Analysis of toxic load calculations and fluctuation concentrations modeling for the assessment of atmospheric accidental release

ABSTRACT
Computing the effect zones around industrial facilities requires using modelling tools. For the specific case of accidental scenarios involving toxic cloud dispersion, it is necessary to make use of acute toxicity threshold values. Those thresholds can be given in terms of concentration or in terms of toxic load. The toxic load is commonly evaluated by extensions of the Haber’s law that corresponds to an integration in time of concentration. The improvements achieved in the atmospheric dispersion modelling now enable to predict the intermittency of the toxic cloud. However, such new approaches raise questions about the relevance of the toxic load evaluation, knowing that many parameters which characterize biological reality and the whole process of the dose-response should be taken into account. To achieve a deterministic model, it is necessary to pool research efforts between the communities of toxicologists and the atmospheric dispersion modellers.

CONTEXT AND OBJECTIVES
For the specific case of accidental scenarios involving toxic cloud dispersion, characterizing the effect zones around industrial facilities requires using modeling tools and make use of acute toxicity threshold values. A common practice consists in calculating toxic effects with the total inhaled dose. This total dose is estimated by integrating the concentration evaluated by atmospheric dispersion modelling. The toxic load is commonly evaluated by extensions of the toxicologists’ law that corresponds to an integration in time of concentration, intended to account for this effect by using an exponent (example : n > 2 for ammonia) to the concentration inhaled. There are several extensions of the toxic load model that have been proposed to take into account that a toxic cloud is always intermittent in the real life. Indeed the concentration cloud is always varying due to many phenomena: atmospheric turbulence, moment of the release, etc.

A lot of scientific efforts have been produced to better assess fluctuations in the concentrations; however the inhaled total dose is estimated without taking into account physiological process that modify the accumulation process (Hilderman, 1999) of the total dose. In the same time there is a lack of knowledge to assess physiological response for very short time, i.e. less than 10 minutes. Therefore, difficulties exist in regulatory guidelines for very short time and for some chemical to determine load toxic thresholds.

The objective of this work is to estimate by a simple kinetic model, on the basis of concentration time series: for example, the effective arterial blood concentration that is expected to exceed a toxicological value. For each of this external concentration signal, the arterial blood concentration is calculated and compared to the safe target arterial blood concentration. This comparison allowed analyzing effects of an external atmospheric concentration on the dynamic of the effective arterial blood concentration.

MATERIAL AND METHOD
In order to illustrate intermittency impacts, we choose a Halocarbon extinguishing agent (2,2-dichloro-1,1,1-trifluoroethane or HCFC-123) which is a gaseous compound under normal aircraft operating conditions. Halocarbons are relatively non toxic at recommended use concentrations (Tabscott and Spigel, 2002). No observable adverse effect level (NOAEL) and the lowest observable adverse effect level (LOAEL) are given in the Table 1 for 2,2-dichloro-1,1,1-trifluoroethane.

RESULTS AND DISCUSSION
Three time series of external concentrations were taken as input of the toxicokinetic model. These time series correspond to three scenarios of atmospheric concentration exposure with the same mean concentration of 20 000 ppm exposure, corresponding to the LOAEL concentration, and the same toxic load, D(x), corresponding to a non-steady time varying concentration:

\[ D(x) = \int_0^T C(x,t) \, dt \]

First condition exposure : steady state exposure (LOAEL) of 20 000 ppm

Second condition exposure : repeated exposure to 10 000 ppm during 3 s with exposures to 30 000 ppm during 3 s

Third condition exposure : 10 000 ppm during 30s then 30 000 ppm during 30 s

Although the mean external concentration and external dose are equivalent for the three scenarios, we observed that the peaks of arterial blood concentration exceed to 5%, 20% and 50% the target arterial concentration for HCFC-123.

REFERENCES

Authors would like to thank the French Ministry of Environment which financially supports this project.