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

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#### 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. 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 or superheated liquid (with or without rainout), or vapour; unpressurised or pressurised releases; and continuous, time-varying or instantaneous releases. For flammables, ignition may lead to rising fireballs, jet fires, pool fires and vapour cloud fires or explosions.

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), and "validation" against experimental data to show how closely the mathematical model agrees with the experimental results. The current paper includes an overview on how the above verification and validation is carried out for the latest consequence models in the hazard assessment package Phast and the risk analysis package Safeti.

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<sub>2</sub>, hydrogen, chlorine, HF etc.).

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

#### 1. INTRODUCTION

Consequence and risk assessments for the releases of hazardous materials are often produced using integrated software packages which seek to model a sequence of events and outcomes from the original loss of containment through to downwind flammable and toxic effects on human populations. Establishing overall confidence in these assessments requires that each stage in the calculations is accurately modelled. This paper presents such an overview, based on relevant published material.

Typical release scenarios involve liquid, two-phase or gas releases from vessel or pipe work attached to vessels:

- First discharge calculations are carried out to set release characteristics for the hazardous chemical (including depressurisation to ambient).
- 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

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