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A Matter of Life and Death: Validating, Qualifying and Documenting Models for Simulating Flow-Related Accident Scenarios in the Process Industry

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This paper describes an integrated approach for validating, qualifying and documenting numerical models for simulating complex systems. Although the example used to illustrate the process entails simulations of accident scenarios in the petroleum and process industries by means of computational fluid dynamics (CFD), the methodology is not restricted to any particular model or system. CFD tools are applicable to various aspects of societal safety, including transportation, storage and use of various energy carriers, as well as malicious attacks involving toxic gas or condensed explosives. The approach adopted involves a continuous process where relevant validation cases are classified according to the physical phenomena involved, and prioritized based on parameters such as relevance for typical applications of the model system, measurement quality and repeatability, availability of data, spatial scale, materials or substances used, etc. A model evaluation protocol (MEP) provides guidelines for prioritizing the various validation cases, and for evaluating the simulation results. Statistical methods and visualization techniques are employed for describing the validation range and the associated uncertainties of the model system. Use of the methodology is illustrated for a typical application of the commercial CFD tool FLACS: large-scale gas explosions in congested geometries. The results highlight some of the inherent challenges associated with the interpretation of results from large-scale experiments, and demonstrate how such challenges can be addressed during the model evaluation process. The methodology can be extended to include sensitivity studies and advanced optimization schemes for key model parameters.

1. Introduction

Major disasters continue to cause severe losses in the process industry and society in general. The majority of the 100 largest property losses in the hydrocarbon industries from 1972 to 2011 involved fires and explosions (Marsh, 2012). The Macondo disaster in 2010 demonstrated the devastating effects such accidents can have on the environment (DHSG, 2011). Many organisations have adopted quantitative risk analysis (QRA) as part of their approach for achieving satisfactory levels of safety (Vinnem, 2007). However, there are significant uncertainties associated with most risk assessments, including the completeness of the hazard identification processes, lack of relevant data for estimating the frequencies of events such as loss of containment and ignition of flammable mixtures, and the topic of the present work: how accurate are the models used for estimating the consequences of specific hazardous events?

Many accidents in the process industry involve complex fluid flow phenomena, with or without chemical reactions (Mannan, 2012): release and dispersion of toxic, asphyxiating, radioactive or flammable material in gaseous, liquid or solid form; gas, vapour, mist, dust or hybrid explosions; detonation of condensed explosives and propagation of blast waves; jet and pool fires; etc. The type of models used for assessing the consequences of such events range from the analytical expressions and empirical correlations or nomographs in standards and guidelines, to phenomenological tools of varying complexity, and finally sophisticated numerical model systems that solve conservation equations for fundamental parameters such as mass, momentum and energy. Regardless of the complexity of the models, it is essential for the

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quality of QRAs, and hence for safety and security, that risk analysts understand the underlying assumptions and inherent limitations of the tools they use, as well as the level of accuracy they can expect in the results. Both government bodies and industry show increasing awareness of the need to qualify models for particular applications, for instance by requiring modellers to demonstrate the capabilities of their models by reproducing results from specific sets of experiments (Ivings et al., 2007).

The validation and documentation process represents a fundamental challenge for developers of any model system that aspire to describe a wider range of physical phenomena, or other initial and boundary conditions, than the ones that can be mapped out by a finite number of experiments. Although the governing equations for turbulent fluid flow are well established (Bradshaw, 1994), analytical solutions are primarily of academic interest, and discrete solutions by direct numerical simulation (DNS) can still only be realized for relatively simple systems. Models based on large eddy simulations (LES) have gained increasing popularity in recent years. However, within the context of simulating industrial accident scenarios, most commercial CFD tools still rely on turbulence models based on Reynolds-averaged Navier-Stokes (RANS) equations (Launder and Spalding, 1974), often complemented with sub-grid models to account for the influence of objects that cannot be resolved on the computational grid. For turbulent reactive flows it is necessary to add models for chemical reactions, and to couple the resulting model system (Hjertager, 1982). Several CFD codes for engineering applications have adopted the concept of turbulent burning velocity S_T for simulating premixed combustion. The speed of the propagating flame front relative to the unburnt mixture is determined by an empirical expression on the form:

$$S_T \propto u'^{A}\, L^{B}\, S_L^{\,C}\, \nu^{D} \tag{1}$$

where u' is the root-mean-square of the turbulent velocity fluctuations, L is a turbulent length scale, S_L is the laminar burning velocity, and ν is kinematic viscosity (or thermal diffusivity). Table 1 summarizes some published values of the exponents in Eq. (1). It is evident that the values from literature span a considerable range, and in Section 4 it will be shown how the validation system can be extended to parameter optimization. Figure 1 shows the geometry model implemented in the commercial CFD code FLACS for the test rig that will be used to illustrate the methodology presented in this paper.

Table 1: Examples of exponents in Eq. (1) from published combustion models; see references for details.

Publication	*A*	*B*	*C*	*D*
Bray (1990), used in FLACS v9.1	0.412	0.196	0.784	-0.196
Peters (1992,1999)	0.500	0.500	1.000	-0.500
Bradley et al. (1992)	0.550	0.150	0.600	-0.150
Zimont and Mesheriakov (1988)	0.750	0.250	0.500	-0.250
Kerstein (1988)	0.875	0.375	0.500	-0.375
Sensitivity range investigated in Figure 7	0.412-0.536	0.196	0.784	-0.196

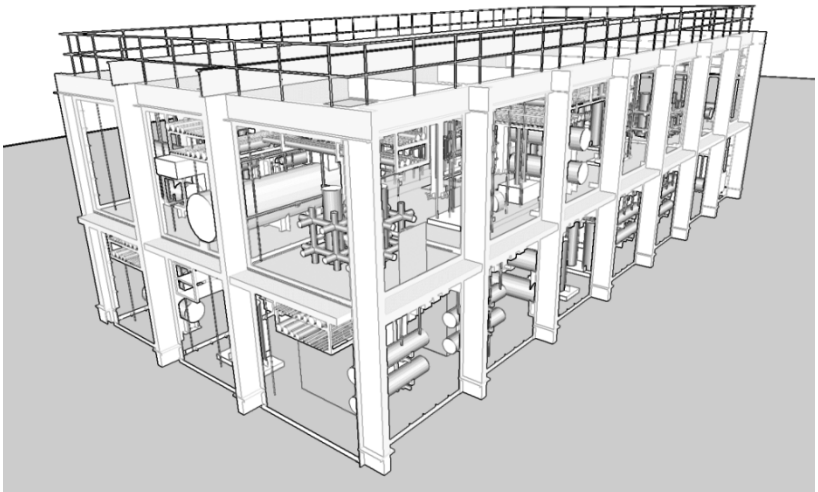

Figure 1: Geometry model implemented in FLACS for the HSE test rig; dimensions 28 m x 12 m x 8 m.

2. Experiment and simulations

The methodology for validating, qualifying and documenting models for simulating flow-related accident scenarios in the process industry will be illustrated for two repeated test series performed in a congested offshore module (Evans et al., 1999): one series of five repeated experiments with central ignition (*Alpha*), and one series of six repeated experiments with end ignition (*Beta*). The work was commissioned by the UK Health & Safety Executive (HSE) and executed by BG Technology on the Spadeadam test site. There were changes in the level of congestion between the two series, but all experiments were performed with mixtures of natural gas and air for equivalence ratios in the range 1.05-1.14. The mixtures were ignited by low-energy electrical discharges under initially quiescent conditions. The simulations have been performed with the commercial CFD code FLACS v9.1 (GexCon, 2011; Pedersen and Middha, 2012).

3. Methodology and results

Figure 2 shows a schematic representation of the proposed methodology. Each potential validation case, or *instance*, is classified according to the physical phenomena it represents. Relevant validation cases can be experiments, accidents, detailed simulation results, or analytical solutions to idealized problems. The schemes for classification and prioritization are illustrated in Figure 3. The categories defined for validating modules in the CFD code FLACS include: wind (atmospheric flow); release and dispersion; fire; gas, mist, dust and hybrid explosions; and blasts generated by condensed explosives or physical explosions. Each category is further divided according to specific criteria, such as degree of congestion and confinement in the case of gas explosions. The experiments in the HSE rig would typically belong to group 1B in Figure 3. It is a challenge to define objective and unambiguous scales for categorizing validation cases based on relevance, spatial scale, repeatability, etc. However, as long as a significant number of cases are simulated the resulting uncertainty has limited influence on the outcome of the overall analysis.

Basic characteristics of each instance are registered in a database, together with relevant data for the cases where the average score exceeds a certain threshold. Of particular concern with respect to predicting the consequences of major accidents in industry is the lack of repeated large-scale experiments of high quality. In this respect, the two test series from the HSE rig are quite unique. Figure 4 shows that the repeatability is somewhat limited in both series, and Figure 5 shows measured and simulated pressures as a function of distance from the ignition point. The spread in experimental results highlights the inherent limitation with respect to the accuracy that can be achieved in CFD simulations.

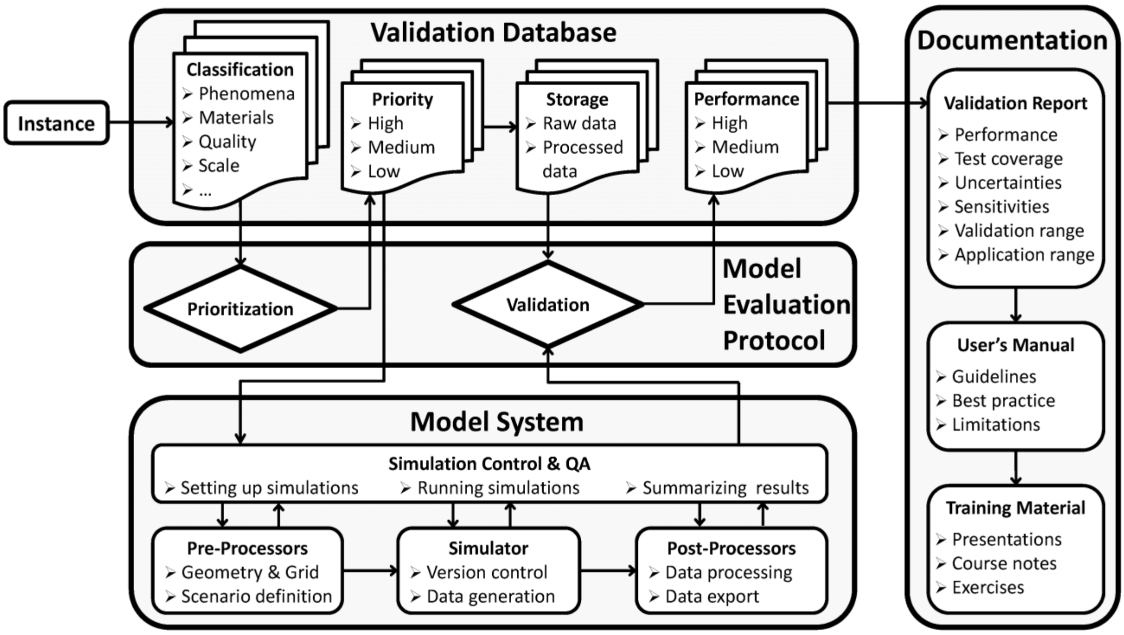

Figure 2: Flow chart illustrating the work flow and main components in the integrated system for validating, qualifying and documenting models for process safety applications.

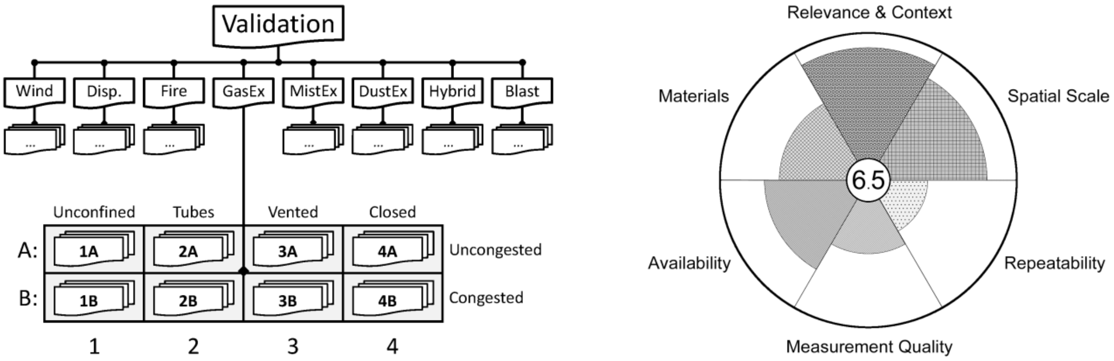

Figure 3: Classification of validation cases (left), and categories for prioritization (right).

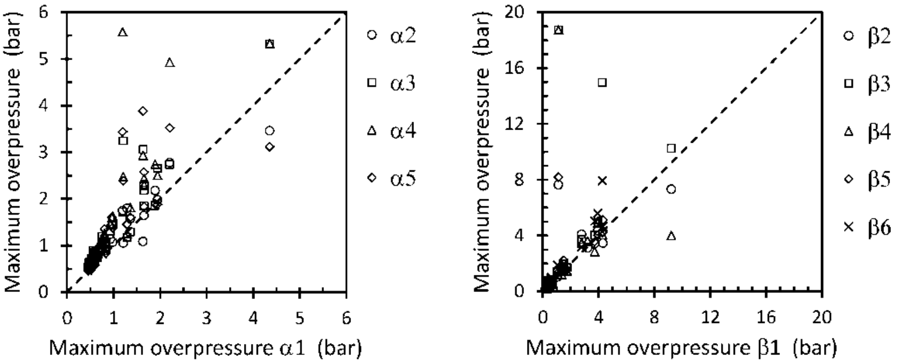

Figure 4: Spread in experimental results for repeated tests in the HSE rig; end ignition on the right.

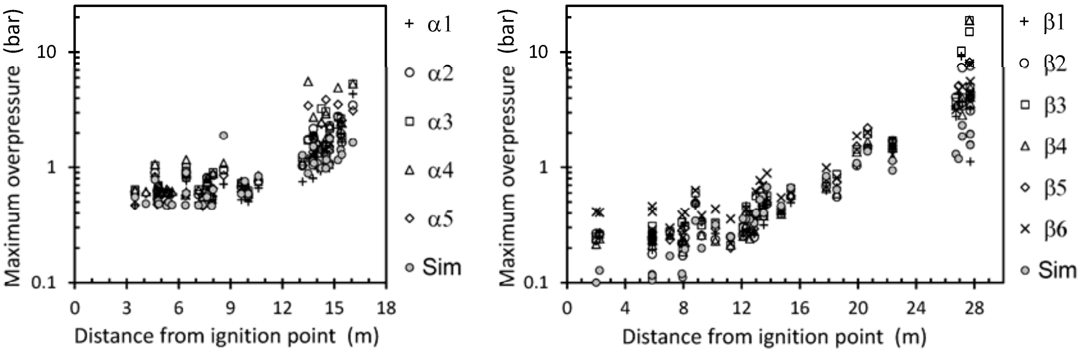

Figure 5: Maximum measured and simulated pressures in the HSE rig as a function of distance from the ignition point to the respective sensors; end ignition on the right. The experimental data were obtained after smoothing the pressure traces with a 1.5 ms moving average. The simulation results were obtained with FLACS v9.1 and cubical grid cells of size 0.8 m.

The validation cases that are registered in the database will be simulated according to their assigned priorities, with particular focus on sensitivity analysis for variables such as critical model constants, spatial and temporal resolution, initial and boundary conditions, etc. The model system includes tailor-made tools for setting up, documenting and running simulations, quality assurance (QA), and utility programs for data extraction and data reduction. Standard file formats for storing experimental data allows for visualization of experimental and simulated results directly in the post-processor for the CFD tool. The performance of the model system is determined based on criteria outlined in the model evaluation protocol (MEP), which for most practical purposes follows the recommendations from MEGGE (1996). Figure 6 summarizes simulation results for five grid resolutions: 0.4, 0.5, 0.8, 1.0 and 2.0 m cubical cells. The 2 m grid is clearly too coarse for this problem, with only four cells across the flammable cloud, and it is not surprising that these simulations severely under-predict the explosion pressures for both central and end ignition.

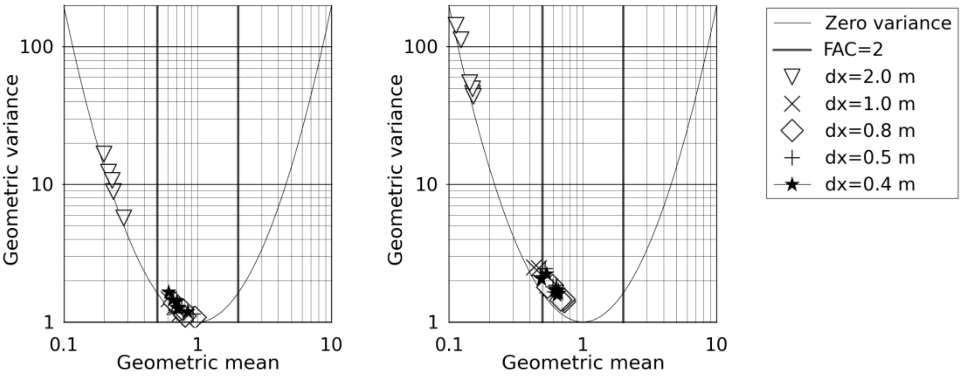

Figure 6: Geometric mean vs. geometric variance for the ratio of the predicted maximum overpressure to the observed maximum overpressure for five grid resolutions; end ignition on the right.

For the remaining grid resolutions, the results from the CFD simulations are in fairly good agreement with experimental values. The model under-predicts the mean explosion pressure, particularly for scenarios with end ignition. However, Figure 5 shows that the main reason for this deviation can be traced to a limited number of pressure sensors located in the far end of the module. The same measurements are the primary cause of the spread in experimental results shown in Figure 4. It should be noted that FLACS has been developed for simulating deflagrations, not detonations, and that the spatial and temporal resolution in the simulations probably would need to be increased significantly in order to capture the most extreme pressure peaks observed for scenarios with end ignition. The results highlight the need for developing reliable criteria for predicting deflagration-to-detonation transition (DDT) in complex geometries. Previous validation work has shown that FLACS performs significantly better for geometries with a higher degree of confinement (Foisselon et al., 1998). As indicated in Figure 2, the validation framework is designed to facilitate documentation of the software, including compilation of comprehensive validation reports. The content of the validation database can be made available to users of the software through an online web interface. Selected parts of the validation results should be included in user manuals and training material for the CFD tool. The instances in the validation database will also be used for automated testing of the software.

4. Parameter optimization

Once the system illustrated in Figure 2 is operational, it is straightforward to perform sensitivity studies and parameter optimization. CFD codes for engineering applications rely on empirical constants, such as the exponents in the S_T correlations in Eq. (1). Figure 7 illustrates the potential for parameter optimization: by increasing the value of the exponent A for u' in the Bray correlation by 30 %, the model predictions for both experimental series change from severe under-prediction to slight over-prediction. Table 1 shows that the modified value, $A = 0.536$, is still well within the range of values that have been reported for this exponent by other researchers. To modify the default values of model constants in a commercial CFD tool, such as FLACS, would obviously require a thorough analysis of numerous experimental results. However, once the validation database has been populated, the actual optimization process may proceed according to methods known from chemical kinetics (Davis et al., 2004).

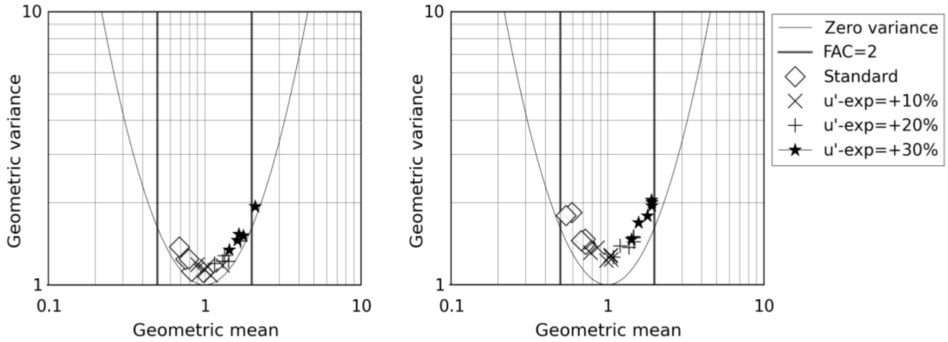

Figure 7: Geometric mean and geometric variance for the ratio of the maximum predicted overpressure (0.8 m grid cells) to the maximum observed overpressure for different values of the exponent A in Table 1.

5. Conclusions

Developers of complex model systems for industrial applications can benefit significantly from adopting an integrated approach to testing, validation, qualification and documentation. The proposed model evaluation process entails a continuous process towards an extensive database of prioritized validation cases. Standards for file formats, prioritization criteria, model evaluation, documentation, etc. facilitate efficient validation, test driven development, QA, and preservation of corporate knowledge. It is straightforward to extend the methodology to include sensitivity studies and optimization schemes for key model parameters. Major disasters continue to cause severe losses in the process industry and society, and better validated and more accurate models for consequence assessment may turn out to be a matter of life and death.

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