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Global sensitivity analysis of the ADAM dispersion module: Jack Rabbit II test case

Luciano Fabbri *, Maureen Heraty Wood, Ivano Azzini, Rossana Rosati

European Commission, Joint Research Centre (JRC), Ispra, VA, Italy

HIGHLIGHTS

- A global sensitivity study and an uncertainty analysis of consequence models are presented.
- The study is conducted on the atmospheric dispersion module of the ADAM modelling consequence tool.
- The reference accident scenarios used in the study were constructed by using the trials of the Jack Rabbit II exercise.
- Dispersion model inputs having most/least significant impact on the model outcome are identified.
- It might be beneficial to include sensitivity and uncertainty analyses as routine activities of consequence modelling.

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ABSTRACT

This paper provides the result of a parametric sensitivity study conducted on the atmospheric dispersion module of the Accident Damage Analysis Module for consequence assessment, developed by the European Commission to support the EU competent authorities for the implementation of the Seveso Directive in their countries or other legislation associated with chemical safety and security. A variance-based Global Sensitivity Analysis was conducted on a series of reference scenarios build by using the trials of the Jack Rabbit II coordinated model inter-comparison exercise, in order to establish the impact of input parameters on the model output uncertainty.

1. Introduction

Consequence modelling, and atmospheric modelling of toxic and flammable clouds in particular, provides decision-making support to various functions associated with industrial risk management, enforcement and oversight, including risk analysis, land-use and emergency planning, inspection and monitoring, and the preparation and review of safety reports. The outcome of consequence calculations are of fundamental importance for estimating potential damage and risk associated with incidents generated by the release of hazardous chemicals. These calculations are also essential for selecting control measures to prevent and mitigate the effects of a loss of containment of a dangerous substance, and also, in case of the failure or insufficiency of existing control measures, for decision-making surrounding chemical emergency response planning and preparedness.

For a given accident scenario, the outcome of consequence modelling depends on a significant number of inputs associated with the discharge phenomenon, the properties of the substance involved, the environmental and meteorological conditions, and the specific internal input parameters of the models involved. Whilst the simulation results might be quite insensitive to certain inputs, a critical variation on the model output might be observed by varying other input parameters, which would result in a serious drawback when these parameters are characterised by a large degree of variability or uncertainty. Despite current understanding of modellers about which parameters may have greater influence on model output, there are several situations in which, given the complexity of the phenomenon involved, the model behaviour may be counter-intuitive. On the other hand, the outcome of a given accident scenario, as obtained through consequence modelling, can be strongly influenced by the input parameter choice. Hence, it is particularly important to increase the model knowledge by fully analysing the impact of input parameters on the model output. For such a purpose, it is

* Corresponding author.
E-mail addresses: luciano.fabbri@ec.europa.eu (L. Fabbri), maureen.wood@ec.europa.eu (M.H. Wood), ivano.azzini@ec.europa.eu (I. Azzini), rossana.rosati@ec.europa.eu (R. Rosati).

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particularly helpful to apply sensitivity analysis techniques that allow quantifying the uncertainty affecting the model based on the input variability. Then the evaluated uncertainty can be apportioned to different sources of uncertainties in the model inputs by ranking their relevance (Saltelli et al., 2008).

The simplest approach is to focus on the local impact of the inputs on the model output, by varying single parameters at a time and holding the others constant. Such an approach, which is normally identified as local sensitivity analysis, has the clear drawback of producing an outcome that is strongly dependent on the specific values assigned to the fixed parameters. Moreover, it does not allow the investigation of non-linearities and interactions among the different sources of variability (Campolongo and Saltelli, 1997). In order to overcome these problems, global sensitivity analysis is normally considered, in which all the inputs are varied simultaneously and the sensitivity is evaluated over the entire range of input parameters. Such an analysis can be applied to provide the overall ranking of different inputs in terms of their impact on the model output, highlighting the more significant inputs that can be the focus of efforts to reduce uncertainty in the system. Inputs identified as having negligible effect might be discarded, thereby reducing the number of variables required to perform calculations. The latter option could benefit real-time simulation in particular.

Global sensitivity analysis is a widely applied, mature discipline. The scientific literature contains several cases where process safety engineers have indicated application of sensitivity analysis techniques in a consequence-modelling context (Bubbico and Mazzarotta, 2008; Cormier et al., 2009; Pandya et al., 2008, 2012). In addition, it has also been demonstrated that global sensitivity analysis can be applied routinely in consequence analysis to identify the relevant aspects of accident consequences and to restrict the scope of simulation studies for preventive purposes (Gant et al., 2013).

This paper presents our findings from a global sensitivity study of the atmospheric dispersion module of the ADAM modelling tool. This tool was recently developed by the Joint Research Centre of the European Commission (EC) to support Competent Authorities in the European Union (EU) and European Economic Area (EEA), and associated research institutions, in the implementation of the Seveso Directive (2012/18/EU) in their countries, as well as government and research organisations of EU Accession and Candidate Countries, and European Neighbourhood Policy countries involved in chemical accident prevention and preparedness (Fabbri et al., 2017). The analysis was conducted by using selected trials of the Jack Rabbit II coordinated model inter-comparison exercise, to build the reference case (Mazzola et al., 2020).

2. Methodology

2.1. ADAM modelling tool

ADAM is a European Commission (EC) modelling tool for consequence assessment of chemical accidents developed and managed by the Major Accident Hazards Bureau (MAHB) of the EC's Joint Research Centre. This tool is designed to address the overall consequence assessment cycle of an industrial accident, including the unintended release of a hazardous substance (i.e., loss of containment), the rainout and pool vaporisation, and the final physical effect and its impact on human health associated with thermal radiation from chemical fires, blast effects of vapour cloud explosions, and inhalation of toxic chemical vapours. The overall structure of ADAM consists, therefore, of three interconnected calculation modules: source term, physical effects, and vulnerability. The first module refers to the implementation of models for source term calculation, that is, the estimate of the amount of substance released and the associated parameters that fully characterise the release process. This estimate requires the knowledge of the type and amount of substance involved in the accident scenario, the physical and storage conditions, the type and mode of rupture, the release time if limited by the operator intervention, and the environmental conditions. The second module uses the outcome of the first module to estimate the effects, resulting from the loss of containment and subsequent sequence of events, in terms of, depending on the substance, a concentration of a toxic after airborne dispersion, thermal radiation from a chemical fire, or overpressure/impulse from a vapour cloud explosion. The third module is designed to transform the exposure to physical effects, as calculated by the second module, into effects on the surrounding community by using lethality or damage levels. This is normally obtained by using probit functions, or alternatively, reference thresholds such as Protective Action Criteria (PAC) for inhalation toxicity or other empirical average criteria for fires and explosions.

For atmospheric dispersion of toxic or flammable clouds, ADAM uses an in-house modified version of SLAB, which is a model developed by the Lawrence Livermore National Laboratory (Zeman, 1982; Ermak, 1990). This model is based on spatially averaged conservation equations of mass, momentum, energy, and species and produces spatially averaged cloud properties by calculating similarity function coefficients as a function of the downwind distance. In ADAM, the SLAB algorithm has improved the precision of the output by applying a coding strategy that significantly increases the number of points generated by the calculations, resulting in higher resolution consequence maps. All environmental data, which are coded and fixed in the original software, are taken directly from the ADAM database and correspond to the specific environmental conditions of the scenario under study. In addition to these modifications, ADAM introduces some major modelling improvements, specifically: (*i*) an alternative calculation of the average concentration for instantaneous releases, (*ii*) the calculation for time-varying releases, (*iii*) the inclusion of the contribution from pool evaporation in case of rainout, and (*iv*) the extension of the calculation to cover downward jets. The first item overcomes the inherent error present in SLAB, that is, the simplification of the time average concentration calculation by performing a variable transformation from time to downwind distance via the velocity of the puff centre-of-mass. However, this correction applies only to catastrophic scenarios. It is not relevant for the test cases used in the study described in this paper. By contrast, the other three corrections are very much relevant for the Jack Rabbit II case. In particular, both the source term's time dependence, and the contribution from pool evaporation to the vapour jet, were processed and recombined by using a proprietary algorithm, described in detail by Fabbri et al., (2017). Results were also validated against experimental data available in the literature (Fabbri et al., 2018; Fabbri and Wood, 2019).

Notably, an extension of the dispersion module to include downward jets was implemented because the Jack Rabbit II model inter-comparison exercise conducted some trials under this release configuration. (The original SLAB is applicable to vertical and horizontal jets only.) This extension was implemented in both the source term and dispersion modules. For the source term, the difference in the jet direction has a significant impact on the calculation of the rainout routine. In particular, if the jet trajectory was downward, rather than horizontal, its momentum was considered in the correction of the droplets lifetime flight, and in turn of the overall rainout. For the dispersion, the original source area defined in the SLAB model has likewise been modified to account for the different release geometry associated with a downward jet, and the initial velocity of the plume has been taken as the wind speed in the proximity of the release.

The structure of the ADAM software uses separate calculation libraries for each step of the consequence assessment cycle. This feature greatly facilitates the development of a customized programme for executing all necessary runs of each combination of input parameters, taking into account a wide variety of potential input ranges.

2.2. Global sensitivity analysis

In order to simultaneously explore the entire input space and fully assess the model output uncertainty, a global sensitivity analysis was carried out by applying variance-based methods, which are powerful and well known techniques (Saltelli et al., 2010).

To do so, the study applied Sobol' method, a variance–based technique that relies on the estimation of the model output sensitivity through the so-called ANOVA decomposition (Sobol', 1993). Under certain defined conditions, this method allows the unique decomposition of the total variance of the outcome $Y = f(\mathbf{X})$ into terms of increasing dimensionality, referring to the partial variances associated with uncertain model inputs $\mathbf{X}=(X_1, \ldots, X_d)$. In particular, Sobol' method allows the computation of the terms of the variance decomposition via the estimation of a multidimensional integral using Monte Carlo techniques, and propagating the input uncertainty thought the model via the generation of (pseudo-)random samples. The inputs are considered as independent variables, therefore, their variability is characterised by their marginal probability density functions. In this way, the uncertainty/-sensitivity analysis can be directly based on the distributions of the inputs. Specifically Sobol' method is based on the variance decomposition into summands of increasing dimensions, as follows:

$$V(Y) = \sum_{i=1}^{d} V_i + \sum_{j>i}^{d} V_{i,j} + \cdots + V_{1,\ldots,d} \tag{1}$$

where $V(Y)$ is the total variance of Y and V_i and represents the partial contribution to the variance of the input i individually (first-order effect), the second-term $V_{i,j}$ expresses the measure of the joint effect of the pair (X_i, X_j) on Y, followed by the terms referring to the joint effect of the triple, and so on until the higher order interaction $V_{1,\ldots,d}$. Each term in equation (1) can be computed by straightforward Monte Carlo integration. By dividing equation (1) by the total variance V, the decomposition gives normalized values in the range 0–1, which are known as Sobol' sensitivity indices:

$$\sum_{i=1}^{d} S_i + \sum_{j>i}^{d} S_{i,j} + \cdots + S_{1,\ldots,d} = 1 \tag{2}$$

The *Main or First-order Effect* S_i of the input X*i* corresponds to the conditional variance $V(E(Y|X_i))$, where $E(Y|X_i)$ denotes the expectation of Y conditional on a fixed value of X_i; consequently, it is given by:

$$S_i = \frac{V(E(Y|X_i))}{V(Y)} \tag{3}$$

A high value of S_i is associated with the considerable individual effect of the input X_i on the model output uncertainty.

The *Total effect* S_{Ti} of the input X*i* is associated with the increased uncertainty deriving from all possible interactions between inputs (Sobol', 1993; Homma and Saltelli, 1996). This can be obtained as difference:

$$S_{Ti} = 1 - \frac{V(E(Y|X_{\sim i}))}{V(Y)} \tag{4}$$

where the unity expresses the total variance of the investigated model, and $V(E(Y|X_{\sim i}))$ is given by all terms of any order that do not include the input X_i (~i indicates all terms but *i*).

Further, given the law of total variance, the Total Effect of X_i can also be defined as:

$$S_{Ti} = \frac{E(V(Y|X_{\sim i}))}{V(Y)} \tag{5}$$

First-order Effect S_i is normalized between 0 (no effect) and 1 (the input is responsible for the entire uncertainty). The value 1 expresses the whole variance. Consequently, the sum of all S_i is equal (no interactions) or lower than 1. The Total Effect sensitivity index S_{Ti} expresses the sum of all the effects of any order involving the same input. The S_{Ti} of an input is always equal (no interactions) or greater than the S_i of the same input. The main properties of Sobol's sensitivity indices main properties are summarized in Table 1.

Table 1
Sobol' sensitivity indices main properties.

Formula	Explanation
$0 \le S_i \le S_{Ti} \le 1$	Always when inputs are independent
$\sum_{i=1}^{d} S_i \le 1$	Always when inputs are independent
$\sum_{i=1}^{d} S_i = 1$	Additive model (no interactions)
$1 - \sum_{i=1}^{d} S_i \gg 0$	Indicator of the presence of interactions

Several numerical methods exist to estimate both first-order and total order indices (e.g., Sobol, 2001; Saltelli et al., 2010; Shao et al., 2017). In the present work, we use the so-called radial sampling strategy proposed in Saltelli et al. (2010), which requires the generation of two independent matrix samples **A** and **B** of size N by d, where N is the sample size and d the number of variables. In addition, a third dependent sample indicated as $\mathbf{Ab^i}$ matrix is derived for each investigated input X_i from A and B. The $\mathbf{Ab^i}$ matrix is equal to the matrix A except for the *i*-th column which is replaced with the value of X_i taken from B (the *i*-th column of the sample B). For each model input, the sensitivity indices are estimated on the basis of the output vectors $f(\cdot)$ obtained by the evaluation of the three samples (A, B, and Ab^i), in the following way:

$$\widehat{S}_i = \frac{1}{N} \frac{\sum_{j=1}^{N} f(\mathbf{B}_j)\left[f\left(\mathbf{Ab}_j^i\right) - f(\mathbf{A}_j)\right]}{\widehat{V}} \tag{6}$$

while the estimation of the total index results:

$$\widehat{S}_{Ti} = \frac{1}{2N} \frac{\sum_{j=1}^{N}\left[f(\mathbf{A}_j) - f\left(\mathbf{Ab}_j^i\right)\right]^2}{\widehat{V}} \tag{7}$$

The sensitivity indices have a natural interpretation since they represent the fraction of the total variance of the model output in relation to any individual input (main effect or first-order index) or combination thereof (total order index). By determining the main and total effect sensitivity indices, it is possible to assess the model sensitivity to input parameters by using the following scheme:

- Input X_i associated with the highest Main Effect are very influential by themselves (indicating a direct influence);
- Input X_i associated with very low Total Effect have a very small uncertainty impact on the output both directly and because of their interactions.

In particular, inputs characterised by a low or null Total Effect can vary across a range of uncertainty without making a significant contribution to the model uncertainty (variance of the output). In some cases, significant model simplification is possible when irrelevant inputs are identified, such that their presence do not affect the output variance. Consequently, whilst the value selected for the input (or group of inputs) with a significant Main Effect is extremely important, the value selected for the input with a low Total Effect may be quite unimportant.

2.3. Definition of the test cases

Three of the nine Jack Rabbit II experiments selected for the initial phase of the inter-comparison exercise, Trials 1, 6 and 7 (Mazzola et al., 2020), were used to build the reference case for this sensitivity study. The releases of pressurised liquefied chlorine simulated in the study described in this paper consist of aboveground orifice discharges from a horizontal vessel that disperse under stable to neutral atmospheric conditions. The initial amount of pressurised chlorine present in the tank for these trials was 4.5 tonnes, 8.4 tonnes and 9.1 tonnes, respectively. The discharge orifice in each trial was 6-inches (0.152 m) in diameter. In Trials 1 and 6, the orifice was located on the underside of the vessel and

Table 2
List of model inputs, and associated range of values applied in the sensitivity analysis. The Ref. Values are the inputs used for the simulation of JR II Trial 1.

Model Inputs	Min.	Max.	Ref. (Trial 1)	Description
Discharge and pool evaporationrowhead				
Ts (°C)	5	30	17.5	Storage temperature
φ (%)	20	80	42.3	Tank filling level
z_{0n} (m)	$0.5{\cdot}10^{-3}$	$10{\cdot}10^{-3}$	$5{\cdot}10^{-3}$	Substrate roughness in prox. of release
κ ($Wm^{-1}K^{-1}$)	0.207	1.3	0.222	Substrate thermal conductivity
α (m^2s^{-1})	$0.25{\cdot}10^{-6}$	$1{\cdot}10^{-6}$	$0.984{\cdot}10^{-6}$	Substrate thermal diffusivity
Weather and Environmentalrowhead				
T_a (°C)	5	30	17.5	Ambient temperature
H (%)	5	80	25	Humidity
u_{10} (ms^{-1})	0.5	10	1.45	Wind speed at 2m
L^{-1}(m^{-1})	0	0.124	0.124	Inverse Monin-Obukhov length
z_0 (m)	$0.5{\cdot}10^{-3}$	$500{\cdot}10^{-3}$	$0.5{\cdot}10^{-3}$	Terrain roughness (for dispersion)
Model (internal)				
σ_G (m)	1	2	1.4	Geometric spread
Z_{0p} (m)	$0.1{\cdot}10^{-3}$	$0.5{\cdot}10^{-3}$	$0.23{\cdot}10^{-3}$	Pool roughness length
SMD	1. 2. 3. 4.[a]		2.[a]	Correlation for droplets' SMD

[a] 1. TNO; 2. CCPS; 3. Modified CCPS, 4. JIP Phase III (see Fabbri et al., 2017 for detailed description).

the released jet was directed vertically downwards onto a concrete from a height of 1 m. In Trial 7, the orifice was in a position of the tank that led to a 45-deg jet downwards from the horizontal.

Since tank geometry, the hazardous substance (chlorine), substance storage state (pressurised liquefied), and failure type (jet release from a 6-inch orifice) were the same for all three trials, all input parameters related to the aforementioned aspects were kept fixed for this study. All other inputs of the ADAM-SLAB model associated with the discharge phenomenon and weather conditions were varied in a reasonable range of values to analyse their influence on the model output. In particular, the overall initial quantity present in the tank, the storage conditions (gauge pressure and temperature), the jet direction (vertical downward and horizontal), and the meteorological conditions (wind speed and atmospheric stability) constituted the main differences between the three trials. Thus, all these parameters were varied accordingly for the sensitivity analysis of the ADAM-SLAB atmospheric dispersion module.

Considering that jet direction would affect the release significantly, it was decided to conduct separate studies for the case of (*i*) vertical downward, (*ii*) horizontal, and (*iii*) vertical jets. Whilst the first corresponds directly to Trials 1 and 6, the other two do not have a direct correspondence with any of the other trials selected. Although Trial 7 is just in between case (*i*) and (*ii*), no trials are representative of case (*iii*). Nonetheless, it was decided to include case (*iii*) in the analysis in order to explore a higher spectrum of cases and to see whether there are differences in the importance of input parameters for different scenarios that might result from the same component type.

The storage parameters (gauge pressure and temperature) were reduced to one (temperature), represented by the saturation condition that ensures the stored substance remains in a pressurised liquefied state. In particular, the storage temperature could vary between 5 and 30 °C, with corresponding storage gauge pressure in the range of 3.5–8 bar. The overall initial amount of substance present in the tank varied according to the filling level parameter, a value that could fluctuate across a rather large range to represent all conditions between 'almost full' and 'almost empty'.

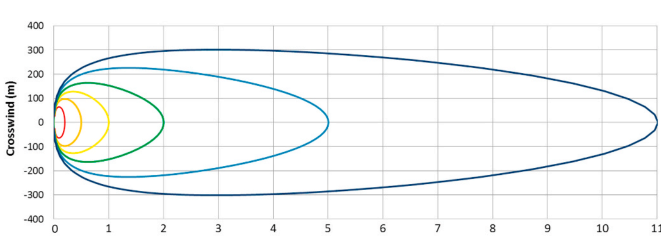

Fig. 1. Iso-concentration curves computed by ADAM. The progressive concentration values are those reported in Table 3 (from the inner to the outer curve).

Parameters describing the substrate in the proximity of the release are often characterised by a certain degree of uncertainty (e.g., heat conduction of concrete is highly affected by the production method due to possible differences in porosity). Hence, the main properties (roughness, thermal conductivity and diffusivity) were also included in the sensitivity analysis, even though the substrate in the proximity of the release was the same for all trials involved.

The meteorological inputs of wind, ambient temperature, and terrain roughness were allowed to vary, whilst in order to reduce the number of variables, the ground temperature was set as equal to the ambient temperature. The inverse Monin-Obukhov length, expressing the atmospheric stability could vary across a range of values from neutral to unstable to stable conditions (equivalent to Pasquill stability class in the range D-F). Irradiation was set to zero since this condition was common to all trials.

Finally, a number of internal model parameters that are specific to the rainout calculation module of ADAM, and that can be modified in the default parameters of the software, were also included in this study. All these parameters have considerable influence on the rainout, a phenomenon that often leads to a reduction of cloud concentration combined with extended duration of the dispersion phenomenon. Specifically, the Sauter Mean Diameter (SMD) is a characteristic measure of the average dimension of droplets formed during post-expansion, where the liquid mass fraction of the jet will break by mechanical forces and/or flashing. The modelling of this process is rather complex, since the atomisation produces many different droplet sizes according to a certain distribution pattern. Although there are a variety of different droplet distributions that can be selected in ADAM, it was decided to use the log-normal distribution (Woodward, 2014) for the purpose of this sensitivity study. This distribution is fully characterised by two parameters, the so-called geometric spread (that is, the standard deviation of the normalized drop size distribution), and the SMD. In ADAM the geometric spread is set by default to 1.4, and the *modified CCPS correlation* is used to estimate the SMD (Witlox and Harper, 2013; Fabbri et al., 2017). For the purposes of this study, the geometric spread was varied across a range of values, and all implemented SMD correlations were used. Finally, the evaluation also included the pool roughness length parameter that is used in the GASP pool evaporation model implemented in ADAM. This parameter is particularly critical because it has a direct impact on the wind profile, and therefore is highly influential on the overall evaporation process, but is very difficult to estimate. In ADAM, this parameter is set to 2.3 mm by default, which is the recommended value suggested by Brighton (1987). Table 2 shows the model inputs selected for examination and the range of values assigned

Table 3
Comparison of chlorine concentrations computed by ADAM and measured experimentally at different downwind distances for JR II Trial 1.

Downwind distance (km)	ADAM concentration (ppmv)	Exp. peak concentration (ppmv)[a]
0.2	14417.7	5202.8
0.5	3335.1	3348
1	1019.5	1137.1
2	304.7	356.6
5	58.3	49.9
11	12.9	20.4

[a] (Mazzola et al., 2000).

to them. For all 13 parameters, independent and uniform distributions (between the indicated minimum and maximum values) have been assumed. The SMD is the only variable to which only discrete values are assigned. Column 'Ref.' of Table 2 gives the data input used to simulate Trial 1of the Jack Rabbit II intercomparison exercise. The dispersion plume computed by ADAM using these values is depicted in Fig. 1. The different curves were obtained by using progressive iso-concentration values equivalent to the concentrations obtained at downwind distances of: 0.2, 0.5, 1, 2, 5, and 11 km, respectively. These distances correspond to the sensors' positions of the field trials. The comparison of the concentration values computed by ADAM to the peak concentrations of the field trials is given in Table 3, which shows a good agreement. The only exception is given by the first point at 200m i.e., in the very near field. This might be due to the presence of the CONEX obstacle array in the proximity of the release, that produced an increase of turbulence and in turn of the dispersion rate (Mazzola et al., 2000).

For the purpose of the sensitivity and uncertainty studies, across all possible model outputs, this analysis was conducted by considering the downwind distances from the release sources in which the plume reached concentration levels of chlorine of 15,000, 1500, and 15 ppmv. This range of values facilitates exploration of variation in the model output in the near, mid and far-field, respectively. The target height was set to 0.3m, which corresponds to the sensors' vertical position in the Jack Rabbit II field trials.

3. Results

The uncertainty and sensitivity analyses were conducted in order to evaluate the variability of the output given the model input uncertainties (see Table 2). The propagation of the input uncertainties into the reference model output (the downwind distances associated with concentration levels of 15,000, 1500, and 15 ppmv) were performed using Monte Carlo simulations of the ADAM-SLAB model. Therefore, two independent Monte Carlo matrix samples **A** and **B** of size "N x d" (N = 3000, d = 13) were generated. Each matrix column referred to the values of an individual input sampling based on its probability density function (see Section 2.2). Each row of the matrix represented a set of model parameter values that were used to evaluate the model.

All tests were performed by using MATLAB 2018a (matworks.com) in conjunction with the C++ calculus libraries of ADAM.

3.1. Vertical downward jet reference case

This case consists of a vertical downward jet emanating from a horizontal cylinder containing liquefied pressurised chlorine. The first 10 inputs, together with their variability range (see Table 2), cover different scenarios that differ from each other in terms of volume of substance contained in the tank, and storage, meteorological, and environmental conditions. Reference values of these 10 inputs can be set to reproduce Trial 1 of the Jack Rabbit II inter-comparison exercise. The last three parameters of Table 2 are internal to the model and refer to the rainout process. Reference values of these parameters were taken from the default values of ADAM.

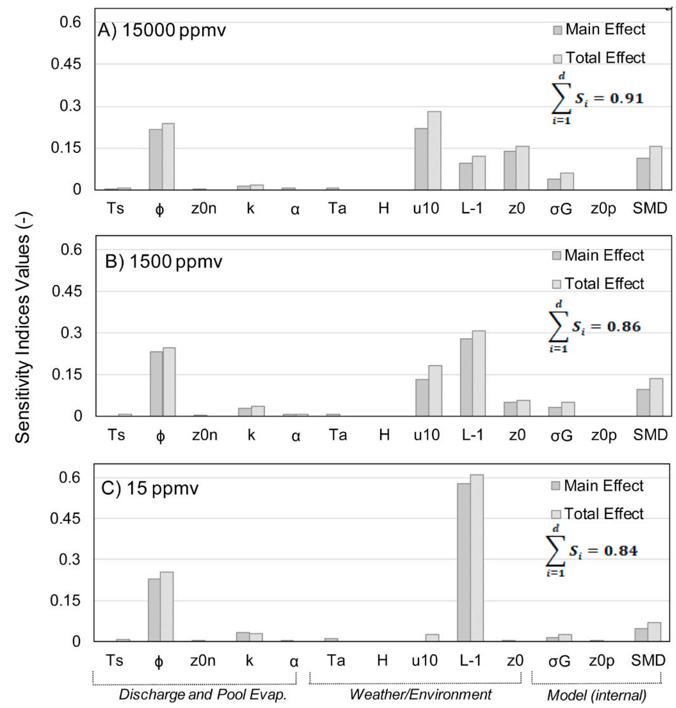

Fig. 2. Vertical Downward jet: Main and Total sensitivity effects for ADAM model inputs given in Table 2.

The sensitivity analysis was conducted on the entire set of 13 uncertain inputs in Table 2. The Sobol' Main and Total Effect indices (Sobol', 1993; Homma and Saltelli, 1996; Jansen, 1999) were calculated using a radial sampling strategy (Saltelli et al., 2010).

The results are given in Fig. 2, where the indices associated with the different inputs are reported for the three model outputs (downwind distances associated with the three different concentration levels).

A point to note is that the summation of Main Effect indices ranged between 84 and 91%, demonstrating that a large part of the model variability is explained by the direct impact of individual inputs. At the same time, the relative importance and behaviour of each input varies quite significantly for the three different model outputs.

For the discharge and pool evaporation parameters, the only input showing a certain relevance is the filling level φ that accounts for more than 20% of the variability of the overall model outcome. This parameter is directly related to the total amount of released substance, and its importance is quite independent of the model outcome as defined by the reference concentration level. Surprisingly, the storage temperature has indices well below 3% in all selected cases, despite the fact that this parameter is directly associated with the storage pressure and, in turn, with the discharge flow rate. This means that, in the present case, the overall amount of the toxic contained in the tank, and in turn the part thereof released in the atmosphere, plays a more important role than the flow rate, a direct input parameter of the dispersion model.

Concerning the weather and environment related parameters, as expected, the wind speed u_{10}, and the inverse Monin-Obukhov length L^{-1}, play the major role. Interestingly, L^{-1} is extremely important in the far field (15 ppmv) driving alone more than half of the variability of the outcome, whilst its relevance decreases significantly in the proximity of the release source (15,000 ppmv). By contrast, the wind speed shows the opposite behaviour, having the highest impact in the near field, by dominating the mass transport of the downward jet in the downwind direction. In the far-field, this parameter has a quite meaningless individual impact, although it shows indirect effects ($S_{Ti} \gg S_i$). In other words, its direct impact on the model output is less important than the inverse Monin-Obukhov length, although it plays still a role though its dependencies. Terrain roughness z_0 has less importance, with quite

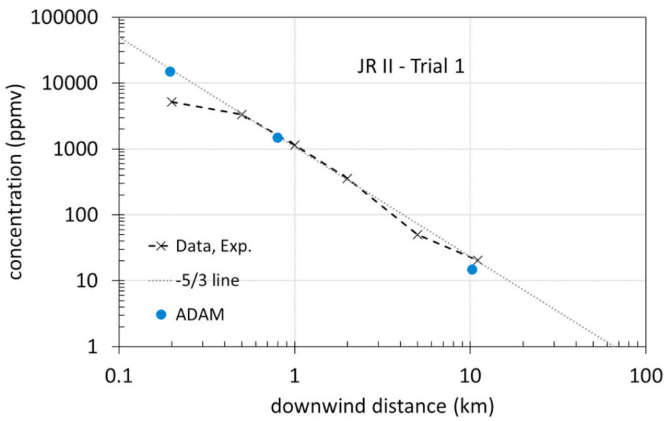

Fig. 3. JR II trial 1, concentration vs. download distance.

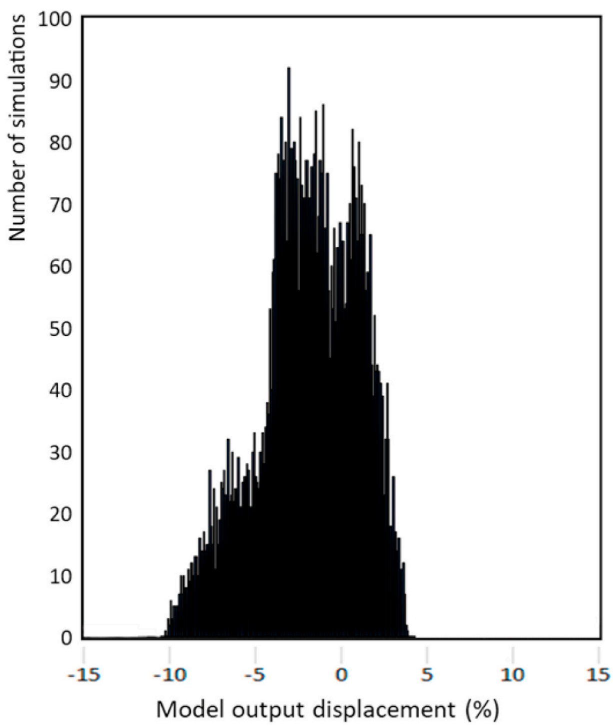

Fig. 4. Number of simulations vs. the model output at the reference concentration level of 15,000 ppmv in terms of displacement from the reference value obtained by fixing the 13 inputs at the reference values of Table 2. Model output: downwind distance at 15,000 ppmv concentration level. (Scenario: Vertical downward jet.)

negligible values in the mid and far-field, and slightly higher values for the near-field.

All internal model parameters have a relatively modest impact, making the highest contribution in the near-field. Amongst them, the droplets' size correlation SMD is the only one that achieves a 10% impact or greater in the far and mid field.

In sum, given our assumptions, the global sensitivity analysis reveals that 4 out of 13 inputs (namely, storage temperature, substrate roughness in proximity of the release, humidity, and pool roughness length) are definitely negligible, with total order sensitivity indices ($\widehat{S}_{Ti}$) that are consistently below 3% for all three model outputs (15,000, 1500, and 15 ppmv). It is particularly interesting to assess the impact of these low significance parameters on the model output uncertainty. Thus, with the whole set of the 13 inputs set to their reference values in column 'Ref' of Table to (so as to reproduce trial 1 of the Jack Rabbit II inter-comparison exercise), a first run of the ADAM-SLAB model was performed. Since the model outputs selected for the sensitivity analysis were the downwind distances at which the plume reaches three fixed values of concentration (15,000, 1500, and 15 ppmv), the simulation was conducted for these three reference values. The result is presented in Fig. 3, where, as a reference, the ADAM simulation is also compared to the experimental concentration data measured during the Trial as taken from Table 3 (Mazzola, 2020). A point to note is that the ADAM points follow quite well the empirical correlation $C_{max} \propto x^{-5/3}$, found by Hanna et al. (2016, 2017). Again, in the very near field ADAM tends to under predict the experimental concentration as previously mentioned (see section 2.3).

Table 4
Uncertainty analysis for the vertical downward jet conducted for the three model output (i.e. downwind distance at reference concentration levels).

Model output	Average Error (%)	Std. deviation (%)
15,000 ppmv (near field)	−1.9	3.1
1500 ppmv (mid field)	−2.4	2.3
15 ppmv (far field)	−4.3	3.5

The purpose of this uncertainty analysis is to assess how the uncertainty on the input parameters propagates to the final model outcome, allowing quantification of the possible vertical displacement of ADAM points in Fig. 3 consequent of the variation of input parameters from their reference values. Given the results of the sensitivity study, only 4 inputs with Total Effect below 3% have been included in the uncertainty analysis. The model output simulations were conducted by executing 10,000 simulations according to Sobol' sequence, in order to demonstrate that the input parameters with lowest Total Effects have insignificant impact on the model output within the considered variability range, and as such, they may be ignored.

Fig. 4 represents a typical outcome from the set of simulations conducted for the near field model output (15,000 ppmv). The histogram of the figure refers to the entire set of simulations, in which the value along the x-axis represents the displacement (%) of the model output from the reference value (obtained with the 13 reference inputs of Table 2). This displacement shows the difference in outcomes resulting from variation of *only* the 4 least important inputs. In the present case, the displacement is characterised by an average of ca. −2% with a standard deviation of about 3%. This figure represents the average error of the final estimate of the model outcome when only the value of the least important variables is allowed to fluctuate in the selected ranges. In other words, by fixing the values of the 9 most significant input parameters, while varying the values of the least important inputs, one arrives at the average error of the model output that would be achieved in the case of lack of knowledge of the least significant parameters.

The results of the analysis on all the three model outputs is given in Table 4. Notably, the model outcome variability is comparable in the three cases, and rather low in absolute terms if compared to the typical uncertainties of dispersions models. This means that by guessing the values of the least important input parameters, the average error introduced will never be greater than 4%, which may be considered acceptable for most purposes.

3.2. Horizontal jet reference case

As previously mentioned, a pure horizontal jet did not directly correspond to any trial of the Jack Rabbit II inter-comparison exercise. Due to the modelling differences, this reference case was introduced in this analysis to assess whether the overall conclusions of the sensitivity study might be similar for different jet directions. Thus, by using same criteria and methods of the case involving the vertical downward jet, the sensitivity indices were calculated and reported in Fig. 5, with Main Effect indices summation in the 78–85% range, which shows that also for this case model variability is meanly explained by the direct impact of individual inputs. Also looking at the single input parameters, the

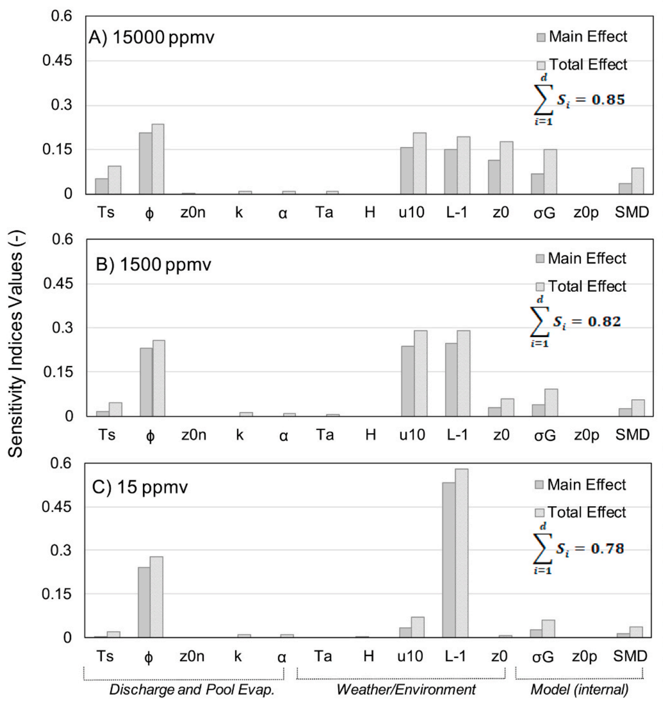

Fig. 5. Horizontal jet scenario: Main and Total sensitivity effects for ADAM model inputs given in Table 2.

Table 5
Uncertainty analysis for the horizontal jet conducted for the three model outputs (i.e. downwind distance at reference concentration levels).

Model output	Average Error (%)	Std. deviation (%)
15,000 ppmv (near field)	4.3	4.7
1500 ppmv (mid field)	3.6	3.9
15 ppmv (far field)	−0.3	2.5

results are quite consistent with the previous case, with a constant contribution of the filling level φ that accounts for more than 20% of the importance for the three model outputs. However, the results of this analysis indicate that the storage temperature is slightly more important here than in the other cases. This fact is not surprising, since storage temperature is directly associated with storage pressure, and thereby plays a definitive role in increasing the momentum of the jet in the downwind direction. This is particularly evident in the near field.

Similar behaviour is present also for weather and environment related parameters, although the inversion of the role played by the u_{10} and L^{-1} between the far and the near fields is somehow less pronounced. Model parameters shows similar behaviour, although there seems to be an inversion between the role played by the geometric spread σ_G, which relates to the droplets' distribution and SMD, the initial droplet size after post expansion. Due to the complexity of the rainout process and the differences in the pool formation mechanisms (higher and closer to the tank for downward jets and smaller but displaced further in the jet direction for horizontal jets) it is rather difficult to draw any conclusion from this result, also in light of the fact that the mentioned differences are quite limited.

In this case 6 out of 13 inputs with total order indices ($\widehat{S}_{Ti}$) are consistently below 3% for all three model outputs, namely, ambient temperature, humidity, pool roughness length, and substrate properties in proximity of the release (roughness thermal conductivity and diffusivity). (The latter are mainly responsible of the heat exchange between the rainout pool and the terrain.) By fixing all of the remaining 7 (most significant) parameters the uncertainty analysis was conducted as for the vertical downward case. The results are given in Table 5, showing the average displacement of the model output (downwind distance for the reference value of concentration) together with the corresponding standard deviation.

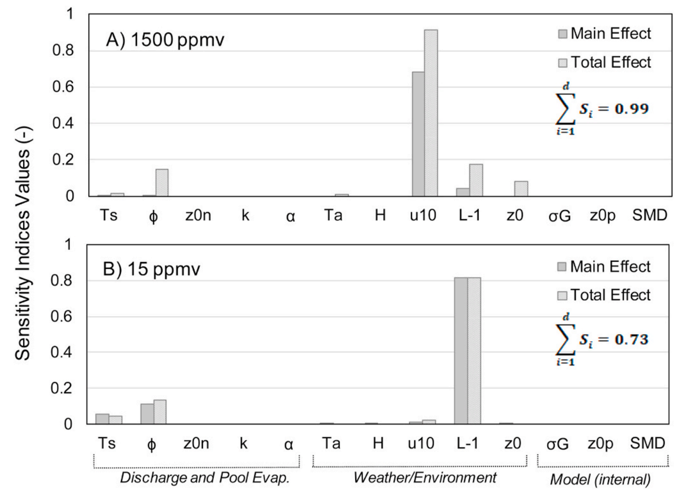

Fig. 6. Vertical jet scenario: Main and Total sensitivity effects for ADAM model inputs given in Table 2.

3.3. Vertical jet reference case

The last reference case is the vapour vertical jet from a hole on the top of the vessel. This case differs significantly from the previous cases (consisting of metastable liquid discharges undergoing rapid depressurisation at the hole plane exit, i.e., a flash phenomenon). Since the rupture occurs above the liquid level, a sudden depressurisation will take place within the vessel. Therefore, a completely different source term model must be employed. In addition, the analysis applies a different dispersion model from the previous cases. Whereas the dispersion model normally consists of two separate moduli involving (*i*) the initial vertical plume rise, and (*ii*) the subsequent move of the plume in the downwind direction. Not surprisingly, the result of the sensitivity analysis is also quite different from the previous cases. First of all, the highest concentration selected for the definition of model output (15.000 ppmv) was never achieved in the simulations. Therefore, the sensitivity analysis could only be applied to the two model output with lower concentrations, as shown in Fig. 6.

As for the majority of vertical jets, the current simulations confirmed absence of rainout and, in turn, absence of pool formation. Consistent with this result, all input parameters associated with the rainout modelling and with the pool evaporation were shown to have sensitivity indices equal to zero. It consists of the parameters of the substrate near the release (roughness z_{0n}, thermal conductivity and diffusivity) and the internal model parameters (σ_G, z_{0p} and SMD). Moreover, the filling level φ, a parameter directly associated with the amount of substance in the tank, is the only input parameter of the discharge series that accounts for more than 20% of the variability of the model outcome. Similar to the other cases, the wind speed u_{10} and the inverse Monin-Obukhov length L^{-1} play the major role even if with reverse importance in the mid and far fields. Terrain roughness is accountable for nearly 10% of the variability of the model output, but only in the mid field, whilst in the far fields its contribution is negligible.

According to the sensitivity analysis results, the inputs with Total Effect indices consistently below 3% for the two model output were greater than before (8 out of 13), and they were selected for the uncertainty analysis. The results are given in Table 6. The average errors are practically equal to zero for both model outputs.

Table 6
Uncertainty analysis for the vertical jet conducted for the two model outputs (i.e. downwind distance at reference concentration levels).

Model output	Average Error (%)	Std. deviation (%)
1500 ppmv (mid field)	−0.1	0.7
15 ppmv (far field)	0	0.5

4. Conclusions

A global sensitivity analysis was conducted on the ADAM-SLAB dispersion module. Three different reference cases associated with pressurised-liquefied chlorine orifice discharges from a horizontal vessel were built for this purpose. The resulting dispersion of chlorine vapours was assumed to have occurred under stable to neutral atmospheric conditions. The test cases were based on the trials of the recent Jack Rabbit II inter-comparison exercise and as such, retained all model input parameters referring to shared characteristics of the different trials (vessel geometry, storage state, and discharge orifice size). All other relevant input parameters (substance amount, storage and environmental conditions) were varied in a reasonable range to analyse their influence on the model output. The jet direction assumed in each case relates to the position of the equipment failure and its value was varied to incorporate all possible situations (downward, horizontal, and vertical jet direction).

The global sensitivity analysis showed that the filling level φ that accounts for the overall quantity of substance contained in the vessel is consistently the only important input in the group of discharge and pool evaporation modelling parameters. Concerning the other parameters, a quite different behaviour was identified for the different distances associated with the model outputs. In particular, in the far field, that is, the distance associated with the smallest concentration values-the atmosphere stability (the inverse Monin-Obukhov length) plays the most important role, accounting consistently for more than half of the variability of the outcome. In the near field, the number of parameters that drive the model output tends to increase, with the downwind wind as the dominant parameter.

The undertaken uncertainty analysis, in line with the main conclusions of the sensitivity analysis, showed that, by fixing all input parameters with a Total Effect sensitivity index above a certain level (3% in our case), and by varying the least significant parameters in the selected input range, the model output variability is always much below (in absolute terms) if compared to the typical uncertainties of dispersions models. This finding is in line with the main conclusions of the sensitivity analysis. The analysis is scenario-oriented rather than model-oriented, that is, it focuses on the influence of different inputs in relation to scenario outcomes, rather than the dispersion model performance. Nonetheless, the outcomes of this study also suggest a comprehensible way forward for reducing the number of input parameters for the ADAM-SLAB dispersion model and maintaining a comparable level of model accuracy at the same time. Further study is necessary to analyse whether some of the general conclusions found in the present case may be extended to a broader range of scenario types (e.g., catastrophic releases, failure type, dispersions under stable to neutral atmospheric conditions) and to release of toxic substances other than chlorine.

CRediT authorship contribution statement

Luciano Fabbri: Conceptualization, Methodology, Writing - original draft. **Maureen Heraty Wood:** Supervision, Writing - review & editing. **Ivano Azzini:** Software, Data curation. **Rossana Rosati:** Methodology, Validation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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