Sensitivity Analysis and Parameter Optimization for the Improved Modelling of Gas Explosions

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1 Introduction

The accidental release of flammable gas or liquids may have severe consequences, as experienced after the Macondo disaster in 2010 [1]. Quantitative risk assessment (QRA) is an important part of the effort directed towards gaining higher safety levels in the process industries. Advanced computational fluid dynamics (CFD) models are often used to predict the consequences of potential accidents.

The fluid flow in large scale gas explosions will ultimately become turbulent. While the modelling of turbulent flows represents a challenge in itself [2], a gas explosion will also have a reaction zone where chemical energy is released. In addition, the effects of the surrounding geometry may be significant for the flame acceleration. A range of instability phenomena will cause a flame to transition from the laminar state and enter the turbulent regime of flame propagation. At the higher flame velocities a deflagration to detonation transition (DDT) may occur. In order to represent gas explosions in industrial process facilities with a CFD model, the grid resolution needs to be significantly larger than the scales where the chemical reactions interact with the flow. A range of subgrid models is therefore necessary to close the system of equations. The coupling of these submodels with the fundamental equations will ultimately require some *tuning* of empirically determined parameters within their range of experimental uncertainty.

In order to systematically investigate the effect of perturbations of empirical parameters on the model result, the method of sensitivity analysis is proposed [3], [4]. Davis *et al.* [4] present an approach that uses sensitivity analysis to optimize the active parameters, in order to get model results that are as close as possible to a set of experimental target values. In this paper, the same approach is applied to the gas explosion model in the CFD tool FLACS [5].

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2 Theory

The concept of sensitivity analysis is often used in the field of chemical kinetics to determine which of possibly thousands of parameters are rate-limiting [4]. The approach is useful for any complex system where the number of variables involved makes it challenging to have a complete understanding of their influence on the model results. The turbulence and combustion models that are used in the FLACS solver constitute such a complex system.

With a solid knowledge of how the results of a system vary when the input is perturbed, it is possible to foresee the effect that a model change will have. More specifically, model results can be predicted with a response surface [6], expressed as a function of model parameters in the form of a second or third order polynomial

$$\eta = a_0 + \sum_{i}^{L} a_i x_i + \sum_{i}^{L}\sum_{j\geq i}^{L} a_{ij} x_i x_j + \sum_{i}^{L}\sum_{j\geq i}^{L}\sum_{k\geq j}^{L} a_{ijk} x_i x_j x_k \;, \tag{1}$$

where η is the model response, L is the number of active parameters, and x_i is the ith parameter k_i normalized by its nominal value $k_{i,0}$ and uncertainty factor f_i

$$x_i = \frac{ln\left(\frac{k_i}{k_{i,0}}\right)}{lnf_i} \;.$$

If the curvature of η is too high to be described by Eq. 1, a logarithmic response surface may be more appropriate

$$\ln \eta = a_0 + \sum_{i}^{L} a_i x_i + \sum_{i}^{L}\sum_{j\geq i}^{L} a_{ij} x_i x_j + \sum_{i}^{L}\sum_{j\geq i}^{L}\sum_{k\geq j}^{L} a_{ijk} x_i x_j x_k \;, \tag{2}$$

The response surface can be expressed as a multivariate Taylor expansion of the model response $\eta(\mathbf{x})$ around **x=0** [4]

$$\begin{aligned} \eta(\mathbf{x}) \;\; = \;\; & \eta(0) + \sum_{i}^{L} \left.\frac{\partial \eta}{\partial x_i}\right|_0 x_i + \frac{1}{2}\sum_{i}^{L} \left.\frac{\partial^2 \eta}{\partial x_i^2}\right|_0 x_i^2 + \sum_{i}^{L}\sum_{j>i}^{L} \left.\frac{\partial^2 \eta}{\partial x_i \partial x_j}\right|_0 x_i x_j + \frac{1}{6}\sum_{i}^{L} \left.\frac{\partial^3 \eta}{\partial x_i^3}\right|_0 x_i^3 \\ & + \frac{1}{2}\sum_{i}^{L}\sum_{j\neq i}^{L} \left.\frac{\partial^3 \eta}{\partial x_i^2 \partial x_j}\right|_0 x_i^2 x_j + \sum_{i}^{L}\sum_{j>i}^{L}\sum_{k>j}^{L} \left.\frac{\partial^3 \eta}{\partial x_i \partial x_j \partial x_k}\right|_0 x_i x_j x_k + ... \end{aligned} \tag{3}$$

Davis *et al.* [4] propose to utilize the relation

$$\left.\frac{\partial \eta}{\partial x_i}\right|_0 = \eta(0) s_i \ln f_i \;, \tag{4}$$

where $\eta(0)$ is the nominal, unperturbed model response value and s_i is the first order sensitivity coefficient. The coefficients of the surface in Eq. 1 can thus be determined up to the second and partially third order by computing the first order sensitivities, $s_i = \partial \ln \eta(0) / \partial \ln k_i$ and $s_{\pm i,j} = \partial \ln \eta \left[\mathbf{x}(\pm\alpha)_i\right] / \partial \ln k_j$, where $\eta\left[\mathbf{x}(\pm\alpha)_i\right]$ is a vector of normalized parameters, whose elements are 0, except for the ith parameter, which is perturbed by α, $\mathbf{x}(\pm\alpha)_i = [0, 0, ..., x_i = \pm\alpha, ..., 0]$. The second order coefficients are found by differentiating the first order sensitivities. Some of the third order coefficients can also be obtained by using the first order sensitivities, resulting in a response surface of higher accuracy without an increased computational cost.

When a reliable model response surface is at hand, the active parameters can be optimized for a given case by minimizing a least-squares objective function

$$\sum_i \left[1 - \frac{\eta_i(\mathbf{x})}{\eta_{expt,i}}\right]^2 , \tag{5}$$

where $\eta_i(\mathbf{x})$ is the model response to a certain parameter **x**, and $\eta_{expt,i}$ is an experimental target value [4].

3 A system of empirical parameters

Several CFD models developed for engineering applications use the concept of a turbulent burning velocity, where an empirical correlation determines the relative importance of the root mean square (rms) turbulent velocity fluctuation u', some characteristic length scale l, the laminar burning velocity S_L, and the kinematic viscosity ν for the propagation velocity of the turbulent flame front. In general, turbulent burning velocity correlations are often given on the form

$$S_T \;=\; F\left(u', l, S_L, \nu\right) \;\sim\; u'^A \, l^B \, S_L^C \, \nu^D \, . \tag{6}$$

The literature proposes a range of possible values of the exponents in the empirically derived correlations [7], see Table 1. Although the correlations may apply for somewhat different turbulent flow regimes, the range in values suggests that the system is a candidate for systematic parameter optimization.

Reference	**A**	**B**	**C**	**D**
Bray (1992) (used in FLACS) [8]	0.412	0.196	0.784	-0.196
Peters (1999) [9]	0.500	0.500	1.00	-0.500
Bradley (1992) [10]	0.550	0.150	0.600	-0.150
Zimont (1988) [11]	0.750	0.250	0.500	-0.250
Kerstein (1988) [12]	0.875	0.375	0.500	-0.375

Table 1: Examples of turbulent burning velocity correlations.

4 The target values

Naturally, the target values for model optimization must be determined with care, as reliable experimental results are essential. A comprehensive framework for evaluation and classification of experiments is therefore needed [7]. The target values in this work are picked from a test matrix where gas explosion experiments are classified according to the degree of congestion and confinement of the geometry. See Figure 1 for an overview of all categories for the gas explosion (GasEx) application of FLACS.

Three experiments from the category *1B: Unconfined, congested* are used here to illustrate how the method of using sensitivity analysis for response surface development can be applied to the gas explosion model in FLACS. Two repeated test series (*Alpha* and *Beta*) commissioned by the UK Health and Safety Executive (HSE) were performed in an open, congested offshore module [13], using natural gas. For the MERGE test series, the geometry consisted of dense pipe racks in unconfined gas clouds [14]. Here, the *B* configuration with methane is used. In the unconfined, congested category, the solution may be expected to be particularly dependent on the empirical turbulent burning velocity correlation. A first order sensitivity analysis of the maximum overpressure obtained in two representative monitor points confirms that the exponents in Table 1 are among the active parameters. Figure 2) shows the first order sensitivities. Note that monitor points with a higher number are further away from the ignition point.

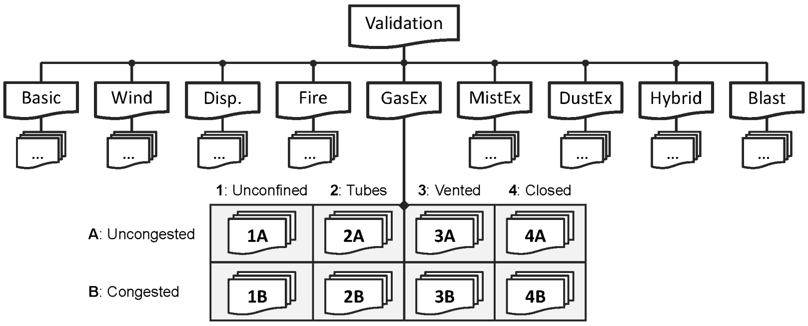


Figure 1: A classification scheme for the GasEx application of FLACS [7].

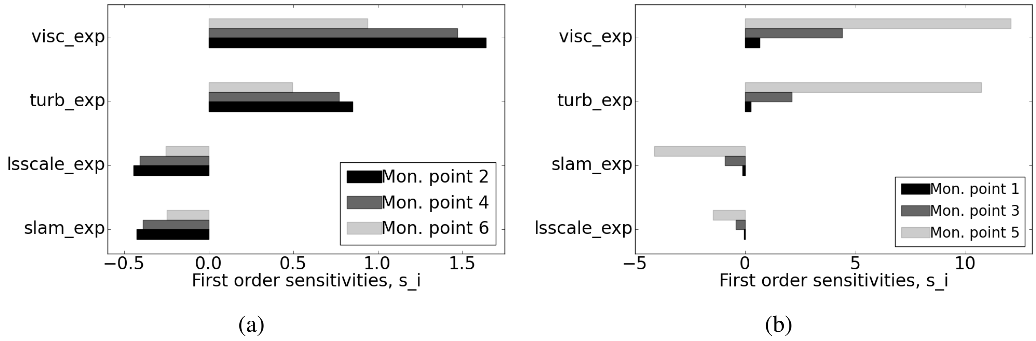


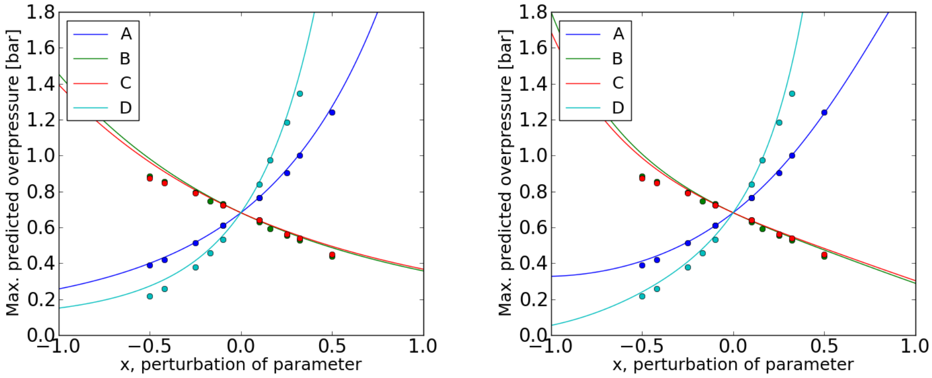
Figure 2: First order sensitivity analysis of the maximum overpressure to a selection of empirical parameters, obtained in two monitor points for the MERGE *B* (a) and HSE *Beta* (b) configurations.

5 Results and discussion

Response surface polynomials of second order, partial third order and logarithmic response surfaces of second and partial third order were constructed according to Eqs. 3 and 4. The *finite difference approximation*, also called the *brute force method* was used to compute the coefficients. The method may be computationally expensive, however, it is simple to apply as only the ODE solver itself is needed [15]. The brute force approach is considered to be feasible for the relatively low number of active parameters studied here, i.e. the exponents A, B, C and D given in Eq. 6 and Table 3. The uncertainty factor was set to $f_i = 2$ for all exponents.

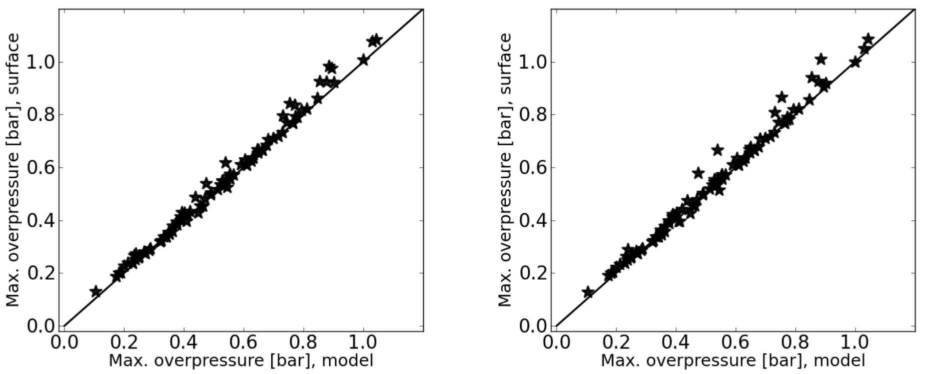
The results for each of the experiments show the same general trends. A logarithmic response surface gave the best agreement towards the edges of the uncertainty span. The model and surface response (i.e. the maximum overpressure) in a representative monitor point for the MERGE B experiment are plotted in Figure 3. The projections of the four dimensional surface onto the plane where only one parameter is varied at a time are shown. Figure 4 shows the agreement between the model and the response surface for all parameters described in Table 3. The scatter plots indicate that for this example, second and partial third order give roughly the same accuracy for the chosen sample points. The accuracy decreases as the parameters are perturbed more than $\pm 50\%$ of their uncertainty range. Meanwhile, the response surface seems to be capable of predicting the model response with a satisfying accuracy closer to the nominal response value.

A first optimization of the model system was done by minimizing the function in Eq. [5], for the maximum overpressure in the monitor point used in Figure 3(b). The parameters A, B and C were allowed to vary. The results indicate that an exponent A of ~ 0.7, an exponent B of ~ 0.25, and an exponent C of ~ 0.6 might be the most appropriate for this particular example. Naturally, no definite conclusions can be reached before a similar study has been undertaken for a wide set of validation cases, for each of the categories shown in Figure 1.



(a) (b)

Figure 3: Model (dots) and response surface (lines) for (a) a second order logarithmic surface and (b) a partial third order logarithmic surface, legend labels defined according to Table 1.



(a) (b)

Figure 4: Model and response surface agreement for (a) a second order logarithmic surface and (b) a partial third order logarithmic surface.

6 Summary and further work

This paper proposes the use of sensitivity analysis to analyze the influence of empirical parameters on the model response of a complex CFD gas explosion model, FLACS. Response surfaces in the form of second and third order polynomials were constructed. Reliable response surfaces can be used to optimize the empirical parameters – so as to ensure an improved fit of the model to a range of reliable experiments. The exercise of computing the first order sensitivities is valuable simply because of the gained insight into the behaviour of the model. However, an extensive literature review is necessary to determine the uncertainty span of the active parameters. Target values must be specified with great care. A comprehensive evaluation and classification framework is essential for ensuring the quality of the experimental data. The examples considered here illustrate this approach, and the results suggest that sensitivity analysis may be a powerful tool for further CFD model development and systematic model improvements.

References

[1] DHSG (2011). Final report on the investigation of the Macondo well blowout, Deepwater Horizon Study Group (DHSG), 1 March 2011

[2] Hanjalic, K. and Launder, B. (2011). Modelling turbulence in engineering and the environment: Second-moment routes to closure, Cambridge University Press, 1st edition

[3] Rabitz, H., Kramer, M. and Dacol, D. (1983). Sensitivity analysis in chemical kinetics, Annual Review of Physical Chemistry, 34: 419-461

[4] Davis, S.G., Mhadeshwar, A.B., Vlachos, D.G. and Wang, H. (2004). A new approach to response surface development for detailed gas-phase and surface reaction kinetic model optimization. Int. J. of Chemical Kinetics 36(2): 94-106

[5] GexCon AS (2012). FLACS v10.0 User's Manual, http://www.flacs.com, accessed 05.01.2013

[6] Frenklach, M. (1984). Systematic optimization of a detailed kinetic model using a methane ignition example, Combustion and Flame, 58(1): 69-72

[7] Skjold, T., Pedersen, H.H., Bernard, L. Middha, P. Narasimhamurthy, V.D., Landvik, T., Lea, T. and Pesch, L. (Unpublished). A matter of life and death: Validating, qualifying,and documenting models for simulating flow-related accident scenarios in the process industry. Chemical Engineering Transactions 31: 6 pp

[8] Bray, K.N.C. (1990). Studies of the turbulent burning velocity. Proceedings of the Royal Society of London: Mathematical and Physical Sciences 431(1882): 315-335

[9] Peters, N. (1999). The turbulent burning velocity for large-scale and small-scale turbulence, Journal of Fluid Mechanics, 384: 107-132

[10] Bradley, D., Lau, A.K.C. and Lawes, M. (1992) Flame stretch rate as a determinant of turbulent burning velocity Philosophical Transactions: Physical Sciences and Engineering 338, 359-387

[11] Zimont, V.L. and Mesheriakov, E.A. (1988). A model of combustion of partially premixed gases, in: Structure of gas flames, Proceedings of international colloquium, Part I.I, Novosibirsk: ITPM SO AN SSSR, 35-43 (in Russian).

[12] Kerstein, A.R., (1988). Pair-exchange model of turbulent premixed flame propagation, Proceedings of the Combustion Institute, 21: 1281-1289

[13] Evans, J.A., Exon, R. and Johnson, D.M. (1999). The repeatability of large scale explosion experiments, Offshore Technology Report OTO 1999 042, Health & Safety Executive, October 1999, www.hse.gov.uk/research/otopdf/1999/oto99042.pdf, accessed 15.01.2013

[14] Mercx, W.P.M. (1994). Modelling and Experimental Research into Gas Explosions. Overall final report for the MERGE project. CEC contract STEP-CT-0111(SMA)

[15] Turányi, T. (1990). Sensitivity analysis of complex kinetic systems. Tools and applications. Journal of Mathematical Chemistry 5(3): 203-248