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Methodology for global sensitivity analysis of consequence models

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ABSTRACT

A methodology is presented for global sensitivity analysis of consequence models used in process safety applications. It involves running a consequence model around a hundred times and using the results to construct a statistical emulator, which is essentially a sophisticated curve fit to the data. The emulator is then used to undertake the sensitivity analysis and identify which input parameters (e.g. operating temperature and pressure, wind speed) have a significant effect on the chosen output (e.g. vapour cloud size). Performing the sensitivity analysis using the emulator rather than the consequence model itself leads to significant savings in computing time.

To demonstrate the methodology, a global sensitivity analysis is performed on the Phast consequence model for discharge and dispersion. The scenarios studied consist of above-ground, horizontal, steady-state discharges of dense-phase carbon dioxide (CO_2), with orifices ranging in diameter from ½ to 2 inch and the liquid CO_2 stagnation conditions maintained at between 100 and 150 bar. These scenarios are relevant in scale to leaks from large diameter above-ground pipes or vessels.

Seven model input parameters are varied: the vessel temperature and pressure, orifice size, wind speed, humidity, ground surface roughness and height of the release. The input parameters that have a dominant effect on the dispersion distance of the CO_2 cloud are identified, both in terms of their direct effect on the dispersion distance and their indirect effect, through interactions with other varying input parameters.

The analysis, including the Phast simulations, runs on a standard office laptop computer in less than 30 min. Tests are performed to confirm that a hundred Phast runs are sufficient to produce an emulator with an acceptable degree of accuracy. Increasing the number of Phast runs is shown to have no effect on the conclusions of the sensitivity analysis.

The study demonstrates that Bayesian analysis of model sensitivity can be conducted rapidly and easily on consequence models such as Phast. There is the potential for this to become a routine part of consequence modelling.

1. Introduction

Consequence modelling is used in the process industries for many purposes, from plant design to risk assessment and incident investigation. In many applications, the inputs to the consequence model (e.g. operating temperature and pressure, wind speed) are either poorly defined or they feature a large degree of variability. It is important in these cases to know the effect of the range in input conditions on the model predictions. The results may be quite insensitive to certain inputs, but for some inputs a small difference may produce a critical change in the study outcome. With experience, modellers can often develop an understanding of the important factors in a given situation, but in complex multi-phase reacting flows this may be challenging, and model behaviour can sometimes be counter-intuitive.

The purpose of a sensitivity analysis is primarily to determine which input parameters have a significant effect on the model outputs. Knowing which factors are important can be useful in driving model refinement and in producing more reliable predictions. For example, in the analysis of dense gas dispersion in the Buncefield Incident, Gant and Atkinson (2011) initially found that the model predictions were sensitive to the slope of the ground and the presence of obstacles. As a consequence, to refine their model they used detailed topographical data from a site survey to construct the final Computational Fluid Dynamics (CFD) geometry.

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This type of uncertainty that can be reduced through improved knowledge of the system is known as *epistemic* uncertainty.

Another type of uncertainty that cannot be reduced in this way, known as *aleatoric* uncertainty, arises from the inherent variability in the physical system or environment that is being modelled. For instance, in modelling atmospheric dispersion there is a natural uncertainty in the wind speed due to the random nature of atmospheric turbulence. To account for this, the wind speed may be expressed in terms of a probability distribution that represents the likelihood of the wind speed taking a particular value over time. In a risk assessment, where the objective is to determine the cumulative risk over a year, the results from multiple simulations for a range of wind speeds may be combined and weighted using this distribution to account for the range in likely values.

In a sensitivity analysis, it is also beneficial to identify the inputs that have a negligible effect on the model output. This information can be used to limit the number of simulations required in a given study. For example, in a risk assessment involving a jet fire, if the ambient wind is demonstrated to have practically no effect on the thermal dose predictions, the risk assessment may not need to consider running multiple jet fire simulations for a range of different wind speeds, which may considerably reduce the total computing effort required.

The issue of sensitivity and uncertainty in consequence modelling has long been appreciated, and a number of examples can be found in the literature (Carpentieri, Salizzoni, Robins, & Soulhac, 2012; Jahn, Rein, & Torero, 2008; Khoudja, 1988; Witlox, Stene, Harper, & Nilsen, 2011). Often the approach used in these studies to examine model sensitivity has consisted of selecting a baseline case and then varying one input parameter at a time, i.e. local sensitivity analysis. This choice has often been taken due to the limitations of computing time and the ease of interpreting the results.

In recent years, a more rigorous approach to model sensitivity analysis has started to be applied to process safety applications, e.g. Brohus, Nielsen, Petersen, and Sommerlund-Larsen (2007) and Pandya, Gabas, and Marsden (2012). In the latter study, a global sensitivity analysis was performed on the consequence model Phast (DNV, 2012), where multiple input parameters were varied at the same time in order to understand the interactions between the different inputs. The calculations involved running Monte-Carlo experiments on Phast directly, with sample sizes of 20,000 simulations and computing times of around 24 h, using several computers in parallel.

Despite these examples of global sensitivity analysis being applied to consequence models, such analyses have yet to become widely used by engineers in the chemical process safety industry. This has perhaps been due to the perception that such exercises are time-consuming and costly, and the fact that much of the literature describing sensitivity analysis is aimed at mathematicians rather than practising engineers.

The aim of the present work is to demonstrate an approach to global sensitivity analysis that is easy to use and can be applied routinely to consequence modelling for process safety applications. The approach involves running a consequence model around a hundred times and then using the results to construct a statistical model (essentially a curve fit, or response surface). This statistical model is then used to undertake the sensitivity analysis and identify important input parameters. The statistical analysis is undertaken here using the Gaussian Emulation Machine (GEM) software produced by Marc Kennedy and colleagues at Sheffield University (Kennedy, 2005). This software is freely-available for non-commercial use, and features an easy-to-use Graphical User Interface (GUI) and good documentation.

The process safety scenarios examined consist of horizontal, above-ground, steady-state discharges of high-pressure carbon dioxide (CO_2). Consequence model predictions have been obtained using the discharge and dispersion models contained in the hazard assessment software package Phast (DNV, 2012). Seven key Phast model input parameters have been varied and the results analysed for main effects and interactions.

2. Methodology

2.1. Phast

Phast is a hazard-assessment software package produced by DNV Software for modelling atmospheric releases of flammable or toxic chemicals (Witlox, 2010; Witlox & Oke, 2008). It includes methods for calculating discharge and dispersion, and toxic or flammable effects (see Fig. 1). A principal component of Phast is the Unified Dispersion Model (UDM), which incorporates sub-models for two-phase jets, heavy and passive dispersion, droplet rainout and pool spreading/evaporation. The model can simulate both unpressurised and pressurised releases, time-dependent releases (steady-state, finite-duration, instantaneous or time-varying), buoyancy effects (buoyant rising cloud, passive dispersion or heavy-gas-dispersion), complex thermodynamic behaviour (multiple-phase or reacting plumes), ground effects (soil or water, flat terrain with uniform surface roughness), and different atmospheric conditions (stable, neutral or unstable).

Three key papers have been produced by DNV Software on CO_2 release and dispersion modelling using Phast. In the first of these, Witlox, Harper, and Oke (2009) described an extension to PHAST version 6.53.1 to account for the effects of solid CO_2. The modifications consisted principally of changing the way in which equilibrium conditions were calculated in the expansion of CO_2 to atmospheric pressure, to ensure that below the triple point the fluid conditions followed the sublimation curve in the phase diagram. Furthermore, two-phase vapour/solid effects instead of vapour/liquid effects were included downstream of the orifice

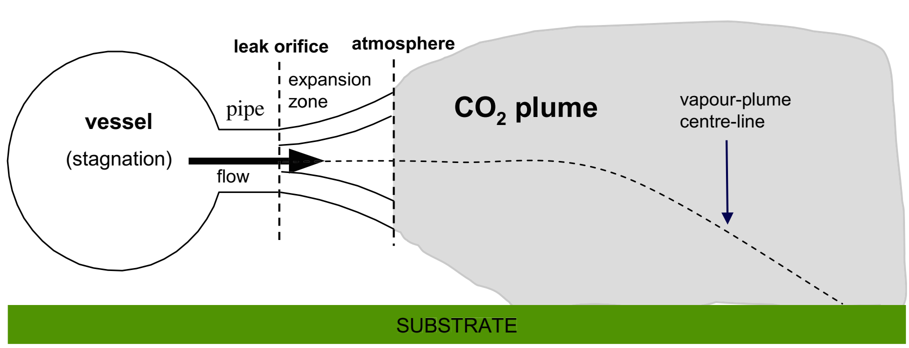

Fig. 1. Phast discharge and dispersion model.