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Uncertainty Quantification of Heavy Gas Release Over a Barrier

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ABSTRACT: In this study a procedure for input uncertainty quantification (UQ) in computational fluid dynamics (CFD) simulations is proposed. The suggested procedure has been applied to a test case. The test case concerns the modeling of a heavy gas release into an atmospheric boundary layer over a barrier. The following uncertain parameters are investigated in their respective intervals: release velocity (18 m/s, 22 m/s), release temperature (270 K, 310 K) and the atmospheric boundary layer velocity (3 m/s, 7 m/s). The Stochastic Collocation (SC) method is used to perform the probabilistic propagation of the uncertain parameters. The uncertainty analysis was performed with two sets of sampling grids (full and sparse grids) for the uncertain parameters. The results show which of the selected uncertain parameters have the largest impact on the dispersed gas plume and the local concentrations in the gas cloud. Additionally, using sparse grids shows potential to reduce the computational effort of the uncertainty analysis.

In the external safety community, significant efforts are made to predict and calculate the necessary safety measures in order to prevent third parties from harm and injury in case of a hazardous or toxic gas release. One of the safety measures in case of a heavy gas release makes use of the parameter effect distance, which is defined as the distance from the toxic gas release point at which the concentration falls below a certain limit.

The dispersion of gasses in the atmosphere depends on the properties of the released gas, the environmental conditions such as weather conditions but also the built environment which might lead to an increased mixing of the released gas with the surrounding medium. Usually, barriers and walls are needed to reduce or prevent toxic gas exposure to humans (Fthenakis (1995)). Barriers are vertical solid objects placed near the release point in order to dilute or delay the dense gas cloud. All the above-mentioned parameters could affect the dispersion pattern and effect distances of the gas release.

Computational Fluid Dynamics (CFD) is being used in industries to predict the effect distances and is capable of predicting the interaction of the released gas with the atmospheric boundary layer and the barrier. However, the prediction of effect distances with CFD could be sensitive to different sources of uncertainties, especially in the physical parameters of the release gas and atmospheric conditions. Thus, quantifying the uncertainty in the prediction of the effect distance as a consequence of uncertainties in these physical parameters is of great importance for safety purposes.

There are three sources of uncertainties associated with each simulation result: numerical, input parameter, and model (form) uncertainties (Oberkampf and Roy (2010)). Methods are developed to quantify each source of uncertainties in order to verify and validate the predictions versus the measurements (Witteveen et al. (2011)).

Additionally, CFD calculations are often computationally expensive and require significant efforts from setting up the computational mesh to post processing the results. For propagation of the input parameter uncertainty, performing (pseudo-)random sampling is practically impossible for a CFD calculation. For this purpose, an efficient uncertainty analysis scheme that requires less computational effort is essential.

In this paper, the effect of input parameter uncertainties on a heavy gas release over a barrier is quantified. A procedure was developed for quantifying input parameter uncertainties including; parameter selection, expert judgment, sensitivity analysis, and input uncertainty propagation. As a result of this analysis, confidence levels for the prediction of effect distances for a specific release scenario are estimated. Additionally, an indication on the feasibility of employing efficient methods to propagate input uncertainties will be given.

1. UQ METHODOLOGY

A step-by-step procedure for performing an input parameter uncertainty quantification is proposed which is shown in Figure 1. It was aimed to propose a general framework which could be used for any input parameter uncertainties study. This procedure is based on four consecutive steps which are required for input parameter uncertainty quantification;

- Identification
- Characterization
- Propagation
- Estimation

The first step is to identify the system boundaries and input parameters. The next step is to characterize the input parameters by quantifying the ranges of parameters’ variations, dependency, and correlation of parameters and specify the confidence levels corresponding to the ranges of each parameter. The characterization of parameters could be either based on measurement data, the design of experiments method, or an expert judgment framework (Goossens et al. (2008)).

The uncertainty propagation is performed to quantify the effect of characterized input parameters on the quantities of interest. In general, the uncertainty propagation methods in high dimensional parametric spaces suffer from the curse of dimensionality, which means computational cost grows exponentially with the increasing number of input parameters (Doostan et al. (2009)). For computationally expensive calculations, a sensitivity analysis is suggested to be performed prior to the uncertainty propagation step to reduce the parametric dimensionality and the calculation effort of uncertainty analysis.

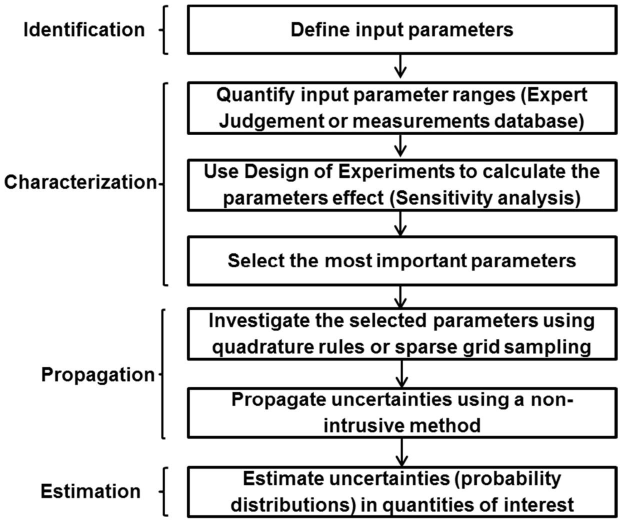

Figure 1: A procedure for uncertainty quantification of input parameters

For uncertainty propagation, the Stochastic Collocation (SC) method is employed in this paper which was first proposed by Xiu and Hesthaven (2005). This method is based on interpolating deterministic samples ($u_i(x,t)$) using Lagrange polynomials at quadrature points ($L_i(\xi)$)

$$u(x,t,\xi) \approx u^i = \sum_{i=0}^{n_s} u_i(x,t) L_i(\xi), \tag{1}$$

$$L_i(\xi) = \prod_{\substack{j=1 \\ j \neq i}}^{n_s} \frac{\xi - \xi_j}{\xi_i - \xi_j}, \quad L_i(\xi_j) = \delta_{ij}, \tag{2}$$

in which δ_{ij} is the Kronecker delta. The approximating polynomial is used to calculate the statistical moments. For instance, the stochastic mean ($\mu_{u,i}(x,t)$) is calculated using a pre-computed weight function (w_k) which depends on the quadrature points (ξ_j) and input parameters distribution function;

$$\mu_{u_i}(x,t) \approx \sum_{k=1}^{n_s} u_k(x,t) w_k, \tag{3}$$

$$w_k = \int L_k(\xi) f_\xi(\xi) d\xi. \tag{4}$$

Tensor grids can be used to extend the SC method to multiple uncertain input parameters. Another method to extend the uncertainty analysis to higher dimensions or reduce the computational effort of the SC method is to use sparse grids. It was shown that the convergence level of sparse grids compared with full grids is comparable with a significant reduction in computational effort, see Bungartz et al. (2004). In the proposed procedure, Smolyak sparse grids are suggested for which a detailed description of grid construction and weight calculations are given by Smolyak (1963).

As a result of uncertainty propagation the probability distribution and statistical moments for quantities of interest will be estimated. As a result of this analysis, confidence levels for the predictions based on non-deterministic simulations will be assessed.

2. CFD DOMAIN

The proposed method for input parameters uncertainty analysis is applied on a test case describing a heavy gas release into an atmospheric boundary layer over a barrier. In the present study, a barrier with a fixed geometry was chosen. Propane was chosen for the heavy gas. A 3D computational domain and grid was generated which is shown in Figure 2. 3D CFD calculations for the proposed test case is required to give a more accurate prediction of the heavy gas cloud topology which occasionally is not correctly captured by 1D Gaussian gas plume models.

The following dimensions for the domain and barrier were chosen;

- Release height: 1m
- Barrier height: 4 m
- Release distance from the inlet: 50 m
- Barrier distance from release: 60 m
- Domain dimension: (550,100,100) m

The grids contain approximately 300,000 nodes. Velocity inlet and pressure boundary conditions were chosen for the inflow and outflow boundaries. By applying a symmetry plane, only half of the domain is solved.

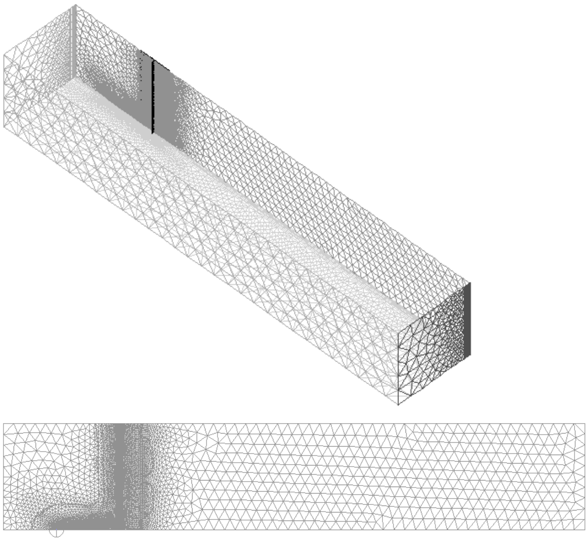

Figure 2: 3D Computational grid (top) and 2D cross section of the computational domain perpendicular to the barrier (bottom)

Steady-state calculations applying the k-ε turbulence model with wall functions were performed. All the calculations were done in ANSYS Fluent v.14. For the heavy gas transport, species transport models were applied. For simplification, the temperature drop due to expansion of propane is neglected.

The atmospheric boundary layer is defined as (Mack and Spruijt (2014));

$$u(z) = \frac{u^*}{\kappa} \ln\left(\frac{z}{z_0}\right), \tag{5}$$

in which u* is the frictional velocity, κ is the Von Kármán constant, and z describes surface roughness.

All the deterministic simulations were performed until the convergence criterion was met (10^{-6}).

3. PARAMETERS SELECTION

According to the procedure in Figure 1, a list of non-geometrical uncertain input parameters in the problem was made. Five input parameters and their variation ranges were identified for the parametric study which are summarized in Table 1. Due to the unavailability of measurement data, the ranges were estimated by aggregating expert opinions. The lower and upper bounds of the parameters are assumed to have a quantile of 5% and 95%. It was also assumed that the parameters are independent and normally distributed.

Table 1: List of input parameters and range of variations (ABL: Atmospheric boundary layer)*

Parameter	Lower	Mean	Upper
Roughness (m)	0.004	0.008	0.012
ABL* velocity (m/s)	3	5	7
ABL* temperature (K)	288	290	292
Release velocity (m/s)	18	20	22
Release temperature (K)	270	290	310

The quantities of interest are effect distances and local propane concentration at the release height. It is important to note that effect distance is computed from the release point. The concentration to determine the effect distance is 1% which is roughly 50% of the propane lower explosive limit (LEL).

In order to reduce the computational effort for the uncertainty analysis with 5 input parameters, a sensitivity analysis by varying one parameter in each simulation, was performed (Figure 3). The figure shows the effect distance for changing one input parameter at a time to its minimum or maximum value. The cost for the sensitivity analysis with the five input parameters is therefore equal to eleven deterministic CFD simulations. The initial results show the significance of each input parameter and based on this analysis, the most dominant parameters were selected for the uncertainty propagation step. These input parameters are atmospheric boundary layer (ABL) velocity, release velocity and release temperature.

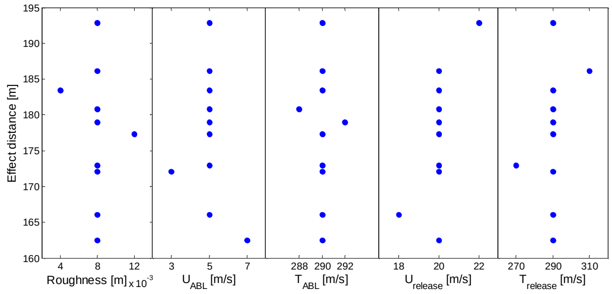

Figure 3. Sensitivity analysis for 5 input parameters

4. UNCERTAINTY PROPAGATION

The first level Clenshaw-Curtis quadrate rules (three samples for each parameter) were used to perform the uncertainty propagation which leads to 27 deterministic simulations for the full grid. This is a significant reduction of the computational cost down from 243 simulations for all five input parameters on the same level. The three-dimensional 1st level full grid and sparse grid collocation points are shown in Figure 4. The corresponding 1st level Smolyak sparse grid gives 7 deterministic simulations, by removing the parameters interaction.

4.1. Deterministic analysis

The CFD calculations were performed for 27 full grid simulations and the effect distance variation with respect to each input parameter was analyzed. Increasing the gas release velocity and decreasing the release temperature leads to an increase in the effect distance (Figure 5, Figure 7). This phenomena is expected to occur due to an increase in the release gas mass flow rate.

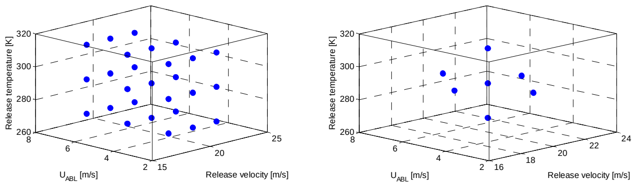

Figure 4. Level 1 full grid with 27 CFD simulations (left) and Smolyak sparse grid with 7 CFD simulations (right)

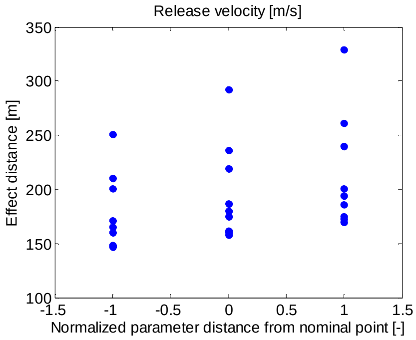

Figure 5. Effect distance variations function of the release velocity

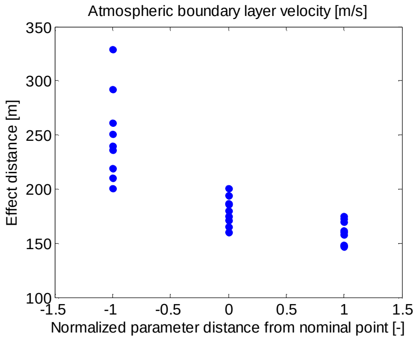

Figure 6. Effect distance variations function of the atmospheric boundary layer velocity

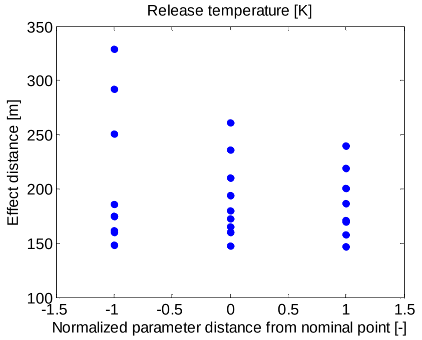

Figure 7. Effect distance variations function of release temperature

A higher atmospheric boundary layer (ABL) velocity, leads to a decrease in the effect distance as a result of change in the shear layer mixing between the background wind velocity and released gas (Figure 6).

The results show that the maximum effect distance occurs at the maximum release velocity and minimum of ABL velocity and release temperature. Contour plots of propane concentration at a plane 1 m from the ground is given in Figure 8 for the maximum and minimum effect distances. It is found that the flow topology changes when the heavy gas approaches the barrier at a higher mass flow rate due to a strong mixing and momentum exchange upstream the barrier.

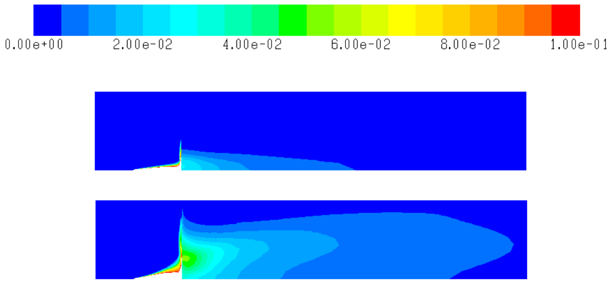

Figure 8.The molar fraction of propane at the plane 1m from the ground for the minimum (top) and maximum (bottom) effect distance. The maximum concentration for contour plot ranges was set to 10% for an easier visualization

4.2. Statistics of effect distance

The uncertainty mean and standard deviation of the effect distance for the first level collocation points is given in Table 2. There is a shift of approximately 7m in the stochastic mean of the effect distance. The considered parameters give a large variation to the effect distance (15% of the mean value).

Sparse grid results show a convergence for the uncertainty mean value of the effect distance. The uncertainty standard deviation is under-predicted. It indicates that interaction of the input parameters contributes to the variation of the effect distance. The statistical moments computed with the sparse grid gives a reasonable convergence compared to the full grid by performing fewer CFD simulations.

The cumulative distribution functions of the effect distance for both full and sparse grids are given in Figure 9. Higher standard deviation of effect distance for the full grid can be seen at the tail of the distribution functions. According to the cumulative distribution function, confidence levels could be estimated for predictions. In other words, the effect distance is predicted to be below 235 m with 95% confidence, given the input specified parameters ranges.

Table 2:Uncertainty mean and standard deviation of the effect distance

	Nominal case	**Sparse grid**	**Full grid**
Simulation points	1	7	27
Mean value (μ)	179.87	186.05	186.30
Standard deviation (σ)	0	25.16	29.72

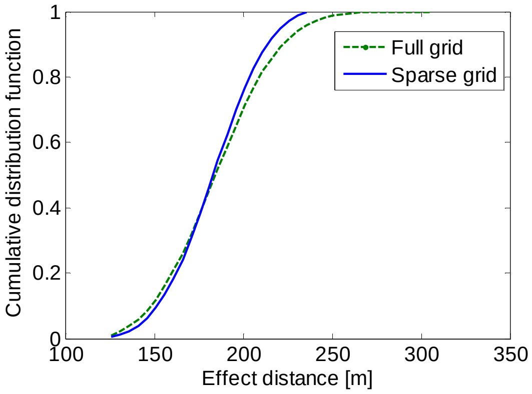

Figure 9. Cumulative distribution functions of effect distance

4.3. Statistics of propane concentration

The uncertainty mean and standard deviation of the propane molar concentration at a plane 1m above the ground with full grid is shown in Figure 10 and Figure 11. The uncertainty mean of propane concentration has its maximum at the release point. The maximum standard deviation occurs at the mixing zone between the release point and atmospheric boundary layer velocity. Additionally, the variations in the topology of the released gas clouds as a result of uncertain parameters can be seen in the standard deviation contours. It indicates that the propane concentration, shape of the gas cloud and the shear mixing zone is affected by uncertain input parameters.

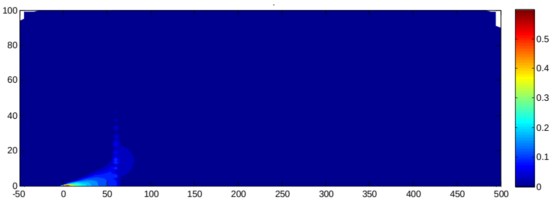

Figure 10. Uncertainty mean of propane molar concentration.

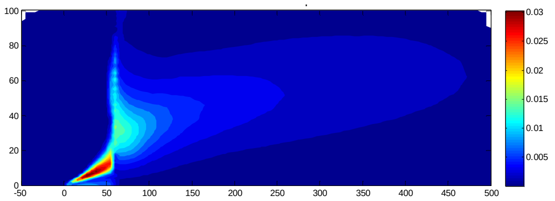

Figure 11. Uncertainty standard deviation of propane molar concentration

5. CONCLUSIONS

A step-by-step procedure for input parameter uncertainty quantification is proposed and it has been applied to a computationally expensive CFD model of a heavy gas release over a barrier.

For the analysis, five non-geometrical input parameters were chosen, of which three significant parameters were selected for input uncertainty propagation. The ranges for these three input parameters were atmospheric boundary layer velocity (3 m/s, 7 m/s), release velocity (18 m/s, 22 m/s) and release temperature (270 K, 310 K). For input uncertainty propagation the stochastic collocation method with the first level Clenshaw-Curtis full grid and sparse grid is used.

The results show that the effect distance is sensitive to the input parameters and the largest variation is observed in the gas plume topology. The interaction between the release mass flow rate and background wind velocity changes the mixing layer and consequently the gas cloud topology and effect distance.

Using sparse grids shows a potential to perform uncertainty analysis with a reduced number of samples and computational effort. Thus, in future work, uncertainty analysis could be performed in higher dimensions while incorporating more input parameters by employing sparse grids.

Performing an input uncertainty analysis is an essential step in applications dealing with safety and hazards. This analysis gives confidence levels to the predictions and additional information with respect to the validity of the simulations.

6. REFERENCES

Bungartz, H.J., Griebel, M. (2004) "Sparse Grids", Acta Numerica: p1-123.

Doostan, A., Iaccarino, G. (2009) “A least-squares approximation of partial differential equations with high-dimensional random inputs”, *Journal of computational physics 228, 4332-4345.*

Fthenakis, V.M. (1995). “Mitigation options for accidental releases of hazardous gases” *International conference on modeling and mitigation the consequences of accidental releases of hazardous materials*, New Orleans, *LA.*

Goossens, L.H.J., Cooke, R.M., Hale, A.R., Rodic-Wiersma, Lj. (2008) ”Fifteen years of expert judgement at TUDelft”, *Safety Science 46, 234-244.*

Mack, A., Spruijt, M.P.N. (2014).”CFD dispersion investigation of CO2 worst case scenarios including terrain and release effects” *Energy Procedia 51,363-372.*

Oberkampf W.L., Roy C.J. (2010). ”Verification and validation in scientific computing“, *Cambridge University Press.*

Smolyak, S.A. (1963). ”Quadrature and interpolation formulas for tensor products of certain classes of functions” *Dokl. Akad. Nauk SSSR 4, 240-243.*

Witteveen, J.A.S., Duraisamy, K., Iaccarino, G. (2011). “Uncertainty quantification and error estimation in scramjet simulation” *Proceedings of the* 17^{th} *AIAA International Space Planes and Hypersonic Systems and Technologies Conference, AIAA-2011-2283, San Francisco.*

Xiu, D., Hesthaven, J.S. (2005). ”High-order collocation methods for differential equations with random inputs” *SIAM Journal on Scientific Computing 27, 1118-1139.*