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Coherent Computational Analysis of Large-Scale Explosions and Fires in Complex Geometries – From Combustion Science to a Safer Oil and Gas Industry

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The present paper demonstrates and discusses the development of a coherent technology for both gas explosion and fire safety assessment in the oil and gas industry based on the Eddy Dissipation Concept (EDC). The physical basis of the concept is recapitulated and the implementation and application of the EDC model in the advanced KFX™ computational fluid dynamics (CFD) technology is presented. The KFX™ simulation technology includes the industrial fire simulation code KAMELEON FIREEX KFX® and the industrial gas explosion simulation code EXSIM™, both extensively validated.

1. Introduction

There is a risk of hazardous releases and uncontrolled ignition of hydrocarbons in the oil and gas industry. Accidents happen with serious, sometimes dramatic consequences where lives are lost, facilities are destroyed, environments are contaminated, economies are threatened and the credibility of the industry is at stake. Even ignition of small releases of flammable substances might develop into a disaster on an offshore platform. To prevent or mitigate explosion and fire related accidents, the industry needs technologies to pre-design the safety measures. This means reliable predictive computational methods that can simulate release and dispersion of hydrocarbons, explosions, fire evolution, dynamic loads from explosions and fires on safety critical structures, production and dispersion of smoke and effects of mitigation measures in realistic, complex geometries. Further, this means technology that can depict results in such a way that decisions can be made by people with different background or experience.
Traditionally, advanced computational fluid dynamics (CFD) based industrial analyses of consequences of gas explosions and fires in complex geometries have been performed using one software tool for prediction of consequences of gas explosions and another software tool for fires. Here a coherent technology for both gas explosion and fire safety assessment in the petroleum industry based on the Eddy Dissipation Concept (EDC) by Magnussen will be discussed and demonstrated. Coherent technology in this respect means similar operational platform built on the same physical basis and no adjustable constants in the physical submodels. This concept of thinking has been materialized in the advanced KFX™ fire and explosion simulation technology which is an integration of the dedicated industrial fire simulation code KAMELEON FIREEX KFX® (Magnussen et al., 2000, 2013) and the dedicated industrial explosion code EXSIM™ (Hjertager, 1991, 1993; Hjertager et al., 1994; Sæter, 1998). KAMELEON FIREEX KFX® is a result of more than 40 years of R&D activities on turbulent flow and combustion led by Professor Bjørn F. Magnussen at ComputIT, the Norwegian University of Science and Technology (NTNU) and SINTEF in Trondheim. The KFX™ software technology is developed in cooperation with some of the world's largest oil and gas companies and is extensively validated. As the fundament of KAMELEON FIREEX KFX® is a general-purpose CFD code for 3-D transient reacting and non-reacting flow, it has a wide operational domain, from gas dispersion and fire relevant problems to low NO_x problems in burners and furnaces. Today, KAMELEON FIREEX KFX® is applied on a daily basis worldwide for

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a large number of practical gas dispersion and fire analyses in the oil and gas industry, and it is recognized as the leading industrial simulation tool for advanced 3-D analyses of fires in realistic, complex geometries. Similarly, the internationally recognized explosion code EXSIM™ is a result of R&D activities on turbulent reacting compressible flows led by Professor Bjørn H. Hjertager since 1980 at Christian Michelsen Institute (CMI), Telemark University College, Tel-Tek and the University of Stavanger in Norway and at Aalborg University Esbjerg in Denmark. The CFD code EXSIM™ has been developed in close cooperation with the oil and gas company Shell and used for advanced industrial 3-D gas explosion analyses since 1989. EXSIM™ is extensively validated and has been SHELL's main gas explosion simulation tool for more than 20 years. At the end of 2014 rights to the EXSIM™ source code was transferred to ComputIT for further development and integration with the KFX™ simulation technology. EXSIM™ has recently been incorporated as the explosion simulation module KFX-EXSIM™ of the KFX™ simulation technology, utilizing powerful features of KFX™ for handling complex CAD geometry models, efficient pre- and postprocessing as well as an USFOS interface for non-linear dynamic structural response analysis.
In industry application the problem owners and decision makers, and the scientists often have very different background of practical and theoretical understanding. It is therefore important to create a common understanding of the problem and the consequences of the results. This is achieved in the KFX™ simulation technology through extensive use of graphics and video animations. Examples from validation studies and large-scale industry applications are given.

2. Modelling turbulent combustion in fires and explosions by the Eddy Dissipation Concept

Even though fires and explosions behave differently due to the degree of non-premixed/premixed combustion taking place, the underlying physics is similar to what we find in any turbulent combustion environment, even if the overall scales and boundary conditions also may be different. In order to have combustible gases reacting with each other, fuel and oxygen must be mixed at a molecular level, the reactants must be sufficiently heated and the reactants need some time to react. In a turbulent reacting flow, the chemical reactions take place in fine structures of the turbulent fluid, i.e. in sheets or vortices whose smallest linear dimension is substantially smaller than one millimetre and where the rate of combustion is largely dominated by the exchange rate of reactants between these structures and the surrounding fluid. These fine structure regions appear in the highly strained regions between the bigger eddies. The reacting structures may be significant hotter than the surrounding fluid. Furthermore, if the exchange rate between the reacting structures and the surroundings becomes so high that the thermal reactions are unable to keep up with the exchange rate, extinction will occur. This needs to be considered when modelling physical processes occurring in gas explosions and fires such as combustion evolution, flame propagation and acceleration, flame stability, ignition and extinction, soot formation, soot combustion, thermal radiation and effects of fire and explosion mitigating measures. In KFX™ the Eddy Dissipation Concept (EDC) forms the basis for the treatment of these processes, i.e. for the modelling of both fires and gas explosions. This concept builds on a turbulence energy cascade model for interstructural energy transfer first proposed by Magnussen in 1975 and reported in Magnussen (1981). An EDC model for turbulent combustion was first set forth by Magnussen and Hjertager (1976), modified by Hjertager (1982) and extended by Magnussen (1981, 1989, 2005). The newest, validated implementation of EDC exists in KFX™ for fire-related simulations (Magnussen et al., 2013), and an older, validated version is presently used in the KFX-EXSIM™ explosion simulation module (Sæter, 1998). However, both EDC versions are based on the same, fundamental reactor concept of thinking for modelling of turbulent reacting flows. A brief summary of the basis for the EDC model is given below.
In turbulent flow, energy is transferred from the mean flow through the largest eddies and further through smaller and smaller eddies and eventually to the fine structures where mechanical energy is dissipated into heat. In EDC, a turbulence energy cascade model connects the fine structure behaviour to the larger scale characteristics of turbulence like the turbulence kinetic energy, k, and its dissipation rate, ε. Characteristic scales from the fine structures can be derived as:

$$u^* = 1.75\left(\varepsilon \cdot \nu\right)^{1/4} \quad \text{and} \quad L^* = 1.43\nu^{3/4} / \varepsilon^{1/4} \tag{1}$$

where u^* is the mass average fine structure velocity, L^* is the characteristic length scale, and v is the kinematic velocity. These scales are closely related to the Kolmogorov scales.
An important assumption in the EDC is that most of the chemical reactions occur in the smallest scales of the turbulence, the fine structures. These fine structures are conceptually treated as well-stirred chemical reactors. The mass fraction occupied by the fine structures is stated as

$$\gamma^* = \left(\frac{u^*}{u'}\right)^2 \quad \text{or expressed by } k \text{ and } \varepsilon \text{ as} \quad \gamma^* = 4.6 \cdot \left(\frac{\nu \cdot \varepsilon}{k^2}\right)^{1/2} \tag{2}$$

The transfer of mass per unit of fluid and unit of time between the fine structures and the surrounding fluid can be expressed as:

$$\dot{m} = 2 \cdot \frac{u^*}{L^*} \cdot \gamma^* \ (1/s) \quad \text{or} \quad \dot{m} = 11.2 \cdot \frac{\varepsilon}{k} \ (1/s) \tag{3}$$

Further, the mass transfer rate between a certain fraction, χ, of the fine structures and the surrounding fluid can be expressed as

$$\overline{R}_i = \frac{\overline{\rho} \cdot \dot{m} \cdot \chi}{1 - \gamma^* \cdot \chi} \left(\frac{\overline{c}_i}{\overline{\rho}} - \frac{c_i^*}{\rho^*}\right) \quad \left(kg/m^3/s\right) \tag{4}$$

and consequently per unit volume of the fraction, χ, of the fine structure regions as

$$R_i^* = \frac{\rho^* \cdot \dot{m}^*}{1 - \gamma^* \cdot \chi} \left(\frac{\overline{c}_i}{\overline{\rho}} - \frac{c_i^*}{\rho^*}\right) \quad \left(kg/m^3/s\right) \tag{5}$$

where * denotes the fine structures, $\overline{\ }$ represents a mean value and i denotes the species.
Here, the reacting fraction, χ, of the fine structures (sufficiently heated to react) is expressed by:

$$\chi = \frac{\widetilde{c}_{pr} / \left(1 + r_{fu}\right)}{\widetilde{c}_{\min} + \widetilde{c}_{pr} / \left(1 + r_{fu}\right)} \tag{6}$$

where $\widetilde{c}_{pr}$ is the local mean concentration of reaction products, $\widetilde{c}_{\min}$ is the smallest of $\widetilde{c}_{fu}$ and $\widetilde{c}_{o2} / r_{fu}$, and r_{fu} is the stoichiometric oxygen requirement. χ, which is a progress variable for the thermal reactions, gives a probability of reaction that is symmetric around the stoichiometric value.

Although the EDC can be used with detailed chemical kinetics, the fast chemistry limit treatment of chemical reactions is sufficient in most fire and explosion simulations of practical interest. Typically, the burnt conditions of the involved major species are then prescribed and we look for the limiting major chemical component. One practical approach can be to assume that the fine structure reactor has reached a state of equilibrium and precalculate the concentrations of major species as a function of mixture fraction and temperature. If we assume that one of the major components, oxygen or fuel, will be completely consumed in the fine structure reactor, Eq. (4) and Eq. (5) can be expressed, respectively, as

$$\overline{R}_{fu} = \frac{\overline{\rho} \cdot \dot{m} \cdot \chi}{1 - \gamma^* \cdot \chi} \cdot \widetilde{c}_{\min} \quad \left(kg/m^3/s\right) \tag{7}$$

and

$$R_{fu}^* = \frac{\rho^* \cdot \dot{m}^*}{1 - \gamma^* \cdot \chi} \cdot \widetilde{c}_{\min} \quad \left(kg/m^3/s\right) \tag{8}$$

where $\widetilde{c}_{\min}$ is the smallest of $\widetilde{c}_{fu}$ and $\widetilde{c}_{o2} / r_{fu}$, and $\overline{R}_{fu}$ is the consumption rate of fuel.

Altogether, this gives the necessary quantitative format for treatment of reacting fine structures in turbulent premixed flames and diffusion flames according to the EDC. One distinctive feature of the EDC way of modelling the combustion physics is that turbulent flame propagation is automatically generated by the EDC and not given by an empirical expression for the turbulent burning velocity. Hence, we believe that the EDC establishes a solid fundamental physical basis for coherent treatment of the interaction between flow and combustion in general. Further details on the EDC and the theoretical reasoning behind the concept are given by Magnussen (2005).

3. Modelling and simulation of flow and combustion in KFX™

KFX™ is a finite-volume CFD code that solves the fundamental conservation equations for three-dimensional, time-dependent, turbulent reacting flow using a non-uniform Cartesian grid. Due to computational modelling and efficiency, KFX™ simulates fires using a CFD solver for incompressible flow, while the KFX-EXSIM™ explosion simulation module of KFX™ uses a compressible-flow solver. Turbulence is modelled with the standard k-ε model including buoyancy terms and standard constants. Combustion is handled according to the EDC, and extinction is modelled from time scales generated by detailed chemistry calculations. Soot formation and combustion is modelled according to modified versions of the models by Magnussen and Hjertager (1976) and Magnussen et al. (1978). The complex soot chemistry is handled by relating soot formation to the carbon content of the hydrocarbon compounds. Further, KFX™ includes a fully coupled pool model that accounts for the interaction of liquid pool spreading, heat transfer and multicomponent mass transfer between the liquid phase and the vapour phase. Moreover, KFX™ includes a fully coupled Lagrangian model for detailed simulation of water-based mitigation systems, such as water mist systems, water curtains, deluge, monitors and sprinklers, as well as simulation of spray fires. In the Lagrangian model, numerical parcels of droplets are followed, and droplet evaporation and break-up are included. Thermal radiation is modelled according to the discrete transport method of Lockwood and Shah (Shah, 1979), and absorption coefficients for water vapour, water droplets, carbon dioxide and soot are included. In the KFX-EXSIM™ explosion simulation module, a quasi-laminar combustion model is applied for the initial laminar flame propagation in a gas explosion.

In KFX™, complex geometries are modelled based on extensive CAD import capabilities. The technology includes a powerful and efficient native KFX™ CAD format that can be used to build complete geometries from scratch or to modify existing geometries imported and converted from another supported CAD format. CAD geometries, including electronic maps of terrain, buildings, modules, process plants, etc., are converted automatically into computational cells for solid constructions or surface/volume porosities used by the calculation model. A porosity/distributed resistance concept for complex geometries is applied to account for effects of subgrid geometry on the flow. A large number of special cells have been developed for boundary conditions of practical interest. There are special cells for high-pressure gas releases and other subgrid models. KFX-EXSIM™ for simulation of gas explosions features automatic optimization of the computational grid for congested areas.

KFX™ results can be presented in several ways, including visualizations in the CAD geometry. Video animations can be generated at observation points inside and outside the computational domain. Furthermore, KFX™ is interfaced with the finite element structure response code USFOS for non-linear dynamic structural response analysis, both for fire loads and explosion loads.

4. Examples from validation work and industry application

KFX™, including the KFX-EXSIM™ module, has been applied in a number of industry analyses ranging from gas dispersion to fire development, gas explosions, water-based fire mitigation, escape route analysis and structural collapse in complex geometries. Fuels may be gases, LNG or liquids for different release and wind conditions. Detailed calculations of temperatures, explosion pressures, thermal radiation, smoke generation and dispersion, fire and explosion loads on structures, visibility, concentrations of species, toxic gases, etc. are performed.

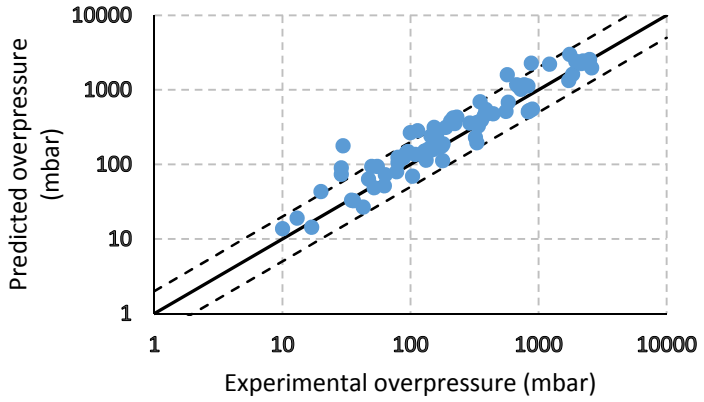

Figure 1: Comparison of maximum predicted and measured overpressures from gas explosion tests

Figure 1 shows examples of predicted and measured explosion pressures from validation of the KFX-EXSIM™ explosion model, including full-scale offshore module gas explosion tests (Selby and Burgan, 1998). Other KFX™ model validation tests are reported by, for example, Magnussen et al. (2013) and Rian et al. (2014).
Figure 2 presents the predicted pressure and drag load on a structure from a KFX-EXSIM™ simulation of a hydrocarbon gas explosion aboard a Floating Production, Storage and Offloading (FPSO) vessel.
Figure 3 shows a visualization of a KFX™ simulation of a catastrophic fire from a large accidental release of hydrocarbons on an offshore platform.

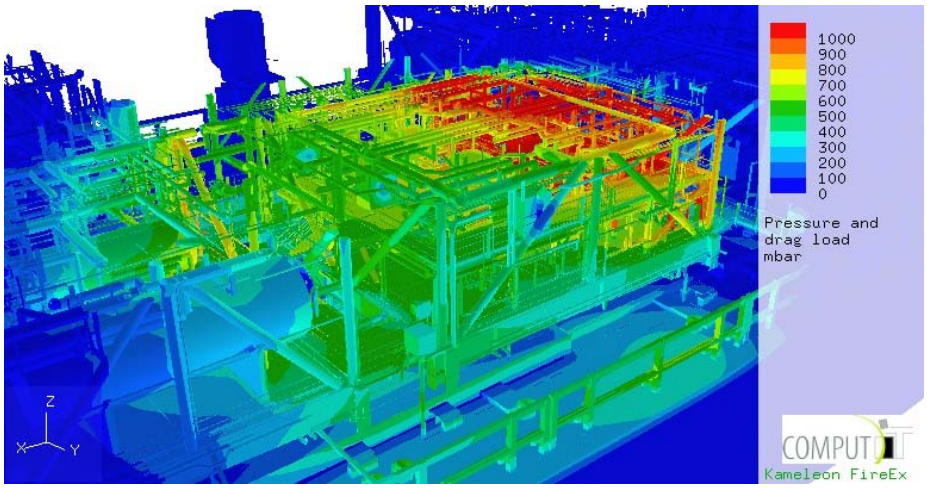

Figure 2: Predicted explosion pressure and drag load footprint on an FPSO structure

Figure 3: KFX™ simulation of a very large fire on an offshore platform

5. Conclusions

It is demonstrated how a general concept, the Eddy Dissipation Concept, for treating the interaction between the turbulence and the chemical reactions in flames can be successfully implemented for CFD-based assessment of safety related scenarios in the oil and gas industry. The KFX™ simulation technology featuring the KFX-EXSIM™ module is capable of simulating gas dispersion, gas explosion, fire and mitigation scenarios

in complex, realistic geometries with high confidence in the computational results. The present simulation technology is extensively used on industry problems.

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