Fire Protection and Explosion Prevention for Hydrogen Safety Technology

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This paper describes main results obtained within the scope of joint project activities concerning the numerical simulation of reacting flow in complex geometries. The aim is the refinement of numerical methods for applied computational fluid dynamics (CFD) using high-performance computations (HPC) to study explosion processes in more detail, especially for hydrogen safety in technical systems. The R&D work is mainly focused on the modelling of the accident-related behaviour of hydrogen in safety enclosures ranging from slow to fast or even rapid flames. Therefore, we have established a modern field code cluster with supercomputing and special modules for specific studies. This new methodology allows the assessment of adequate safety measures to control deflagration-to-detonation transition (DDT) processes and to suppress fires or explosions for industrial safety.

1 Introduction and Objectives

The assessment of the integrity of safety enclosures under severe accident conditions is an important safety issue for industrial power plants. Such studies are under consideration to improve the safety behaviour of technical systems and to reduce the consequences of accidents for the environment as far as possible. To limit the increasing global climate problem and the greenhouse effect, hydrogen technology is a potential future energy option. However, increasing safety requirements have to be fulfilled to minimize industrial risks and to harmonize the safety culture. To control an accidental hydrogen combustion, different safety measures have been developed as part of the defence-in-depth concept with several accident management strategies. However, concerning flame acceleration or hot jet mechanisms, for example, a transition from deflagration to detonation (DDT) cannot be excluded a priori and may produce high explosion loads jeopardizing safety equipment and enclosure systems.

In general, fire and explosion protection is an important safety task in most areas of engineering. For instance, the prediction of hydrogen explosion

loads in safety enclosures under severe accident conditions is relevant for hydrogen demonstration plants with fuel cells or hydrogen-powered vehicles. In this context, Fig. 1 shows a typical flow scheme of a solar H2-plant.

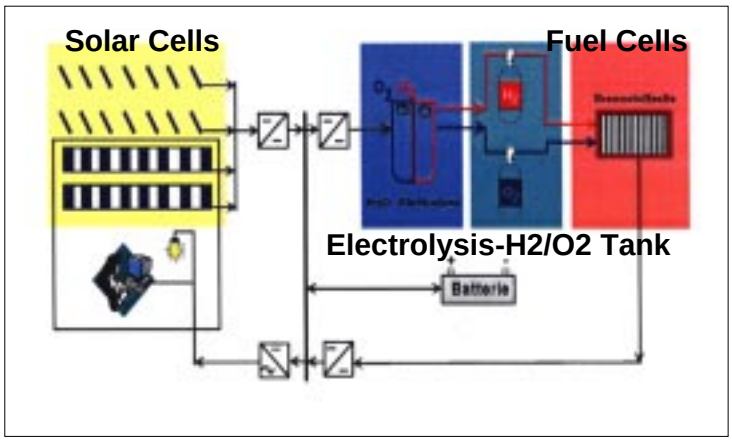

Fig. 1:
Flow scheme of the solar hydrogen demonstration plant operating at FZJ with fuel cells used for an electrical consumption.

Whether or not an accidental transition from deflagration to detonation (DDT) could occur in safety enclosures depends on the specific plant design and the anticipated accident scenario due to the high hazard potential. The DDT phenomena have been studied so far that most of them are qualitatively understood. However, quantitative methods have not yet been established for the objective assessment in large-scale enclosures. DDT is a very complex process associated with turbulent reacting flows and shock wave interactions, and rigorous closure solutions are still in the distant future so that practical approaches are needed. Therefore, it is reasonable to subdivide DDT processes into essential stages, i.e. slow, fast, and rapid flames in the sub/super-sonic regime and to develop suitable software tools capable of numerically defining DDT conditions (criteria) to control the resulting combustion mode and the load response.

For the prediction of hydrogen behaviour, we established special computational fluid dynamics (CFD) modules in a modern field code cluster (MFCC) with supercomputing capabilities, which are suitable for research work as well as for end-user practice. The MFCC represents the state of the art of non-reacting flow simulations (distribution) and reacting flow simulations (combustion) in complex geometries. The establishment of new academic and commercial codes was based on a comprehensive literature review and on our own experience already gained in the EC-H2DDT, the HGF-H2 and the EC-EXPRO project work on CFD/DDT processes, Ref. [1, 2].

2 Computational Physics and Field Codes

The fluid motion can be described by field codes solving the conservation equations for mass, momentum, and energy, which form together with the equation of state a closed mathematical system, i.e. the so-called Navier-Stokes (Na-St.) equations. These governing equations for rate of change + convection - diffusion = source term can be expressed for a general variable (Φ) in the generic form as $\partial (\rho \Phi) / \partial t + \nabla (\rho \Phi \mathbf{u} - \Gamma \nabla \Phi) = S_\Phi$ with the closure terms: (a) Standard turbulence- and combustion models are based on the eddy viscosity (μ) and a two-equation turbulence model (k-eps): $\mu_T = C_\mu \rho k^2 / \varepsilon$ with the eddy life time $\tau_e = k / \varepsilon$. (b) A turbulent combustion model (S_T): $S_T = - A_T \rho (\varepsilon/k) m_{lim}$ and the Damköhler number being larger than unity ($Da = \tau_e / \tau_{ch} > 1$). (c) A shock compression heating (S_C) with a reaction model: $S_C = A_c (\rho / \tau_{ch})$ for $T > T_{ig}$ using the chemical induction time (τ_{ch}) and the ignition temperature (T_{ig}.).

The basic partial differential equations (PDEs) are integrated in a computing domain, using the conservative form of finite volume methods (FVM) with various accurate differentiating schemes and robust solver techniques for the convection, diffusion and source terms for ambient initial and boundary conditions. The resulting set of algebraic equations is solved with direct or indirect algorithms (i.e. iterative or coupled solver), as to: a(p) Q(p) = a(w) Q(w) + a(e) Q(e) for the residual reduction to the defined values and aimed at grid-independent solutions. Here, we distinguish between verification (code-to-code) versus validation (code-to-experiment) from an independent end-user side. For the numerical simulation of transient, compressible, turbulent, chemically reacting flows, we have developed special field codes for specific studies based on reactive Navier-Stokes and on reactive Euler flow solver codes. The software and hardware infrastructure of the modern field code cluster is displayed in Fig. 2 for CFD predictions of engineering flows in complex geometries using high-performance supercomputing systems.

3 Computational Fluid Dynamics and Numerical Simulations

For hydrogen safety studies, we developed modern CFD methods for the analysis of hydrogen behaviour with supercomputing related to software optimization and special applications including improvement, validation, and performance tests. The modern field code cluster developed consists of new modules: **D3UNS, CFX, AIXCO, SHOCKIN, and IFSAS** with pre- and post-processing. Characteristics are hybrid grids, higher order turbulence and

combustion models with various solver techniques, including multi-processing in the PVP and MPP mode executed on **the CRAY supercomputer complex** (J90, T90, T3E) of the FZJ. The modern field code cluster is capable of numerically simulating non/reacting flows of slow, fast, and rapid hydrogen flames in complex geometries and consists of the following innovative CFD methodology, as outlined below, related to main accidental phenomena: (1) Hydrogen distribution in complex geometries, (2) Hydrogen combustion with DDT, (3) Hydrogen explosion loads and resulting loads, and (4) Fire prevention and explosion protection with suppression agents. Major features and main results are, as follows:

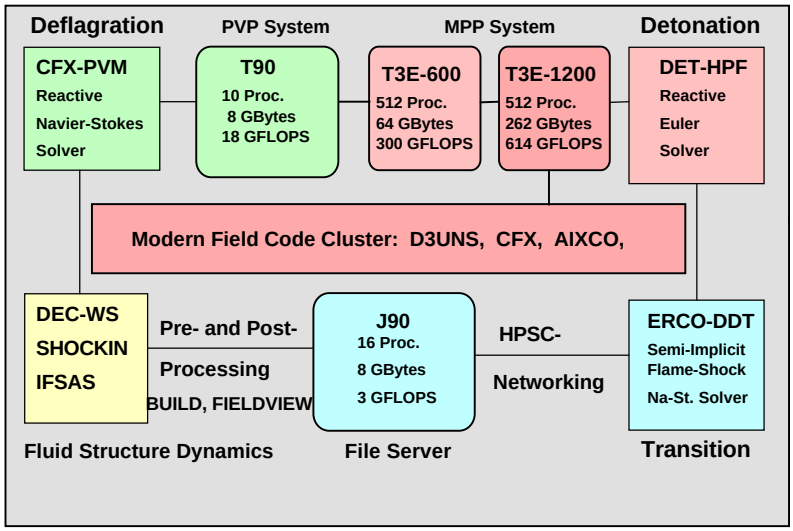

Fig.2: Modern field code cluster with high-performance supercomputing used for CFD flow simulations in complex geometries.

D3UNS code: We developed a new unstructured Navier-Stokes solver for non-reacting flow simulations (hydrogen distribution) consisting of classical turbulence modelling and large eddy simulations (LES) for in/compressible flows, including subgrid scale (SGS) modelling based on extended Smagorinsky models with wall damping and wall laws or dynamic modelling by Germano. The code works quite well on the T3E in the MPP mode and was successfully tested for benchmark cases reported in the literature (e.g. flow around obstacles). The D3UNS code is a sophisticated research tool for the large-scale simulation of engineering flows, especially for turbulent mixing with inertization, making full use of mesh refinement and adaptation using flow field parameters, Ref. [3].

CFX code: For the prediction of non- or reacting flows (hydrogen distribution and combustion) in complex geometries, we significantly improved the CFX software with physical-chemical models. This software consists of CFX-4 version (structured grids) on the T90 and CFX-5 version (unstructured grids) on the T3E with body-fitted coordinates. CFX-5 was

extended for eddy dissipation combustion models (EDM) with flame quenching. Besides classical turbulence models, we implemented a new LES model for in/compressible flows based on a standard Smagorinsky model with modified wall functions. The CFX versions were ported and optimized on the CRAY complex for parallel processing showing a good performance and scalability. The new versions were validated in experiments for hydrogen distribution and combustion (e.g. BMC, RUT, ENEL tests). Empirical parameters were fine tuned for the selected test cases indicating that the experimental results agreed quite well with the numerical simulations. The CFX code system is a comprehensive design and analysis tool for numerical simulations of turbulent reacting flows in complex geometries, Ref. [4].

AIXCO code: For the numerical simulation of hydrogen combustion (flame acceleration and DDT processes), we essentially improved the reactive Navier-Stokes code AIXCO. This code is based on the flamelet combustion model with flame front tracking and shock wave capturing. The flame front is described as a discontinuity between the burnt and unburnt gas, using a level set formulation with appropriate burning laws. The effects of turbulence can be taken into account through improved two-equation models. In addition, a two-step reaction model is implemented to study self-ignition characteristics of various hydrogen-air mixtures based on reduced chemical reaction schemes. We ported, parallized and optimized the AIXCO code on the CRAY-T3E, obtaining good performance tests and reasonable speedup factors. The code has been tested for large-scale RUT explosion tests performed at KI in Moscow with reviewing the DDT modelling. Finally, the code was extended for very large eddy simulation (VLES) using two-scales modelling with down-scaling and up-scaling between the integral and the subgrid scales (e.g. mixing layers). The AIXCO code is a modern research tool for the prediction of turbulent combustion, based on RANS and VLES flow solver options used for combustion engines and hydrogen safety, Ref. [5].

SHOCKIN code: For the numerical simulation of reacting flows related to hydrogen self-ignition (i.e. spontaneous thermal ignition), we developed a new adaptive reactive flow solver code with a two-step reaction model, including reduced or detailed chemistry. The code was validated in H2-DDT experiments performed at SWL of RWTH Aachen showing excellent agreement between experimental and numerical results with detailed insights into the shock wave behaviour. For the first time, H2-DDT test simulations were performed for self-ignition conditions in a large-scale containment model geometry. The code is an advanced research tool for analysing DDT conditions in complex geometries and for hydrogen-air mixtures with additives to prevent explosions, Ref. [6].

H2 safety: These modules of the modern field code cluster were used in hydrogen safety studies for technical systems. Hence, hydrogen control systems are based on mitigation, prevention, or protection measures. For fire protection and explosion prevention, effective suppression agents have been studied recently and already being used in industrial safety, public buildings, and high-tech equipment. The effectiveness depends on the special plant design and the specific requirements, which are still under investigation for process and industrial safety , Ref. [7], with different pros and cons for the safety concepts. Typical control systems studied for fire and explosion protection are, e.g.: (1) Auto-recombiner systems to avoid burnable mixtures, (2) Deliberate ignitor systems to control resulting explosion loads, (3) Dilution, inertization, micro-spray systems to suppress fires. In this context, Fig. 3 compares different fire suppression agents, such as Halon (rejected), FM-200 (modern), and CO2 or N2 (standard).

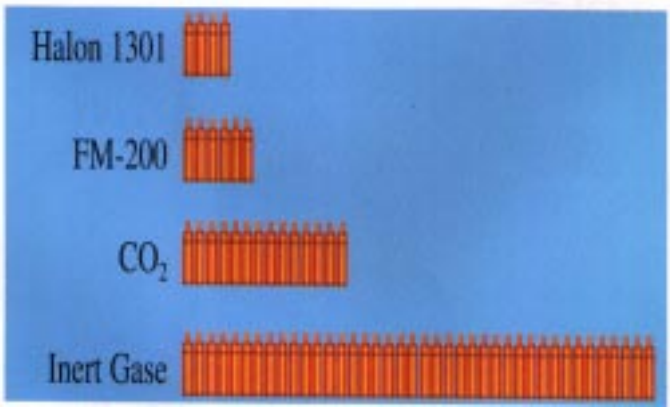

Fig. 3:
Comparison of different fire extinguishing media, e.g. Halon, FM-200, CO2, and inert gas, with regard to a comparable consumption by Kidde-Deugra.

4 Summary and Outlook

We have established a modern field code cluster (MFCC) with new versions of the reactive Navier-Stokes/Euler flow solver codes: D3UNS, CFX, AIXCO, SHOCKIN and IFSAS, to predict fast flames (deflagration), DDT (transition), and rapid flames (detonation) using vector or parallel processing. Characteristics are hybrid grids, higher order turbulence and combustion models with supercomputing and networking. These new field code modules have been optimized on the heterogeneous CRAY-J90/T90/T3E computer complex at FZJ, running in the sequential or massively parallel mode with reduced computing times. With the applied computational fluid dynamics (ACFD) and supercomputing, it is now possible to explore scientific-technical aspects of reacting flows in more detail for realistic safety enclosures, especially for hydrogen safety technology as a future energy option, to limit the global climate problem.

5 Acknowledgments

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6 References

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