METHODOLOGY OF CFD SAFETY ANALYSIS FOR LARGE-SCALE INDUSTRIAL STRUCTURES

Kotchourko A.[1]
[1] **Forschungszentrum Karlsruhe, P.O. Box 3640, Karlsruhe, 76021, Germany**

ABSTRACT

The current work is devoted to problems connected with application of CFD tools for safety analysis of large-scale industrial structures. With the aim to preserve conservatism of overall process of multi-stage procedure of such analysis special efforts are required. A strategy which has to lead to obtaining of reliable results in CFD analysis is discussed. Different aspects of proposed strategy, including: adequate choice of physical and numerical models, procedure of validation simulations, and problem of 'under-resolved' simulations are considered. For physical phenomena which could cause significant uncertainties in the course of scenario simulation, an approach, which complements CFD simulations by application of auxiliary criteria, is presented. Physical basis and applicability of strong flame acceleration and detonation-to-deflagration transition criteria are discussed. In concluding part two examples of application of presented approach for nuclear power plant and workshop cell for hydrogen driven vehicles are presented.

INTRODUCTION

Development of the industry connected with burnable gases and especially with the involvement of hydrogen as energy carrier causes growing interest to safety aspects of design and operation condition of such industry. In case of accident involving considerable amounts of hydrogen, combustion and explosion processes can lead to considerable damages. Very high hazard potential brings to light a need in careful consideration of a methodology of safety analysis applicable for such industry.

Commonly accepted technique for evaluation damage potential used in industry is probabilistic risk analysis. Such analysis makes predictions on the basis of probability of certain event taking into account a severity of its consequences. Nowadays for the consideration of event evolution and evaluations of the consequences, CFD tools are widely used, since they can provide detailed information on process evolution and expected damages. However, it appears that way of CFD simulation utilization is often inadequate or even incorrect.

Which place CFD simulations have to take in safety analysis for industrial applications? What procedure has to be adopted to obtain adequate and reliable results? To obtain answers on these questions, the whole procedure of industrial accident analysis has to be considered. The path of speculations usually adopted in such procedure would include the following main steps:

- Scan for all possible or at least most important by expert assessment accident scenarios.
- Choice of significant scenarios. From significant scenarios large accidents with catastrophic consequences are usually excluded: the probability of such scenarios assumed to be reduced to minimum acceptable by licensing organizations. The rest includes the scenarios for which risk can not be reduced considerable and concentrates on medium and small scale accidents. These scenarios constitute a main body of tasks for CFD safety analysis.
- Scenarios proposed for simulations are numerically modeled. As a result of CFD simulations calculated distribution of gases and blast (pressure) and heat loads resulted from explosion processes in surrounding area of the analyzed constructions are obtained.
- The data on gas distributions and pressure and heat loads are used for evaluation of possible damages in the course of chosen scenario analysis. These evaluations are used in

argumentations submitted to licensing organizations with the aim to demonstrate safety of analyzed object.

Consider now possible sources of inadequacy or incorrectness in this procedure, which can lead to unreliable results:

- Choice of significant scenarios. Usual practice is to submit for numerical simulations only a few scenarios from all chosen. This practice can easily be explained by taking into account that simulations are expensive and time consuming. However, either a systematic study of all significant scenarios is required to obtain data for actually 'worst case' or a preservation of conservatism in scenario selection for simulations has to be demonstrated.

- Scenarios proposed for simulations are numerically modeled. The modeling is performed using the codes in hand and almost never includes a comparison of different codes' predictions. Choice of appropriate codes and models in the codes is completely responsibility of personal performing simulations and therefore a reliability of the results is also a responsibility of this personal. Since modern codes include achievements from many branches of science, such practice implicitly assumes that personal has high qualification in all relevant scientific topics, otherwise a reliability of CFD predictions can hardly be considered as high.

- Even the choice of scenario proposed for simulation can be considered as satisfactory, an influence of multiple factors, which can strongly affect the development of accident, is usually is not taken into account. Such factors, for example, for calculations of gas cloud formation due to pipe leak or rupture, could be: vector of injected gases, external flows (wind), multiple holes with different vectors of injection, etc; for calculations of gas cloud combustion: moment of ignition, place of ignition, external sources of turbulence, etc. To provide a solid basis for making decisions on object safety a systematic accounting of all influencing parameters is required.

- The next important source of inadequacy is CFD codes themselves. Three main such sources can be distinguished:

    - Inappropriate choice of physical and numerical models. In many codes for each individual phenomenon a set of models is frequently available. The choice of proper model is often non-trivial problem and can require very careful consideration.

    - Inadequacy of the code used for simulation or usage of the code beyond its validity domain. Validation procedure of the codes is regularly disordered and nonsystematic. Validity domain in such cases is not well defined what can lead to the utilization of a code beyond its validity limits.

    - Numerous errors connected with quality of calculations. Such errors were analyzed earlier and will not be considered here (see e.g., [1]).

Consideration of the inadequacies connected with scenarios choice is beyond the scope of this work and will not be considered here. The following sections address the problems, which are relevant to CFD tools only, namely appropriate choice of models and validation procedure.

CHOICE OF APPROPRIATE MODELS

To reproduce mechanistically the whole sequence of events in the course of scenario development it is necessary to perform numerical simulations for each event subsequently. Each step in such modeling has to be reliable and conservative.

Requirements to the choice of models

An event sequence of any accident scenario includes a number of individual phenomena. For example, a typical scenario of accident with flammable gases can include the following chain: formation of a source of flammable gas, mixing with air (oxidizer) and formation of flammable mixture (a cloud or a volume filled with mixture), ignition of such mixture, combustion, flame acceleration (FA), fast deflagration, deflagration-to-detonation transition (DDT), detonation. Some of them could be very well understood (and very well numerically modeled, e.g., shock wave propagation), some of them could be described numerically with acceptable accuracy and reliability (e.g., detonation propagation) and some are still far from clear understanding and therefore from accurate numerical description (e.g., DDT).

The first problem in modeling of complex scenario, which can include sequence all three types of individual phenomena, is a problem of appropriate choice of physical and numerical models describing each of events.

For the first and second type of phenomena a special attention has to be paid to a proof that exploiting models are able to produce reliable and conservative results. For the third type it was proposed to replace potentially unreliable calculations by usage of corresponding criteria, estimating possibility that the next event in the sequence occurs. Such criteria should have a character of conditions of necessity. I.e., if some condition is not satisfied, then the expected event will not occur, and if this condition is satisfied then the expected event can take place. In case when the expected phenomenon has higher damage potential, such formulation of criteria guarantees its conservatism. Expressing the same in terms of simulation procedure:

- if condition is satisfied then the simulation has to switch to the calculation of the tested event;
- if condition is not satisfied then the simulation has to remain unaltered.

The choice of models for first and second type of phenomena sometimes can appear to be very complicated. For many phenomena a number of numerical models are available (e.g., a set of models describing radiation has at least 6 different approaches). In case of commercial codes sometimes only obscured indications one can find in the manuals directing a user toward correct choice of model. In many codes only one or few models are included and their choice depends on author’s preferences.

To some extent scientific publications and communications can be considered as an indicator of the model quality. The approved by scientific community models has to be used preferable. However the scientific numerical modeling addresses the problems, which are far from typical industrial scales, and therefore it is not evident *a priori* how good could be the obtained results even in case of using the approved and most advanced models on industrial scales.

Another problem is connected with existing of concurrent approaches in numerical science. For example, in turbulence modeling RANS vs. LES: many articles can be found showing advantages and disadvantages of both methods. Which approach is preferable in every particular situation? Which approach has to be taken as more reliable? If such problem has to be solved by person who is not deeply involved in turbulence modeling, hardly one can expect to find clear and direct indications helping him.

Concluding this section, notice that by present time no systematic evaluation of models and their applicability depending on conditions of their utilization was made. It seems that a need in guideline or hand-book for safety CFD analysis came into sight.

For development of *guidelines* or formulation of a concept of CFD safety analysis a preliminary work for identifications the needs and gaps in existing knowledge has to be done. Preparatory work in this direction was carried out in the frames of EC project NoE ‘HySafe’ with the aim to systematize knowledge and provide starting point for the concept development. Many experts from different branches of modeling are involved. The approach of knowledge systematization adopted in 'HySafe' work targeted to formulation of guidelines is the following:

- Scan for scenarios of possible accidents which could happen in industry tied with hydrogen production, storage, transport, utilization, etc; analysis of the scenarios to determine most typical conditions and phenomena which could be met during scenario development.
- Ranking of the scenarios and identification of most typical and important phenomena; conservatism of scenario choice supposed to be considered here.
- Generalization of the phenomena; formulation of principal phenomena. Since many individual phenomena have strong mutual influence, introduction of intermediate step for phenomena generalization appears to be reasonable.
- Consideration of individual phenomena included in principal phenomena.
- Identification of gaps in physical model for corresponding individual phenomena.
- Identification of gaps in numerical models for corresponding individual phenomena.
- Analysis of the models currently used in CFD analysis, formulation of recommendations on their use and definition of regions of their applicability.
- Formulation of guidelines for CFD analysis of safety problems connected with H_2.

As it was mentioned at the beginning of this section, the development of theoretical backgrounds for some phenomena is still far from its completion and therefore modeling of such phenomena has serious problems. For such phenomena an auxiliary criteria are used.

Criteria for transient phenomena

At the stage of source formation and fuel-air mixing and burnable mixture formation, there are no phenomena, which are so weak understood that require utilization of auxiliary criteria for evaluation their potential to occur. However at the stage of the combustion modeling such lack of confidence or poor knowledge exists and has to be modeled using additional means.

The first such event is mixture ignition. For the sake of overall conservatism during simulations it should be accepted that as soon the mixture can be ignited (as soon it is inside the flammability limits approximately from 4% to 76% vol. H_2 in dry H_2-air mixture [2]), it will be ignited. Notice that the moment and location of ignition is important parameter and can have strong influence on possible damages.

FA criteria

The next phenomenon which strongly influences the route of combustion process is flame acceleration. As it was shown in [3], the possibility of flame acceleration is defined by mixture properties. The experimental data on the combustions in confined volumes from a wide variety of test facilities with the different characteristic lengths and the geometric configurations were analyzed. The analysis showed that strong flame acceleration was observed only for the sufficiently sensitive mixtures (Figure 1).

The parameter, which controls the possibility of flame acceleration, was identified as an expansion ratio σ (ratio between density of unburned and burned mixture at constant pressure). An expression of critical expansion ratio (below which the flame acceleration is not observed) reads as

$$\sigma^* = 0.9 \times 10^{-5} \cdot x^3 - 0.0019 \cdot x^2 + 0.1807 \cdot x + 0.2314, \quad (1)$$

where x is dimensionless activation energy $x = E_a/RT_u$. For hydrogen-air mixtures this parameter is approximately equal to 25 and, therefore, for critical value σ^* gives approximately value of 3.7.

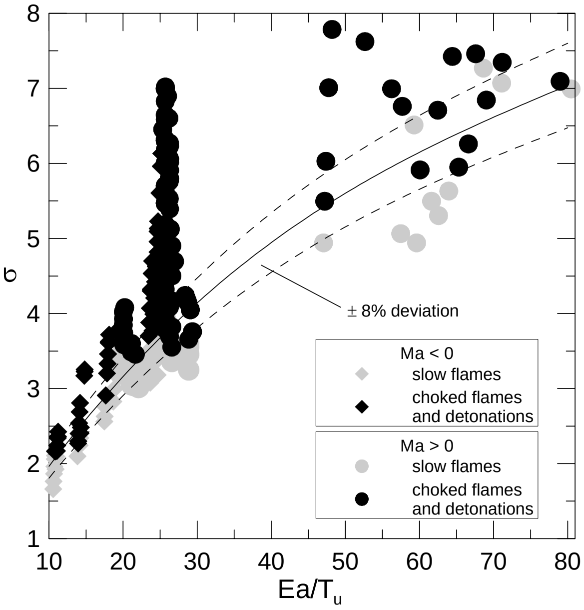

Figure 1. Observed combustion regime as a function of expansion ratio σ and dimensionless activation energy E_a/RT_u for hydrogen-air and hydrocarbon-air mixtures for closed systems. Picture courtesy of authors of [3].

In case of systems with partial transverse venting (as it was shown in [4], see Figure 2) the critical value σ^* is modified proportionally to vent ratio α (ratio between surface of vent and surface of enclosure). The larger is the vent area the more reactive mixtures is necessary for development of fast flames. The resulting expression for critical expansion ratio reads as

$$\sigma_{cr} = \sigma^* \cdot (1 + 2.24 \cdot \alpha),$$

where σ^* is critical expansion ratio for closed systems (Eq. (1)).

On the basis of findings of [3, 4], it is possible to formulate a criterion for strong FA: the mixture can exhibit strong flame acceleration only if its expansion ratio is larger than critical expansion ratio σ_{cr}. This statement has to be supplemented with the following: strong flame acceleration can take place only if there is enough room for actual development of supersonic flame. This geometric limitation is connected with necessity of run-up distance for FA process, which can be evaluated for tube-like configurations as having value of 20-40 diameters (see, e.g., [5]). Such formulated criterion has a character of necessary condition and thus can be directly used for evaluation of FA potential in CFD simulations.

Note, that the proposed criterion has, unfortunately, only limited range of applicability, since it was deduced on the basis of data obtained in confined and confined with partial venting systems. The generalization of this criterion to lower degrees of confinement and to open systems should provide extremely useful information for evaluation of FA potential in safety analysis.

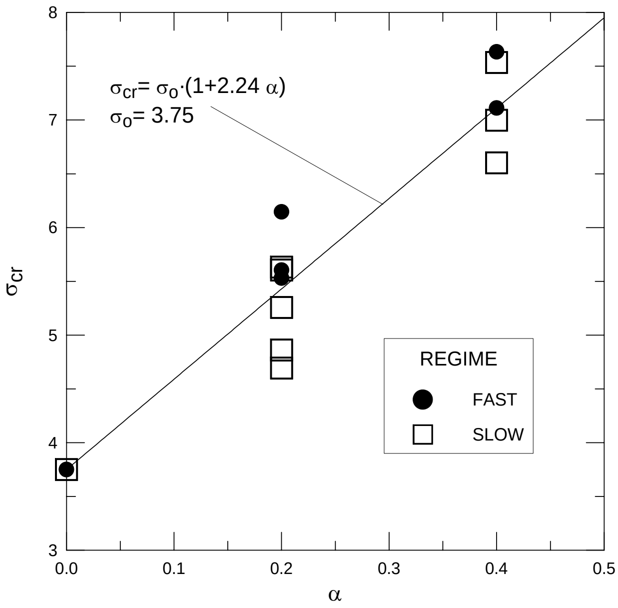

Figure 2. Observed combustion regime as a function of expansion ration σ and vent ratio α. Dependence of critical expansion ratio σ_{cr} on α. Picture courtesy of authors of [4].

DDT criteria

Another critical event, which can affect the regime of combustion, is deflagration-to-detonation transition. For many years many efforts was being made to develop a theory of this event, however it is still far from complete understanding. Due to this fact, the DDT predictions from CFD simulations hardly can have reliable character. To avoid uncertainty in forecast of DDT a criterion for detonation onset was proposed.

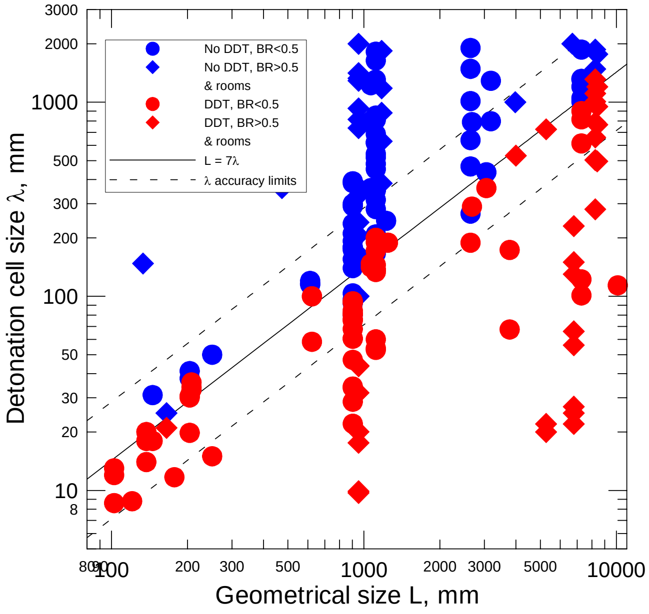

Figure 3. Critical conditions for onset of detonations in rooms and channels with obstacles. Deviations from line L = 7λ are within 30%. Picture courtesy of authors of [6].

For systematization of conditions in which DDT event can take place, numerous sources of data were analyzed in [6]. The literature data and the data from experiments carried out by authors were used. It was shown that depending on geometry of the facility, the mixture of the same composition can exhibit different behavior. In the facilities with characteristic length large than certain value (defined by mixture reactivity) the mixture does detonate, and in smaller facilities the detonation does not occur. The results of analysis are summarized in Figure 3. Solid line $L = 7\lambda$ separate analyzed cases with observed detonation from cases without detonation onset. As it was indicated by authors an accuracy of such separation is within 30% of λ value.

Parameter λ, which is used as characteristic length for characterization of mixture sensitivity, is detonation cell size. Detonation cells are imprint of complex three-dimensional structure of detonation wave and their size is determined by mixture properties only (e.g., H_2 concentration, initial temperature) and does not depend on geometric configuration of detonating mixture. The values of detonation cells are often known only with inaccuracy of 100%, therefore an application of 7λ correlation has to be made with understanding of accuracy of this correlation.

A criterion built on basis of 7λ correlation reads as: for detonation onset to be possible a characteristic size of combustible mixture (cloud or room size) must exceed 7λ (necessary condition). If detonation develops as a transition from fast deflagration, the corresponding criterion for FA has to be fulfilled as well.

Note that this criterion as well as criterion for flame acceleration has limited character of applicability since for non-uniform mixtures with spatially dependent properties (e.g., concentration) assessments of detonation cell size and expansion ratio can have considerable uncertainties in their values. However, by the moment these criteria provide the most reliable methodic on the potential of FA and DDT events.

It is worthwhile to mention here that the exact moment and location of initiation of the considered events have to be chosen maintaining the conservatism of the analysis. For instance, if a mixture at the moment of ignition has formed well premixed cloud with relatively high concentration, there is high probability for such mixture to detonate. On the other hand it could happen that the mixture triggered to high speed deflagration at later time can involve into combustion process much larger amount of hydrogen. To decide which case is more dangerous is not a trivial task. Unfortunately, a systematic study of such effect often is not performed, and as a best estimation an expert guess is taken.

VALIDATION OF THE CODES

Besides the problem of the choice of appropriate models, a problem of confirmation of simulation correctness is exceptionally important. This problem is closely connected with validation procedure. Usual practice of validations implies that codes are tested against available experimental data in conditions similar or equivalent to those which could be presented during safety analysis for real industrial applications. However, typical sizes of industrial applications are often (or almost always) much larger than typical dimensions of experimental facilities. This fact frequently leads to situations in which application simulations are performed with much coarse computational grids than corresponding validation calculations. Even if the validation experiments are carried out on the facilities with sizes close to real sizes, the capabilities of modern computers very rarely allow to perform simulations with grid resolutions dictated by theoretical background of physical models of the codes. For example, jet flows are almost never can be resolved in industrial simulations: in case of distribution calculation in volume of 10 m^3 with 10^6 computational cells with average cell size about 2 cm, a resolution of a jet with 1 cm diameter is evidently not possible. Local grid refinement does not improve situation considerable, since requires enormous computational resources (double refinement of 12.5% of computational volume doubles the total number of computational cells).

Two main issues can be distinguished in the matter of discussion:

- How to prove reliability and conservatism of simulations performed with resolution known to be too low (of so called ‘under-resolved’ simulations).

- How to prove equivalence of conditions of validation calculations and conditions of applications.

‘Under-resolved’ simulations

Let us consider conditions of CFD safety analysis for large-scale industrial applications with modern codes. If the typical size of calculation domain is 10 m × 10 m × 10 m and typical number of calculation cells is about 10^6, then an average computational cell size is about 10 cm (in reality cell size if often varied from 10 cm to 1 m). With such resolution almost all phenomena can be simulated only ‘under-resolved’.

As a good illustration a simulation of turbulent flows, which are quite important for both distribution and for combustion phases of accident analysis, can be considered. In turbulence models the values of the effective transport coefficients are defined by gradients of velocity and gradients of corresponding variables of the resolved part of the flow. It is obvious that with the varying of computational grid size (in case if the finest grid still does not allow to actually resolve gradients) the effective transport will depend on grid size influencing on the evolution of overall process.

Thus a question is raised whether it is possible to use under-resolved calculation to produce reasonable and reliable results. The answer depends on what kind of information should be obtained in the course of simulations. In case of safety simulations the required information has to include data on gas concentration distributions and on expected blast and heat loads as a result of combustion process. In many cases it appears that even the details of physical process are not fully resolved the computations are able to predict reasonable values. As illustration a computation of detonation can be taken. Simulation of detonation on coarse grid does not affect the predicted values of pick pressure P_{CJ} and detonation speed D_{CJ}, even if the chemical reaction completed in one computational cell. However, of course, this problem has to be analyzed carefully for each particular case.

Such analysis has to be included in the validation procedure and minimally should include the following steps:

- recognition of actually required resolution for the particular model;
- determination of the expected impact on model predictions due to the grid coarsening;
- proof of conservatism preservation of model predictions during the grid coarsening.

Quantitative validity domain

Determination of the validity domain of a code as a whole is exceptionally important for acceptability of simulation predictions. The validations are generally performed in conditions as much as possible close to those which are expected in productive calculations. However, an estimation of degree of similarity or equivalence between both of them is always subjective. In some cases only small changes in initial parameters can be followed by complete change of process characteristics or process regime, e.g., increase of hydrogen concentration in mixture from 3% to 4% makes it burnable. Therefore, a need in instruments, which can objectively characterize validity domain of a code, looks apparent.

As an illustration of our attempt for qualification of simple turbulence combustion model (extended Eddy-Break-Up [7]) model working together with 2-equation k-ε turbulence model will be presented. These models were chosen for testing since this combination is still mostly used in industrial simulations and therefore an objective sight on applicability of these models was highly desirable.

Consideration of conditions realized in different industrial applications leads to conclusion that the region of interest for fast turbulent flames can be limited by the turbulence Reynolds number between 10 and 10^6 and Damköhler number between 1 and 10^4.

In the calculations made for determination of COM3D code validity domain [8, 9] turbulence Reynolds number $Re_t = u'l_t/v$ was estimated as $\tau_t k/v$ (here τ_t is characteristic time of turbulent mixing, v is molecular viscosity and k is turbulence intensity), and Damköhler number Da as τ_c/τ_t, here τ_c is characteristic chemical time. Definition of τ_c implies the knowledge of the chemical properties of the mixture and therefore brings some uncertainties in its estimation. Assuming the following approximation of laminar flame velocity $U_L = (\sigma^2 v(T_{max})/\tau_c)^{1/2}$, where σ denotes expansion ratio and $v(T_{max})$ is molecular viscosity taken at maximal temperature, τ_c can be estimated if laminar flame velocities are known. Burning velocities of hydrogen-air mixtures were intensively studied (e.g., [10]) and different approximate formulas are available.

Estimation of the domain limits where extended EBU produces satisfactory results gives the following values: $10^2 < Re_t < 10^6$ and $12.5 < Da < 1250$. This domain covers almost a whole region of interest in industrial applications, excluding relatively narrow part of thickened flames where $1 < Da < 10$ (see Figure 4), and provide therefore a good basis for numerical simulations of the processes involving all types of wrinkled flames.

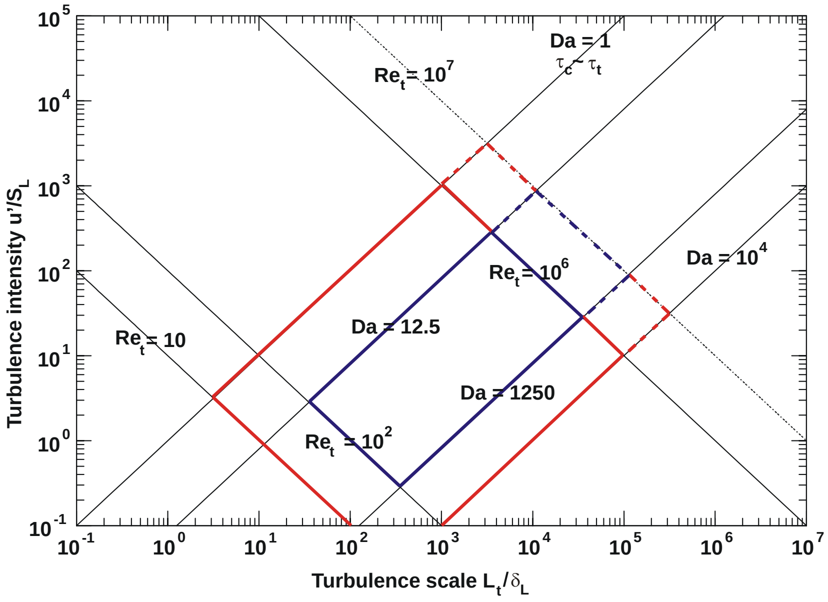

Figure 4. Validity domain of extended Eddy-Break-Up combustion model working with k-ε turbulence model. With red lines a domain of interest for industrial applications is shown. Blue lines shows validity domain for COM3D code. Dotted lines represent a credible extension towards high Reynolds number for large-scale cases.

This example illustrates one of the methods, which can be used for generating an objective determination of validity limits for a particular problem. Indeed, for each individual models' combination a specific study is required. Such work could require substantial efforts; however the implementation of similar methods in code validation procedure can definitely bring much more objectivity in the reliability evaluation of simulation results.

APPLICATION EXAMPLES

To make an example of consecutive application of principles described above, a sample of safety analysis for hydrogen behavior in severe accident scenario in nuclear power plant is presented. In the course of the analysis a special attention was paid on conservatism maintenance at all stages of the analysis.

The considered scenario is so-called ‘small break loss of coolant accident’. The scenario includes consideration of hydrogen release, distribution inside the containment and fast turbulent combustion. The appearance of burnable mixture was calculated first with MELCOR, which simulates sources of hydrogen and steam, and then with GASFLOW, which models distribution phase of accident. The hydrogen and steam concentrations predicted by GASFLOW were used as input to COM3D, which is dedicated for simulation of turbulent combustion.

The grid used in combustion simulation was more than $2 \cdot 10^6$ cells with the cell size of 40 cm × 40 cm × 40 cm. Figure 5 shows the iso-surface of hydrogen concentration of 5% at 0.5 s after ignition. A large portion of in the upper part of the containment has been already burned out.

Concentration distributions were analyzed with the help of FA and DDT criteria with the aim to determine limits of possible location and time of ignition. To provide data on worst case scenario development a systematic study on effect of ignition location, geometry, initial level of turbulence, time of ignition and degree of internal obstruction were made. The results of this set of simulations determined choice of scenario details. Calculated pressure loads on internal constructions and containment walls were delivered to design organization, what allowed them to improve building design for higher safety.

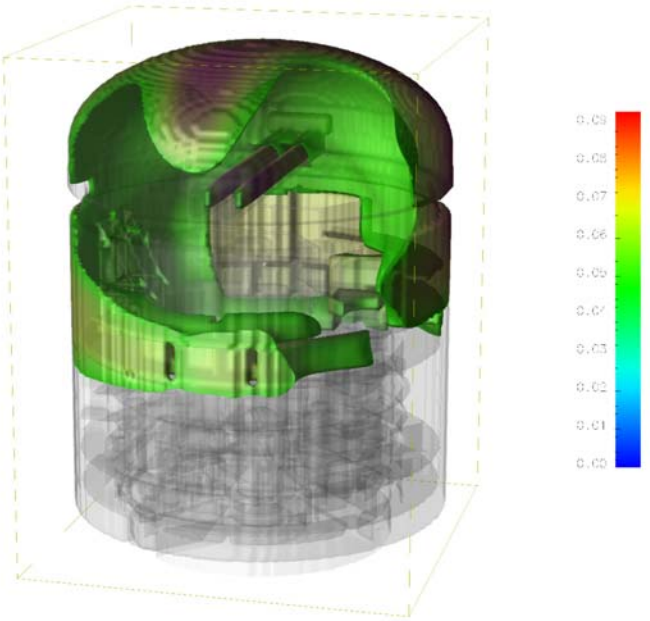

Figure 5. COM3D calculation of turbulent hydrogen-air-steam combustion in reactor containment. Distribution of the hydrogen concentration 0.5 s after ignition (iso-surface for 5% vol.).

Another example of industrial application is devoted to safety analysis of typical workshop cell for hydrogen driven cars. Scenario assumed leakage of stored hydrogen with mixture ignition after hydrogen release. Preliminary analysis showed that possibility of detonation can not be excluded and a worst case scenario with detonation of stoichiometric mixture of hydrogen in air was simulated. A set of computation with the aim to obtain highest acceptable leak was performed. This set of computations included variation of hydrogen mass resulted from the leak. Since conditions in hydrogen-air cloud were predefined (compact stoichiometric mixture), a release and distribution calculations were omitted.

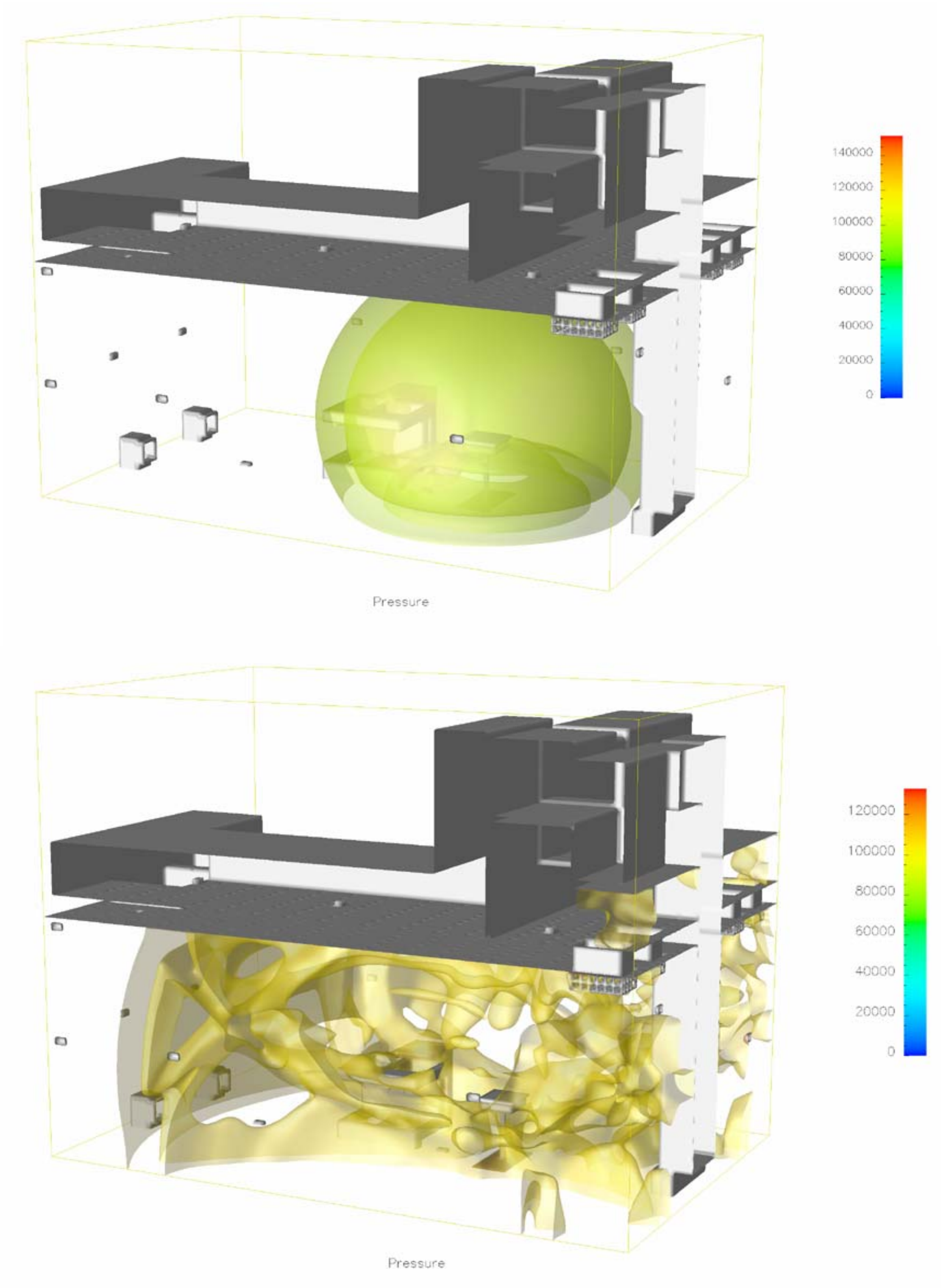

Figure 6. Evolution of pressure waves resulted from detonation of 8 g hydrogen in workshop cell. Iso-surfaces of 50 mbar overpressure at 5 ms after mixture ignition (upper picture) and at 13 ms (lower picture).

In Figure 6 two 3D snapshots of pressure distribution at two different times are shown. Obtained in simulations pressure histories for almost 2000 positions at walls and constructions inside the cell were used for structure analysis by ABAQUS. This analysis allowed to determine maximum permissible amounts of hydrogen inventory at accident conditions, what was necessary for car manufacturers to provide required level of safety during workshop operation.

CONCLUDING REMARKS

In the present work an attempt to systemize the experience gained in the course of multiple safety related projects is made. Many persons and organizations are working in the area of safety, however by the present time systematization and generalization of their experience was not made in full volume. Obviously a need in development of a systematic approach to the problems of safety examinations and in particular to the problems related to CFD simulations as part of safety analysis stands before community involved in this area.

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