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Sensitivity analysis of Phast's atmospheric dispersion model for three toxic materials (nitric oxide, ammonia, chlorine)

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ABSTRACT

We present the results of a parametric sensitivity analysis of a widely used model for atmospheric dispersion of toxic gases, in order better to understand the influence of user-adjustable parameters on model outputs. We have studied 60 min continuous release scenarios for three different products (nitric oxide, ammonia and chlorine), chosen to cover a range of physical characteristics and storage conditions. For each product, we have broken down base-case scenarios into a number of sub-scenarios corresponding to different release conditions which determine physical phenomena (flow rate, release angle, release elevation and atmospheric stability class). The use of statistical tools to analyze the results of a large number of model executions allows us to rank model parameters according to their influence on the variability of a number of model outputs (distances and concentrations), on a per-scenario and per-product basis. Analysis of the results allows us to verify our understanding of the modeling of cloud dispersion.

1. Introduction

The prevention of technological risks requires industrial sites to estimate the consequences of different accident scenarios based on a probabilistic risk assessment. An important contribution to the calculation of the consequences comes from the modeling of atmospheric dispersion, particularly of the accidental release of toxic products. Given the implications in terms of land-use planning, it is important that the calculations be based on the best scientific knowledge available. This subject has motivated numerous studies since the early 1980s through the development of numerical models which are currently used for loss prevention purposes in chemical process engineering. In order to increase confidence in these programs, a subsequent effort has been spent to validate dispersion models by comparing measured and computed data (Calay & Holdo, 2008; Hanna, Hansen, Ichard, & Strimaitis, 2009; Kisa & Jelemensky, 2009; Luketa-Hanlin, Koopman, & Ermak, 2007; Middha, Hansen, & Storvik, 2009) according to recommendations edited by ASTM (2005) for example.

Dispersion models can be classified into three categories, which are, from the less to the more complex, Gaussian models, integral-type models and 3D or computational fluid dynamics (CFD) models.

Gaussian models are derived from the diffusion equation and from observations made by experimental work, i.e. the pollutant concentration follows a Gaussian distribution, whose standard deviations are dependent on the atmospheric turbulence and the distance from the source or the duration since the beginning of the release. These models are appropriate for passive clouds and therefore for the last stage of heavy-gas dispersion (passive dispersion).

Integral-type models are simplifications of the conservation equations for mass, momentum and energy. They model the transitions between different stages of heavy-gas dispersion: slumping and creeping, transition phase and finally passive dispersion. These box models provide relatively easy and fast dispersion estimations. Some of them, like ALOHA, DEGADIS, HEGADAS and Phast's UDM, are among the most popular and widely used in safety engineering applications. Despite the convenience they offer in their application, they appear to have some drawbacks: some physical phenomena use semi-empirical relationships whose parameters have been tuned on field test data; since the trials usually do not include obstacles, they can provide reliable results only in open field conditions.

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In order to analyze the effect of terrain and of large obstacles on gas dispersion, CFD codes (such as CFX, FLUENT, FLACS and FDS) have been developed. This approach (simultaneous resolution of balance equations of mass, momentum and energy) allows a full three-dimensional analysis to be performed. The wind velocity is completely resolved, unlike simpler models where velocity is a single value or a function of height. They can deal with heavy, neutral or light gas dispersion. While providing more detailed results, they require more computational resources and analyst skill. They are starting to play an important role in risk assessments for the process industry because they have the potential better to assess the impact of certain barrier systems and of terrain effects. In this context, a number of recent papers have compared simulation results obtained by CFD and integral models (Fiorucci et al., 2008; McBride, Reeves, Vanderheyden, Lea, & Zhou, 2001; Mouilleau & Champassith, 2009; Pontiggia, Derudi, Alba, Scaioni, & Rota, 2010; Riddle, Carruthers, Sharpe, McHugh, & Stocker, 2004) or aimed to improve turbulence modeling (Pontiggia, Derudi, Busini, & Rota, 2009; Sklavounos & Rigas, 2004), often the main cause of gaps between observations and numerical simulations.

The modeling of the impact generated by an accidental release of hazardous chemical depends on a number of parameters related to the release type, to the product and to the software itself: conditions under which the dispersion occurs (meteorological and environmental), physical properties and toxicity of the chemical and internal parameters of the modeling tool. Simulation results may depend quite strongly on the values chosen for some of these parameters. While flexibility in the parameter choice is useful, it can lead to effect distances that vary considerably when different experts study the same scenario (CCPS, 1996; MEEDDAT, 2008).

An important technique for developing confidence in one's understanding of a model is sensitivity analysis, which evaluates how variations in a model's outputs can be apportioned to variations in the inputs. The most basic sensitivity analysis methods consist of varying input parameters one at a time ("OAT") while holding other parameters at central values, so the sensitivity indices derived are dependent on these central values. More sophisticated sensitivity analysis techniques examine the global response (averaged over the variation of all parameters) of model outputs by exploring the entire input space: these are global sensitivity analysis methods (Saltelli, Chan, & Scott, 2004).

Previous work on sensitivity analysis of atmospheric dispersion models has been limited to OAT methods. In 1989, Kakko published a quantitative sensitivity analysis of the RISKIT program by varying source term parameters, surface roughness and local weather characteristics. Kok, Eleveld, and Twenhöfel (2004) have carried out a sensitivity analysis of NPK-PUFF, a Lagrangian code used to model release scenarios of radioactive contaminants. Ferenczi (2005) undertook an OAT sensitivity analysis of a RIMPUFF code which models radioactive pollutant dispersion. Bubbico and Mazzarotta (2008) have applied an OAT method to 15-min accidental toxic release scenarios of hydrogen chloride, ammonia, trimethylamine and bromine using ALOHA and Trace 9.0 software tools. More recently, Cormier, Qi, Yun, Zhang, and Mannan (2009) have carried out a sensitivity analysis of the CFX CFD code concerning a limited number of parameters (turbulence models, source term and meteorological conditions) to assess the effects on the distance to Lower Flammability Limit and the concentration levels of LNG releases.

This paper presents our work on a global parametric sensitivity analysis of the Unified Dispersion Model (UDM) of Phast, one of the most comprehensive computer programs for the modeling of accidental releases, used by companies and the competent authorities. We present results concerning three materials which are relevant for safety reports: nitric oxide (NO), ammonia (NH_3) and chlorine (Cl_2).

2. Theoretical background

2.1. Dispersion modeling

2.1.1. Phast software tool

Phast (Process Hazard Analysis Software Tool) is a commercial code for consequence assessment developed by DNV Software. It simulates the evolution of an accidental release from the initial point to far-field dispersion, including modeling of rainout, pool vaporization and evaporation, while accounting for flammable and toxic effects. Phast is able to simulate various source terms such as leaks, line ruptures, long pipeline releases and tank roof collapses in both pressurized and unpressurized vessels and pipes, which are combined with Phast's Unified Dispersion Model (UDM) to obtain desired consequence results: for example, i) concentration at a given distance, ii) distance to hazardous concentration of interest, iii) transition through various stages such as jet phase, heavy phase, transition phase and passive dispersion phase, and iv) footprint of the cloud at a given time. Phast version 6.54 has been used in this work.

2.1.2. UDM

UDM models jet, dense, buoyant and passive dispersion including droplet rainout and re-evaporation (Cook & Woodward, 1995; Witlox, 2006). In this model, the simulation of the progression of the cloud resulting from a release follows several phases without discontinuous transitions between them. A similar formulation is used for both continuous and instantaneous releases, with a transition from the former to the latter for short duration releases. The model has been validated against field scale experimental data.

In the case of a continuous release of heavy gas, Fig. 1 shows the different phases of the cloud along downwind distance: jet (elevated, touching down then ground level), heavy, transition and passive (Gaussian concentration profile). The jet phases are dominant initially, followed by the transition phase and the fully passive one. The transition phase is implemented to avoid discontinuities in the cloud behavior between near-field and far-field dispersion.

A set of differential equations is integrated to give the key variables as a function of distance (for a continuous release) or time (for an instantaneous release). These are solved to obtain other variables describing the dispersing cloud. The same type of differential equations is resolved throughout all phases of dispersion (jet, dense and passive), although the terms vary as the cloud passes from one phase to the next. The model equations for the overall behavior of the dispersing cloud implement conservation of total cloud mass, conservation of heat transfer, conservation of momentum and cross-wind cloud spreading in heavy phase.

Total air entrainment (E_{tot}) into a plume is modeled in Phast as the sum of several mechanisms (the meaning of symbols is presented in Nomenclature section):

- jet entrainment (E_{jet}) caused by turbulence resulting from the difference between plume speed and ambient wind speed; it is

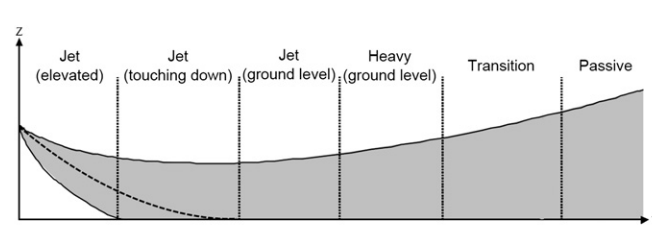

Fig. 1. Dispersion phases according to the UDM (case of heavy-gas behavior). (−−−−−: centerline of the cloud, wind direction according to x).