Numerical simulation of large scale hydrogen explosions in complex geometries

Large hydrogen air clouds represent a serious hazard during severe accidents in nuclear power plants as well as in facilities of the developing hydrogen technology. The accident scenarios are dominated by large time and length scales with complicated boundary conditions. The combustion can proceed as an accelerating turbulent flame with possibly transition to detonation. Such problems require a careful selection of the physical and chemical models as a fully detailed calculation is not yet feasible. An extension of the well known eddy break-up model together with the $k$-$\varepsilon$-model was calibrated at a large set of experiments on different scales. It was demonstrated that this model gives good results for a large range of parameters.

1. Analysis procedure for safety applications

Today's computers do not allow to simulate a complete accident scenario in a nuclear power plant on a fine physical level. Therefore the whole process must be broken down into smaller problems which can be tackled by specialized methods. After the problem has been specified by selecting a plant design, a mitigation concept and an accident scenario, the first step is to calculate the hydrogen release and distribution in the containment. The creation of hydrogen inside the reactor vessel can be modeled by lumped parameter codes like MELCOR [1] which take into account the complex chemical reactions of the reactor materials but do not resolve the details of the flow. Once hydrogen has been created and is released into the containment the distribution of hydrogen and steam is simulated by the cfd code GASFLOW [2]. Depending on the type of accident this distribution phase can last for hours or even days. Therefore the heating of the structures and evaporation of water and condensation of steam must be considered also. During the distribution the hazard potential of the hydrogen-steam-air mixture must be assessed. This is done by applying three criteria. The first criterion are the ignition limits of the mixture. Only when the mixture is within the ignition limits combustion can be initiated. If the mixture can be ignited the next question is whether the flame can accelerate. From a large experimental database the $\sigma$-criterion has been derived [3]. Only if the expansion ratio of the burning mixture is higher than a certain threshold the flame can accelerate. If flame acceleration is possible the third criterion evaluates the possibility of a transition to a detonation (DDT). For DDT to occur the available space compared to the detonation cell size of the mixture must be large enough ($\lambda$-criterion). Depending on the results of the three criteria different combustion codes are used to calculate the further progress of the accident. If only the ignition criterion is fulfilled, the resulting slow flames are investigated with V3D. If flame acceleration is possible, COM3D [4] is used. And if DDT can not be excluded DET3D [5] can be used. The different combustion codes produce as result the loads on the containment structure. In case of a slow deflagration or a standing diffusion flame these are mainly thermal loads. For the faster combustion regimes mechanical loads are more important. The results of these calculations either verify that a given design is sufficient or give indications how the design must be modified, thus starting a new iteration through the whole sequence.

2. The computer code COM3D

For fast turbulent combustion processes the computer code COM3D is used. In this code the Favre-averaged Navier-Stokes equations are solved on a structured grid with constant cell size. Turbulence is modeled by either a standard $k$-$\varepsilon$-model or by the RNG $k$-$\varepsilon$-model. Combustion is described by the extended eddy-break-up model of Said and Borghi [6]. COM3D has been optimized to deal with complex three dimensional geometries with internal obstacles. A variety of explicit solvers including van Leer, Roe and various TVD schemes has been implemented. A more detailed description of the code can be found in [4].

3. Calibration and Validation of COM3D

The combustion model as well as the turbulence model in COM3D contain constants that must be specified. For the $k$-$\varepsilon$-model well known values for turbulent tube flow were used [7]. The single constant in the extended eddy-break-up model was calibrated against experiments performed in the FZK 12m tube. For this tube a large set of
experiments with different hydrogen-air mixtures and obstacle configurations is available. Experiments with different blockage ratios and different hydrogen concentrations were simulated with COM3D. For most of the experiments a value of $C_f = 6.0$ gave good agreement between calculation and measurement. For very lean mixtures the $C_f$ values for best agreement deviated somewhat from this value. An important influence parameter is the geometrical scale of the problem. For larger scales a more violent combustion process can be expected. To cover this effect simulations of combustion processes on a larger scale in the RUT facility (63 m length) of the Kurchatov Institute were performed and compared to experimental data. It was found that these large scale experiments could be simulated with the same model constants as in the small scale experiments. During the simulation the length and time scales of turbulence and combustion were evaluated. This allows to locate the combustion process in the so called Borghi diagram. Collecting this information for many calculations allowed to identify the region in the Borghi diagram for which the extended eddy-break-up model has been calibrated.

4. Application of COM3D to a nuclear power plant containment

The length scale of the RUT facility is of the same order of magnitude as a typical nuclear power plant containment. But of course the total volume of the containment is much larger than the RUT facility. Thus it was possible to perform fast turbulent combustion calculations of a full size reactor containment. The grid for this simulation consisted of approximately 2100000 cells with a cell size of 0.4 m. The accident scenario chosen for the simulation was a small break loss of cooling accident (SBLOCA). In this scenario the release of hydrogen and the subsequent pre-conditioning of the hydrogen-steam-air mixture proceeds for a very long time. The gas distribution at the time of the proposed ignition were calculated with GASFLOW and then imported into COM3D. For the chosen scenario the simulation predicts maximum pressures on the outer containment shell of less than 3 bar. This maximum pressure is well below the design pressure of the containment of 5 bar. Higher pressure values are observed on internal structures in the containment, especially in the steam generator tower near the proposed ignition location.

5. Summary and Outlook

It has been shown that the combustion code COM3D is capable of predicting turbulent combustion processes in large geometric scales. Its application is not limited to nuclear safety investigations. Another possible application is the investigation of accident scenarios in the use of hydrogen as a future source of energy in transportation. However, there are several points that need further attention. The spatial resolution of the code should be increased to cover smaller details of the problem geometry and smaller details of the turbulent flow field. An adaptive grid refinement procedure is presently under development to achieve these goals. Another point for future work is the modeling of turbulent combustion. The extended eddy-break-up model used so far does not cover the whole area of interest in industrial applications. Therefore work is under way to supplement this model with a presumed $\beta$-PDF model.

6. References


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