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Computational Analysis of Large-Scale Fires in Complex Geometries – a Means to Safeguard People and Structural Integrity in the Oil and Gas Industry

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The present paper demonstrates and discusses the development of a coherent technology for fire safety assessment in the oil and gas industry based on the Eddy Dissipation Concept (EDC) by Magnussen. It includes a brief review of the concept and its physical basis which is implemented together with other models into a dedicated fire simulation tool, KAMELEON FIREEX KFX®.

1. Introduction

Fire safety is one of the most important issues in the oil and gas industry. Accidents happen with serious, sometimes dramatic consequences where lives are lost, facilities destroyed, environments contaminated, economics endangered and the credibility of the industry is at stake. A number of serious challenges have to be met by the industry to prevent or mitigate fire related accidents. Questions may be raised, like:

– What about the strategies for accident prevention and mitigation?
– Are the strategies understood and treated at right levels in the organizations?
– Are the companies willing to take lessons from recent accidents or do they feel that they have sufficient knowledge?
– Are the companies aware of and utilizing the best available technologies or willing to pay for necessary technology development?
– Is the intercommunication between different levels in the organization or between companies executed in such a way that the messages are understood and actions executed?

To meet these challenges, the industry needs technologies that can be utilized to pre-design the safety measures. This means predictive computational methods that can handle fire evolution and fire mitigation in complex geometrical environments, methods that can be trusted, and methods that can depict the results in such a way that decisions can be made by people with different knowledge or experience background.

Here, the development of a coherent technology for fire safety assessment in the oil and gas industry based on Magnussen's Eddy Dissipation Concept (EDC) will be demonstrated and discussed. Moreover, this concept of thinking has been materialized in a dedicated fire simulation code, KAMELEON FIREEX KFX® (Magnussen et al., 2010). KFX® is basically a general purpose computational fluid dynamics (CFD) code with a wide operational domain, from gas dispersion and fire relevant problems to low NO_x problems in burners and furnaces. Coherent technology in this respect means similar operational platforms and no adjustable constants in the physical submodels. In industry application the problem owners and decision makers, and the scientists often have very different background of practical and theoretical understanding. A major challenge is therefore to create common understanding of the problem and the consequence of the results. This is achieved in KFX® by extensive use of graphics and video animations. The KFX® software is developed in cooperation with some of the world's largest oil and gas companies and is extensively validated. Examples from large-scale industry applications are given.

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2. Physics of fires

The physics of fires is similar to what we find in any turbulent combustion environment, even though the overall timescale and boundary conditions may be very different. 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 millimeter and where the rate of combustion is largely dominated by the exchange rate of reactants between these structures and the surrounding fluids. The reacting structures may be significant hotter than the surrounding fluid, however under certain conditions the exchange rate between the reacting structures and the surroundings may be so high that the thermal reactions are unable to keep up with the exchange rate, with the consequence of extinction. When modelling fire evolution and fire mitigation, we have to take the preceding into consideration in physical processes occurring in a fire such as the combustion evolution, flame propagation, flame stability, ignition and extinction, soot formation, soot combustion and thermal radiation. In KFX® the Eddy Dissipation Concept (EDC) forms the basis for the treatment of these processes (Magnussen, 2005).

3. Features of EDC

3.1 Characteristics of turbulence

Turbulent behaviour of inertial systems at every level in the space-time continuum seems to display similar characteristics, like vortex structures and structural inhomogeneities. Consequently one may conceive that the interaction between turbulence in fluid flow at different scales can be modelled by the same concept at every structural level. This philosophy has formed the basis for the ensuing energy cascade model and the fine structure models in the Eddy Dissipation Concept.

3.2 Turbulence energy production and dissipation

In turbulent flow, energy from the mean flow is transferred through the bigger eddies to the fine structures where mechanical energy is dissipated into heat. In general, high Reynolds number turbulent flow will consist of a spectrum of eddies of different sizes. Mechanical energy is mainly transferred between neighbouring eddy structures. For the same reason the main production of turbulence kinetic energy will be created by the interaction between bigger eddies and the mean flow. The dissipation of kinetic energy into heat, which is due to work done by molecular forces on the turbulence eddies, on the other hand, mainly takes place in the smallest eddies. Important turbulent flow characteristics can for nearly isotropic turbulence be related to a turbulence velocity, u', and a turbulence length, L'. These quantities are linked to each other through the turbulent eddy viscosity:

$$\nu_t = u' \cdot L' \tag{1}$$

3.3 Modelling interstructural energy transfer

The connection between the fine structure behaviour and the larger scale characteristics of turbulence like the turbulence kinetic energy, k, and its dissipation rate, ε, is in the EDC concept based on a turbulence energy cascade model first proposed by Magnussen in 1975 and reported in Magnussen (1981) and several other publications, see Figure 1.

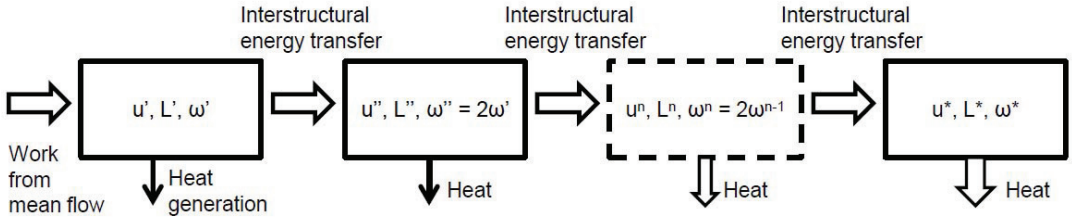

Figure 1: A modelling concept for transfer of energy from large to smaller turbulent structures

The first structure level represents the whole spectrum of turbulence which in an ordinary modelling way is characterized by a turbulence velocity, u', a length scale, L', and vorticity, or characteristic strain rate, $\omega' = u'/L'$. The rate of dissipation can for this level be expressed as

$$\varepsilon' = \zeta^2 \left(12 \frac{u'}{L'} \cdot u''^2 + 15 \cdot \nu \left(\frac{u'}{L'} \right)^2 \right) \tag{2}$$

where ζ is a numerical constant. By working through the energy spectrum and introducing ζ = 0.18 the following characteristic scales for the fine structures are obtained:

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

where u^* is the mass average fine structure velocity, L^* is the characteristic length scale, ε is the rate of dissipation, and v is the kinematic velocity. The scales are closely related to the Kolmogorov scales, and it can be shown that the present cascade model is in accordance with Kolmogorov's model for the energy spectrum of the inertial subrange, the 5/3 law, as well as in close resemblance with the existing, but relatively sparse, data for the viscous dissipation range.

3.4 Fine structures

The tendency towards strong dissipation intermittency in high Reynolds number turbulence was discovered by Batchelor and Townsend (1949), and then studied from two points of view: different statistical models for the cascade of energy starting from a hypothesis of local invariance, or selfsimilarities between motions of different scales, and then by consideration of hydrodynamic vorticity production due to the stretching of vortex lines. It can be concluded that the small scale structures that are responsible for the main part of the dissipation are generated in a much localized fashion. It is assumed that these structures typically consist of large thin vortex sheets, ribbons of vorticity or vortex tubes of random extension folded or tangled in the flow. These small structures are localized in certain fine structure regions whose linear dimensions are considerably larger than the fine structures therein (Kuo and Corrsin, 1972). These regions appear in the highly strained regions between the bigger eddies.

3.5 Reaction space

Chemical reactions take place when reactants are mixed at molecular scale at sufficiently high temperature. It is known that the microscale processes which are decisive for the molecular mixing as well as dissipation of turbulence energy into heat are severely intermittent i.e. concentrated in isolated regions whose entire volume is only a small fraction of the volume of the fluid. The fine structures are responsible for the dissipation of turbulence energy into heat as well as for the molecular mixing. The fine structure regions thus create the reaction space for non-uniformly distributed reactants, as well as for homogeneously mixed reactants in turbulent flow.

3.6 Modelling characteristics of the fine structures

An important assumption in the EDC is that most of the reactions occur in the smallest scales of the turbulence, the fine structures. When fast chemistry is assumed, the state in the fine structure regions is taken as equilibrium, or at a prescribed state. In the detailed chemistry calculations, the fine structure regions are treated as well-stirred reactors. In order to be able to treat the reactions within this space, it is necessary to know the reaction mass fraction and the mass transfer rate between the fine structure regions and the surrounding fluid. It is assumed that the mass fraction occupied by the fine structures can be expressed by

$$\gamma^* = \left(\frac{u^*}{u'} \right)^2 \quad \text{or expressed by } k \text{ and } \varepsilon \text{ as} \quad \gamma^* = 4.6 \cdot \left(\frac{\nu \cdot \varepsilon}{k^2} \right)^{1/2} \tag{4}$$

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

$$\dot{m} = 2 \cdot \frac{u^*}{L^*} \cdot \gamma^* \ (1/s) \quad \text{or} \quad \dot{m} = 11.2 \cdot \frac{\varepsilon}{k} \ (1/s) \tag{5}$$

3.7 Modelling the interstructural mixing processes

The rate of molecular mixing is determined by the rate of mass transfer between the fine structure regions and the surrounding fluid. The various species are assumed to be homogeneously mixed within the fine structures. One can express the mass transfer rate between a certain fraction, χ, of the fine structures and the surrounding fluid as

$$\overline{R}_i = \frac{\overline{\rho}\cdot\dot{m}\chi}{1-\gamma^*\cdot\chi}\left(\frac{\overline{c}_i}{\overline{\rho}} - \frac{c_i^*}{\rho^*}\right) \quad \left(kg/m^3/s\right) \tag{6}$$

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

$$R_i^* = \frac{\rho^*\cdot\dot{m}^*}{1-\gamma^*\cdot\chi}\left(\frac{\overline{c}_i}{\overline{\rho}} - \frac{c_i^*}{\rho^*}\right) \quad \left(kg/m^3/s\right) \tag{7}$$

where * denotes the fine structures, $\overline{\ }$ represents a mean value and *i* denotes the species.

3.8 The reacting structures

When treating combustion reactions, χ designates the reacting fraction of the fine structures. Only the fraction, χ, which is sufficiently heated will react. Several approaches may be applied to quantify the fraction, χ, which certainly is dependent on whether ignited or not. The following rather simple expression has been applied with considerable success:

$$\chi = \frac{\widetilde{c}_{pr}/\left(1+r_{fu}\right)}{\widetilde{c}_{\min} + \widetilde{c}_{pr}/\left(1+r_{fu}\right)} \tag{8}$$

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.

3.9 Detailed chemical kinetics

According to the EDC the preceding gives the necessary quantitative format for full chemical kinetic treatment of the reacting fine structures in turbulent premixed and diffusion flames. The method can readily be extended to treatment of reactions also in the surrounding fluid, which may be necessary for the treatment of for instance NO_x formation, especially in premixed flames.

The mean reaction rate can in this case be expressed as

$$\frac{\overline{R}_i}{\overline{\rho}} = \gamma^*\cdot\chi\frac{R_i^*}{\rho^*} + \left(1-\gamma^*\cdot\chi\right)\frac{R_i^o}{\rho^o} \tag{9}$$

where R_i^o is the reaction rate in the surrounding fluid.

One interesting approach to avoid detailed chemical kinetic treatment, is to precalculate equilibrium concentrations of major species as a function of mixture fraction and temperature, and assume that these values are reached in the fine structure reactor, or to apply simplified reaction mechanisms.

4. Modelling of some physical processes in KFX®

- Turbulence is modelled with the standard κ - ε model including buoyancy terms and standard constants.
- Gas dispersion and species transport are modelled by general transport equations and constants.
- Combustion is treated accordingly to the EDC. Chemistry is treated by algebraic equations based on detailed chemical kinetics.
- Flame propagation is automatic generated by EDC.
- Extinction is modelled from time scales generated by detailed chemistry.
- Soot formation and combustion is treated according to modified versions of the models of Magnussen and Hjertager (1976) and Magnussen et al. (1978). A key issue is to relate soot formation to the carbon content of the hydrocarbon compounds, thus making the computation independent of the complexity of chemistry treatment.
- Water droplets are transported in a Lagrangian way in terms of parcels. Droplet evaporation and break-up are included.
- Radiation is modelled according to the discrete transport method of Lockwood and Shah (Shah, 1979). Absorption coefficients for water vapour, water droplets, carbon dioxide and soot are included (Leckner, 1972).

5. Computational elements of KFX®

- KFX® is a three-dimensional, time-dependent finite-volume CFD code which solves the fundamental conservation equations for turbulent flow and combustion using a non-uniform Cartesian grid.
- The grid system can be generated automatic or manually.
- A large number of special cells have been developed for boundary conditions of practical interest.
- KFX® includes pool spreading models and special cells for high-pressure gas releases.
- KFX® includes powerful CAD import capabilities where 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 KFX® calculation model.
- Results can be presented in a number of different ways, including visualizations in the CAD geometry.
- Videos can be generated at observation points inside and outside the computational domain.
- KFX® is interfaced with structure response models.

6. Examples from industry application

KFX® has been used in a number of industry applications ranging from gas dispersion to fire evolution, fire mitigation by water droplets, escape route analysis and structural collapse in complex geometries.

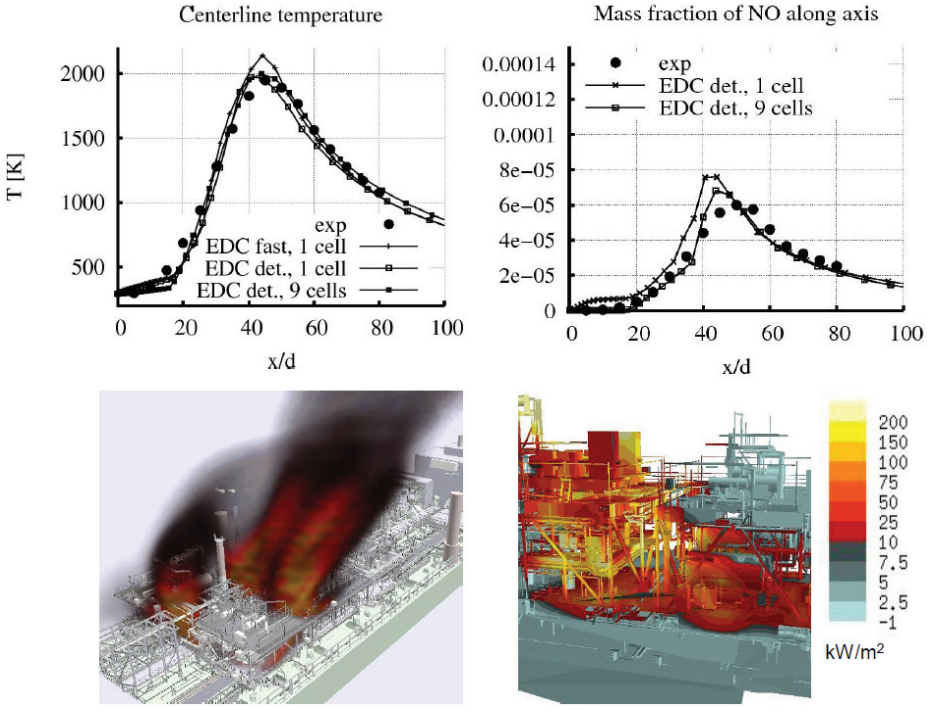

Figure 2: Examples of KFX® simulation results showing EDC with detailed chemistry, TNF D (top), and an FPSO vessel fire, including radiation footprints on structures (bottom)

Figure 3: A 56 m flame from a high-pressure gas release experiment (left) vs. flame predicted by KFX® (right)

Fuels may be gases, LNG or liquids for different release conditions, and external wind conditions are accounted for. The simulations include detailed calculation of temperatures, thermal radiation, smoke generation and dispersion, visibility, concentrations of species, toxic gases, etc. In Figure 2, examples from KFX® simulations are shown where EDC with detailed chemistry is applied for the Sandia TNF D flame (top) and an FPSO vessel fire is visualised (bottom), including a visualisation of the thermal radiation load from the fire on the structures. Figure 3 shows a photo of an industrial large-scale flame from a high-pressure gas release and a KFX® visualisation of the flame based on simulation results.

7. Conclusion

KFX® in its present version is capable of simulating complex fire and mitigation scenarios with high confidence in the computational results. It is extensively used on industry problems (Magnussen et al., 2000, 2004).

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