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VERIFICATION AND VALIDATION OF CONSEQUENCE MODELS FOR ACCIDENTAL RELEASES OF TOXIC OR FLAMMABLE CHEMICALS TO THE ATMOSPHERE

Henk W.M. Witlox*, Maria Fernandez, Mike Harper, Adeyemi Oke, Jan Stene and Yongfu Xu

DNV GL Software, 4th Floor, Vivo Building, 30 Stamford Street, London SE1 9LQ, UK
**Corresponding Author: Tel: +44 20 381 65972, E-mail: henk.witlox@dnvgl.com*

ABSTRACT

Consequence modelling software for accidental releases of flammable or toxic chemicals to the atmosphere includes discharge modelling, atmospheric dispersion modelling and evaluation of flammable and toxic effects:

- First discharge calculations are carried out to set release characteristics for the hazardous chemical (including depressurisation to ambient). Scenarios which may be modelled includes releases from vessels (leaks or catastrophic ruptures), short pipes or long pipes. Releases considered include releases of sub-cooled liquid, superheated liquid or vapour; un-pressurised or pressurised releases; and continuous, time-varying or instantaneous releases.

- Secondly dispersion calculations are carried out to determine the concentrations of the hazardous chemical when the cloud travels in the downwind direction. This includes modelling jet, heavy-gas and passive dispersion regimes, and transitions between them. In the case of a two-phase release, liquid droplet modelling is required to calculate liquid rainout, subsequent pool formation/spreading and re-evaporation from the pool back to the cloud. For heavy-gas releases, effects of crosswind and downwind gravity spreading are present, while for short duration and time-varying releases effects of along-wind diffusion are relevant.. For pressurised instantaneous releases an initial phase of energetic expansion of the cloud occurs. Also, effects of indoor mixing (for indoor releases) and building wakes can be accounted for.

- Finally, toxic or flammable calculations are carried out. For flammables, ignition may lead to rising fireballs (instantaneous releases), jet fires possibly impinging on the ground (pressurised flammable releases), pool fires (after rainout) and vapour cloud fires or explosions. Radiation calculations are carried out for fires, while overpressure calculations are carried out for explosions. For each event, the probability of death is determined using toxic or flammable probit functions.

Testing of the software should ideally include for each consequence model "verification" that the code correctly solves the mathematical model (i.e. that the calculated variables are a correct solution of the equations), "validation" against experimental data to show how closely the mathematical model agrees with the experimental results, and a "sensitivity analysis" including a large number of input parameter variations to ensure overall robustness of the code, and to understand the effect of parameter variations on the model predictions. The current paper includes an overview on how the above verification and validation could be carried out for these consequence models.

Reference is made to the literature for the availability of experimental data. Thus, an extensive experimental database has been developed including experimental data for validation for the above models and scenarios, where many different chemicals are considered (including water, LNG, propane, butane, ethylene, ammonia, CO_2, hydrogen, chlorine, HF etc.). The above verification and validation is illustrated by means of application to the latest consequence models in the hazard assessment package Phast and the risk analysis package Safeti.

Keywords: consequence modelling, model validation, hazard identification and risk analysis