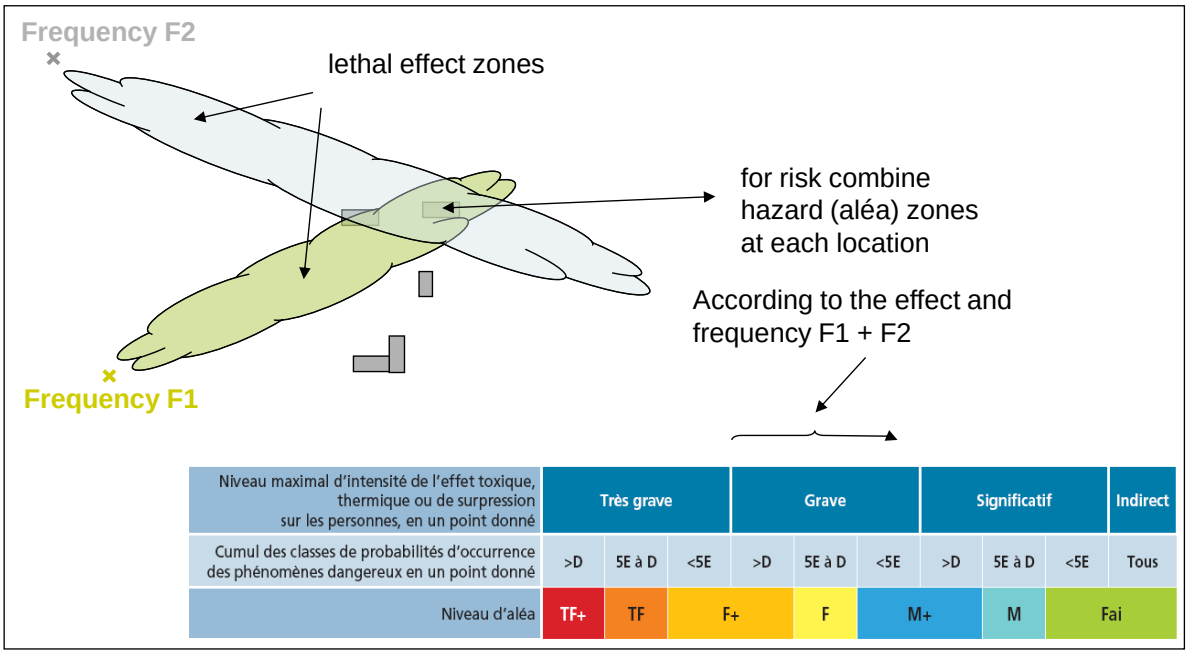


Figure 4. **Definition of PPRT hazard levels ("niveau d'aléa")**
(Figure adapted from presentation by Yvon Mouilleau[x])

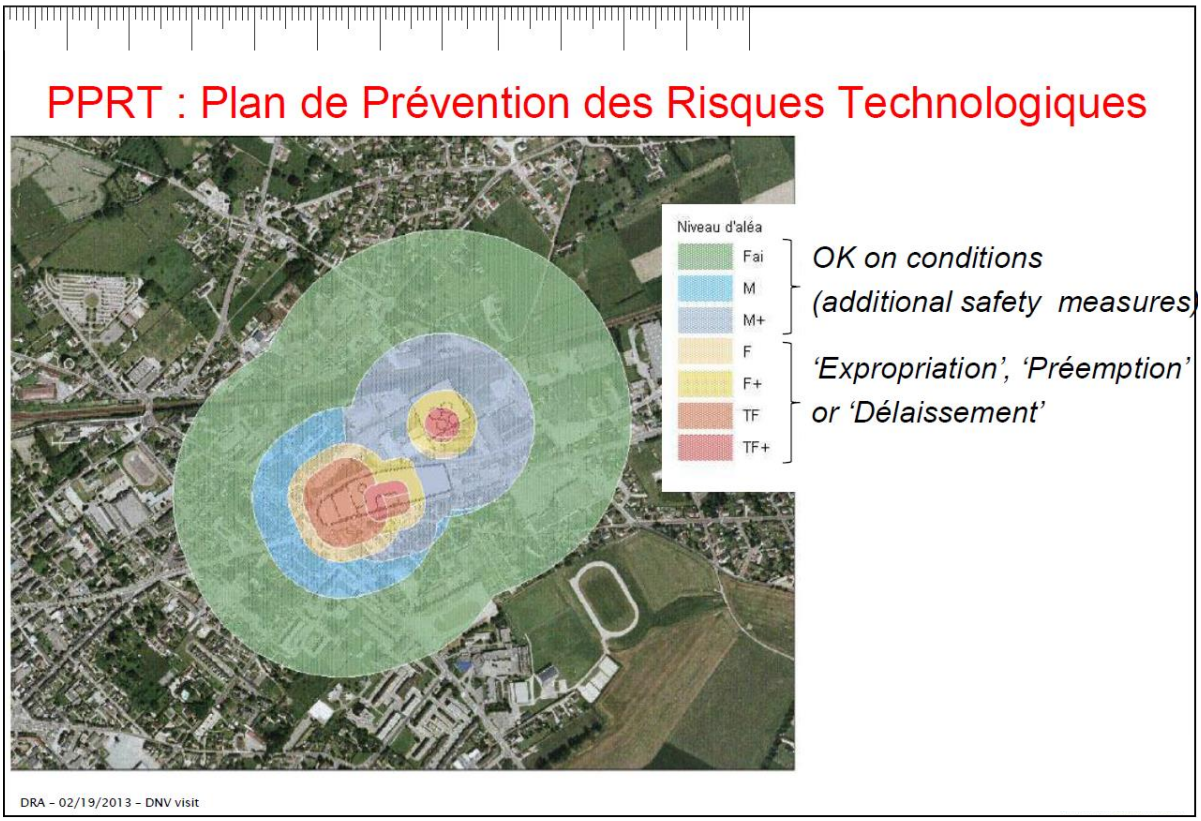


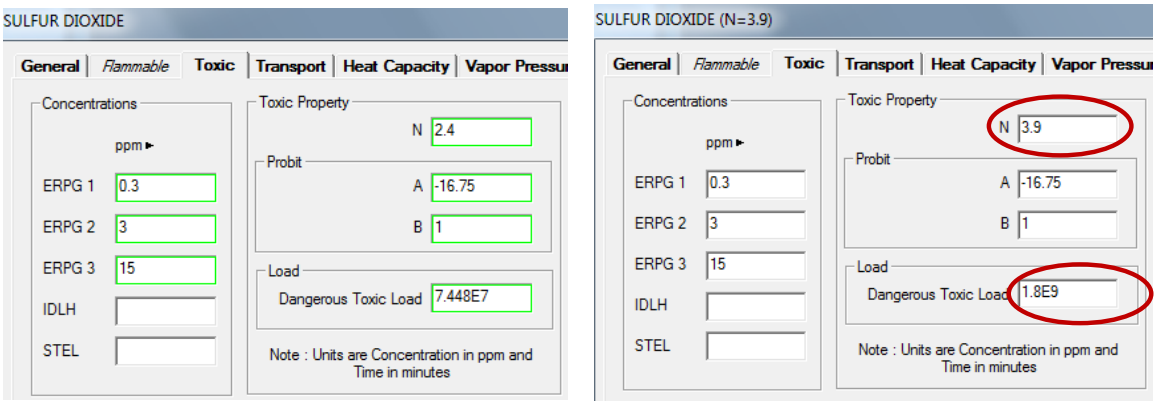
Figure 5. **Example of PPRT cumulative aléa map**

APPENDICES

Appendix A Detailed practical guidance on using Phast 6.7 – example for SO_2 leak

The example of a horizontal leak (100mm orifice, release height 1m) of SO_2 is considered. Storage temperature is 200C and storage pressure is 2 barg. Weather and substrate data are applied according to Section 2.1 (weathers D5 and F3; surface roughness of 0.18m assumed).

In the Material tab, the existing material 'Sulfur dioxide' (with default Phast 6.7 properties) is copied into a new material. In the new material the toxics data are modified according to Table 1, i.e. the material property N=3.9 is applied and the dose DTL^{SEI}=1.8E9 for the minimum 'irreversible toxicity level; see Figure 6. Note that for other materials there may be different N values for different toxicity levels and this would necessitate to general new materials for each toxicity level. However this is not necessary for the current example.



(a) Original default SO_2 properties (b) modified toxic SO_2 properties

Figure 6. New material 'Sulfur dioxide (N=3.9) with modified properties

The following steps now carried out successively according to the method described in Section 2.2.3:

1. First a run is carried out using toxic averaging time = core averaging time = 600s. From this run it can be derived that no QI (Quasi-instantaenous) transition from continuous to instantaneous plume occurs. Thus the cloud is modelled as a steady-state plume with discharge duration of 1494s at all downwind distances (see Figure 7) . Thus the exposure duration t_{exp}^{SEI}= t_{exp}^{SPEL}= t_{exp}^{SELS}=1494s.

2. The averaging time t_{av} is now to be selected as 600 seconds according to INERIS recommendation, and 1494s according to the other (TECHNIP) recommendation. This implies that according to the INERIS recommendation results can be obtained from the above run and no further runs needs to be carried out. According to the other calculation an additional run is to be carried out using toxic averaging time = core averaging time = 1494 seconds.

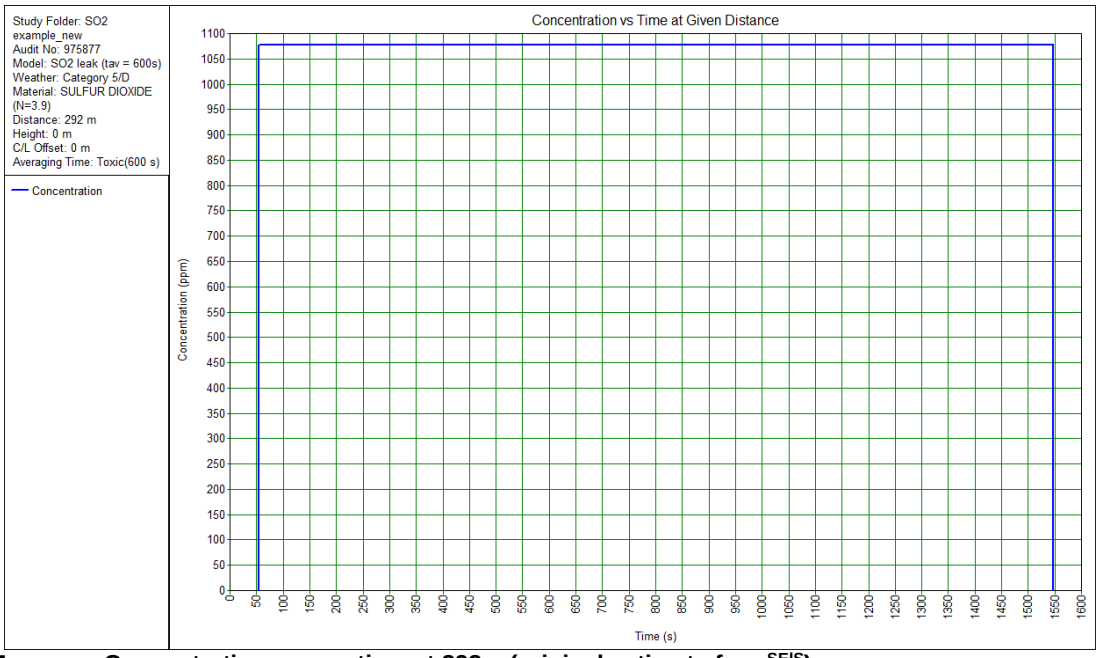


Figure 7. Concentration versus time at 292m (original estimate for x^{SEIS})

The results from both runs are indicated by the Phast graph shown in Figure 8. The blue curve (averaging time = 600s) is used to derive the toxic doses according to the INERIS recommendation, while the yellow curve is used according to the TECHNIP recommendation. The figure also includes a table which includes the distances to SEI, SPEL and SELS according to both methods.

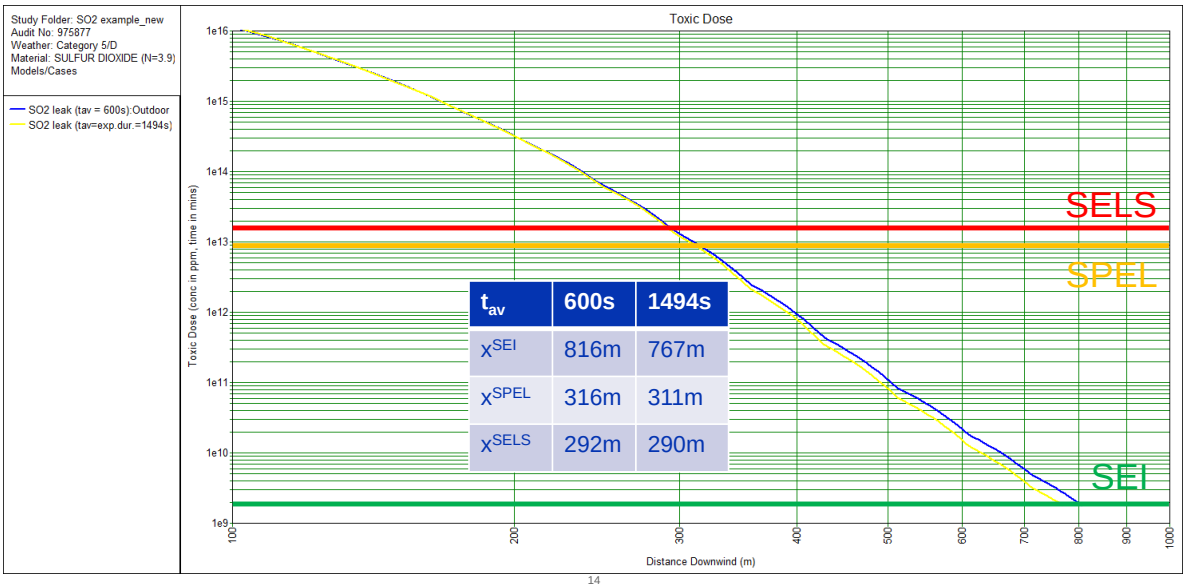


Figure 8. Toxic dose data according to INERIS and other (TECHNIP) recommendation for averaging time

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