TOOL CHAIN FOR SAFETY EVALUATION OF HYDROGEN APPLICATIONS

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Abstract:

This publication presents a methodological toolkit for the determination of direct and indirect hazard potentials in hydrogen applications. The focus is on the generation and propagation of explosive hydrogen mixtures and the propagation of blast waves. The practice- and implementation-oriented approach allows for accurate answers to safety-related questions. As application examples, the atmospheric release of H_2 into the environment through the vent pipe of an H_2 electrolysis container and the sudden release of H_2 in an electrolysis container after a pipe rupture are shown. A 1-D model for the calculation of pressure drop and mass flow as a function of piping and instrumentation diagram is also presented, which is used to calculate input parameters for the CFD simulation in order to reduce the complexity of the simulation model. This enables safe H_2 applications and accelerates approval processes and commissioning.

Keywords: Hydrogen Safety, Hazard Analysis, CFD-Simulation

1 Introduction

Hydrogen plays a crucial role in establishing a renewable and sustainable energy system, mobility and society. The basis for this is that absolute safety is guaranteed in the handling of hydrogen. Hydrogen has the property that it is highly flammable with an ignition energy of only 0.02 mJ, forms an explosive mixture in air over a wide range (4 – 75 %) and is stored in gaseous form at high pressures (> 300 bar) [1,2]. The identification of hazard potentials and its rapid and accurate validation is of crucial importance for safe hydrogen applications. To evaluate potential dangers arising from technical systems working with hydrogen, standards and regulations such as EN IEC 60079-10-1 or EN ISO 12100 are used [3,4].

Additionally, depending on the installation site and the application of a system, there are specific safety requirements for personnel, systems, and the environment, especially in contexts like refinery sites [5,6]. Consequently, a case-by-case assessment is often required to thoroughly evaluate the hazards associated with such systems.

To prevent incidences and derive sufficient and appropriate safety measures, targeting and fast evaluation is necessary during engineering phase and certification processes. Experience in recent years has also shown that the authorities or notified bodies are increasingly demanding an in-depth safety assessment. National standards must be taken into account as well as industry or company-specific requirements. Location-specific conditions have to be considered in order to develop a suitable safety concept.

The tool chain enables the determination of direct hazards such as explosion zones and blast waves as well as indirect hazards such as flying debris. As a direct result, the consequences of damage to people and systems are derived in order to develop suitable safety measures on this basis. Since mobile hydrogen applications are also being used more and more, H_2 propagation at the exhaust openings of venting lines and the spread of explosive atmospheres must also be accurately assessed. This allows safety distances to be defined as a function of the structural and meteorological boundaries.

2 Method

The methodological approach combines classic hazard and risk analyses with thermodynamic and CFD-supported simulation methods. The functional principles of hydrogen technologies as well as their operation modes are integrally considered. The toolchain provides the following individual steps (see Figure 1).

2.1 Structure Analysis and Scenario Definition

The aim of the first step is to develop a profound understanding of the overall system. This involves systematically considering the technology, its integration into the peripherals, the system environment and the legal framework. The technology analysis includes a structured analysis of the entire hydrogen pathway and all supply media, such as coolants, and an evaluation of the technical components. Simultaneously, the thermodynamical parameters pressure and as well as mass flow are assigned to each step of the process. A systematic approach is taken to analysing hazards and risks in accordance with EN ISO 12100 [4]. In addition, the explosion hazards according to ISO 60079 and ignition sources according to ISO 80079-36 are considered [3,7]. Based on this, worst-case scenarios are defined that summarise the impact of all possible cases of damage. The operating states of the system and the thermodynamic state and flow variables form the basis for modelling and simulation.

The general objective is to systematically assess the risks with regard to effects on human health and the environment. This must be carried out using systematic procedures and recognised methods, although there are no recommendations regarding specific methods. It is essential that considerations are documented in a comprehensible manner and that results are reproducible, see [8]

According to [8] existing established methods are

- Concept Safety Review
- Relative Risk Ranking
- Preliminary Hazard Analysis
- What-If-Method and structured What-If-Method (SWIFT)
- FMEA - Failure Mode and Effect Analysis
- HAZOP Analysis – Hazard and Operability Analysis
- Bow-Tie Analysis
- LOPA – Layer of Protection Analysis
- QRA – Quantitative Risk Assessment

Generally, the objective of the listed methods is to reduce the residual risk of complex systems especially with explosion hazard potentials to a level that is acceptable to everyone by taking appropriate measures. When defining appropriate measures, it helps to have precise knowledge of the identified hazards. The presented toolchain helps to develop a profound understanding of the identified hazards and to derive adequate measures.

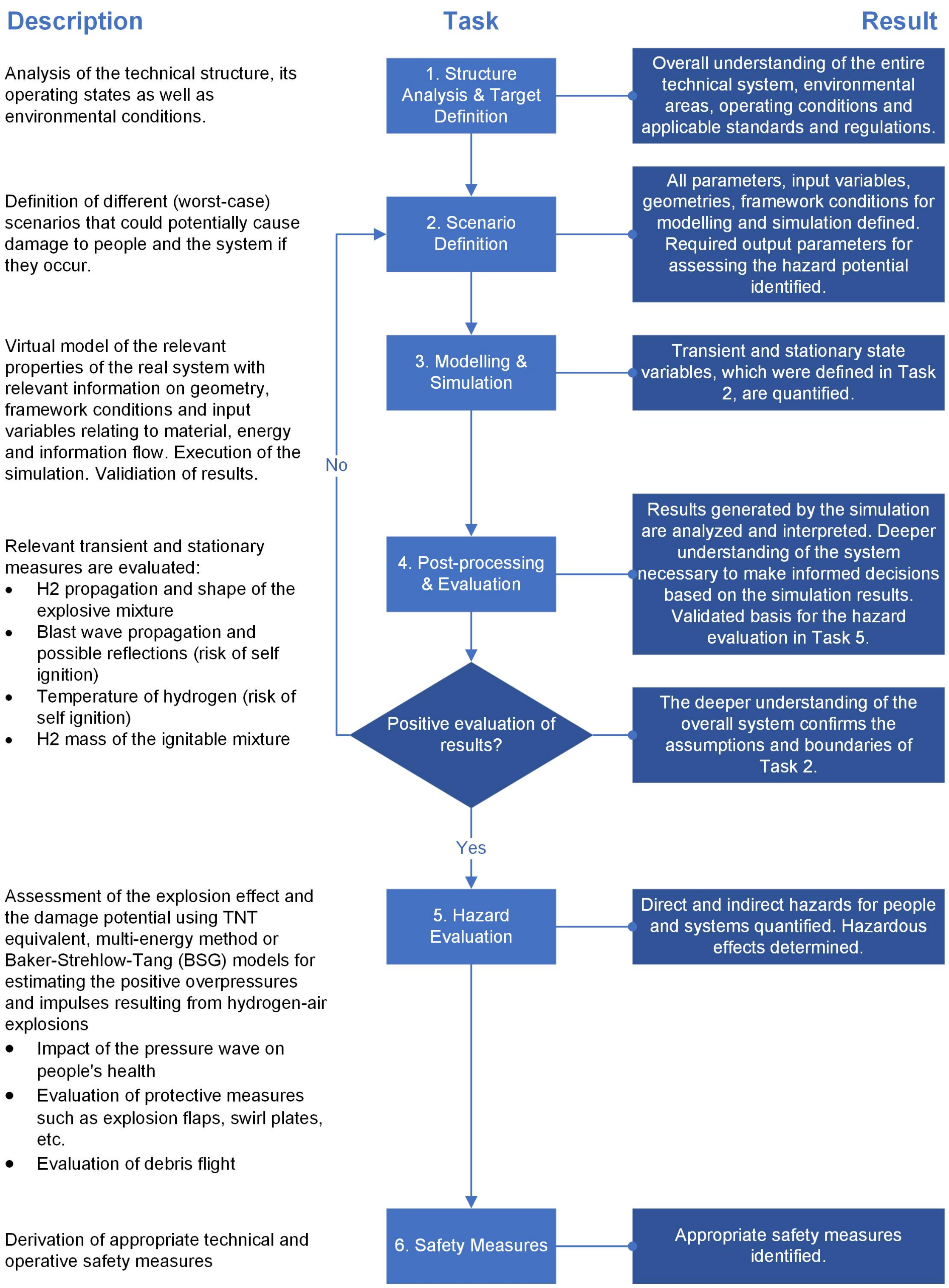

Figure 1: Tool chain for simulation-based hazard analysis

2.2 Submodeling in 1-D for Boundary definitions

Depending on the problem description the use of submodels is necessary to achieve desired results in an adequate timespan. In this subsection we present an example for how a 3-D CFD simulation can be reduced in complexity by using a 1-dimensional (1-D) submodel to calculate the boundary conditions.

In the case of blowing off hydrogen through vent lines of a hydrogen container, the interest lies in the simulation of hydrogen propagation outside the container. Ideally, the simulation would therefore set a boundary condition at the exhaust vessel of the vent line. To do this, however, the mass flow and the temperature of the escaping hydrogen must be known at this surface for every point in time. These properties depend on the nature of the vessel, the starting conditions and the dimensions of the piping up to the vent.

For the scenario described, a 1-D model was used, which consists of a non-adiabatic tank model combined with a model for pipe flows and pipe diameter changes. The non-adiabatic blowdown model of Dadashzadeh, Makarov and Molkov [9] used for the tank is actually only valid for outflows from hydrogen tanks without further piping. In order to take into account, the possibility of a mass flow limitation within the subsequent piping, the overall model is solved iteratively, whereby it is checked in each step whether the sonic velocity is reached first in the piping or the tank valve. It is crucial to consider the effects of real gas when dealing with high pressure hydrogen storage. Therefore the fluid properties were calculated with CoolProp [10].

More advanced geometries or combinations of multiple hydrogen vessels are more complex to solve but can still be simplified by using adequate models like the H2VPATT model from [11].

2.3 Use Case: Hydrogen Dispersion in Atmosphere

The release of hydrogen into the atmosphere is of safety-relevant importance in a large number of applications. Leaks on the one hand, but also process and safety-related blow-outs at the exhaust openings of vent lines, lead to the release of H_2 and the possibility of the formation of an explosive atmosphere with the atmospheric oxygen. At the same time, mobile storage, refuelling and utilization options are becoming increasingly popular [12–14].

The wide range of possible applications means that different exhaust geometries are used (see Figure 2) depending on the construction and there is a wide range of pressures and mass flows released. Current standards and guidelines for the calculation of the propagation such as DVGW G442 [15] or VDI 3783-Blatt1 [16] are only suitable for these calculations to a limited extent. On the one hand, they are not applicable to hydrogen or the exhaust geometries are not represented in them. At the same time the propagation of explosive zones must be precisely known to accurately define safety distances. Therefore, individual analyses based on numerical simulation of the hydrogen release and dispersion in the atmosphere are unavoidable.

The controlled venting of hydrogen via a special vent geometry was considered as a use case in this context. As described in section 2.2, the inlet boundary conditions for such a simulation can be pre-calculated using a 1-D model approach. In this case, the temporal progression of the mass flow and its temperature entering the exhaust was determined and set as an input boundary condition for the CFD simulation. To save complexity and thus computing time, an axisymmetric 2-D simulation was used instead of a 3-D model. The calculated atmosphere has the dimensions of 50 m height and a radius of 30 m and is chosen large enough to avoid any influences of the output boundary conditions on the results.

For the turbulence model the SST k-omega model was chosen as it is computationally efficient and it has been shown before to be effective in the prediction of free jet flow [17]. Before the start of a full simulation, a mesh-independence study and a time-step independence study is conducted to find a good compromise between computational effort and accuracy. To reduce the overall mesh size, it is recommended to use an initial coarse mesh with a refinement in areas that show high gradients in velocity, pressure and hydrogen concentration.

Exemplary results of the method are presented below. Figure 3 outlines the maximum propagation after 10 seconds of discharge of the lower explosion limit (blue) when release out of a special exhaust geometry (Figure 2). The worst-case scenario here was defined as an TPRD triggered safety release, whereby around 8 kg of H_2 is released from a mobile tank at a maximum initial pressure of 934 bar. It also shows the flow pattern of the H_2 propagation with velocity vectors. The results show that the exhaust geometry pushes the explosive mixture into the width, resulting in a high concentration of H_2 close to the ground during the release.

Figure 4 shows the H_2 dispersion at the established exhaust geometry type C according to DVGW G442 [15].

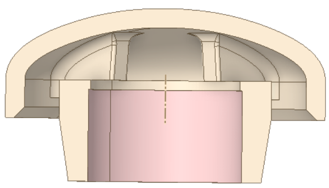

Figure 2: Exhaust vessel geometry

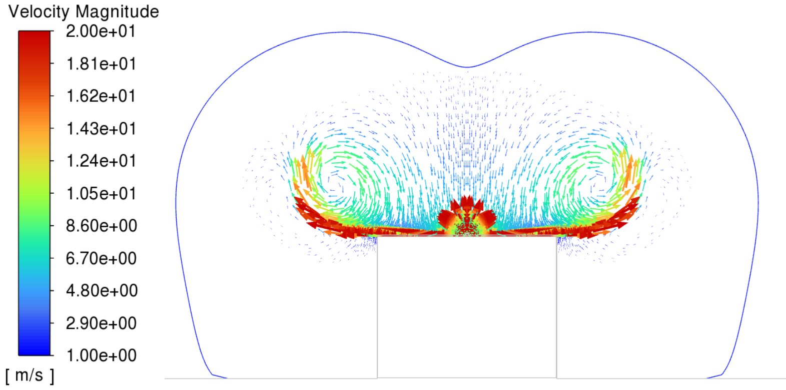

Figure 3: Lower explosion limit (blue) and hydrogen dispersion in atmosphere after TPRD release of H_2

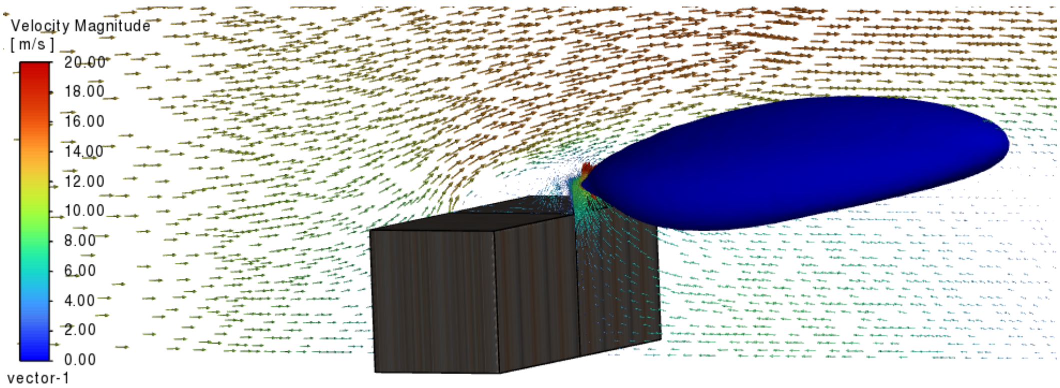

Figure 4: Hydrogen dispersion in atmosphere and flammable gas cloud propagation (lower explosion limit marked blue) at exhaust vessel geometry DVGW 442 – type C

2.4 Use Case: Hydrogen Dispersion in Electrolysers

Decentralized H_2 production means that electrolysers can be used in various industrial applications. The assessment of hazardous situations therefore varies from application and surrounding. In addition, depending on the installation site and application of a system, there are other standard regimes and, above all, specific requirements for the safety of personnel, system and environment, such as for production in a refinery site. Therefore, in the vast majority of cases, a case-by-case assessment is necessary in order to be able to seriously evaluate the hazards that can arise from such a system.

Within this use case the hazard potential of a sudden discharge of hydrogen in an electrolysis container as a result of a rupture in the wall of the dryer is examined.

The container has the dimensions 12.2 m x 2.4 m x 2.8 m. The gas generation system includes 2 PEM electrolysis stacks with a maximum total production capacity of 500 Nm³/h. No hydrogen is actually stored in the electrolysis container, but there is up to 3.8 kg of hydrogen in the lines, the electrolysis stacks, the dryers and other equipment inside the container during operation. The worst-case scenario considered here is that after a sudden rupture of a wall of one of the dryers 3.8 kg of hydrogen inside the container is discharged at the maximum pressure of 35 bar through a tear with a diameter of 80 mm.

Figure 5 illustrates the blast wave resulting from the sudden release of hydrogen at 35 bar. Figure 6 depicts the hydrogen dispersion after 0,1 seconds.

Figure 5: Blast wave propagation in electrolyser container

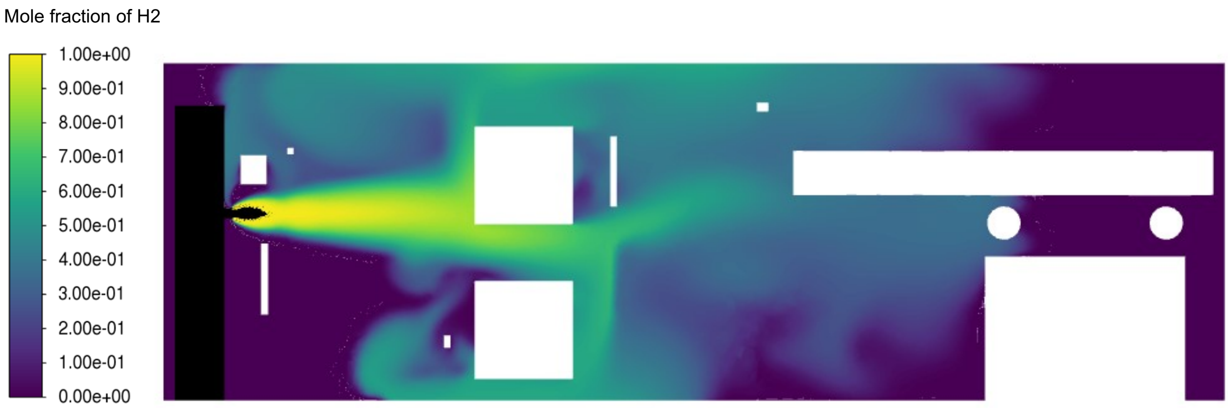

Figure 6: H_2-Dispersion within electrolyser after 0,1 seconds

Based on the simulation results, the following conclusions could be derived:

- Due to the rapid spread of H_2, stationary ventilation is ineffective and detection is too slow to prevent the generation of an explosive mixture.
- The pressure wave opens the electrolyser's double doors, which act as explosion flaps. This effectively transports an explosive mixture out of the container and reduces the likelihood of the container being blown apart in the case of an explosion.
- The escaped hydrogen that is still inside the container peaks at 65 % of the total H_2.
- The area around the electrolyser is fenced off in accordance with the safety distances during operation. However, even in the worst-case scenario, the explosion of the electrolyser will not have any damaging effect beyond the fenced off area.

2.5 Postprocessing and Hazard Evaluation

In the postprocessing of CFD simulations the main areas of interest are the propagation of any blast waves from sudden hydrogen releases and the size and shape of the resulting explosive gas mixture.

The hazards due to blast waves caused by the sudden release of hydrogen are far-reaching, both for people in the vicinity and for the facilities themselves. Depending on how high the overpressure within the blast waves is, the direct consequences for people who are hit by such a blast wave can range from ruptured eardrums to internal injuries and even death. Also, indirect risks due to blast waves can range from simply being knocked over to fatal injuries due to flying debris. Blast waves also have a high damage potential for facilities, as they can lead to the collapse of walls, steel frames or the rupture of pipelines [18]. For these reasons, it is of great importance to understand where blast waves occur, how severe they are and how they propagate so that appropriate measures can be taken to ensure the safety of people. The CFD simulations provide a very good indication of where blast waves are generated and how they propagate, as shown in Figure 5. The magnitude of the resulting overpressure can also be derived and thus the resulting hazards can be assessed according to the tables in [18].

The formation of explosive hydrogen-air mixtures is also of great importance with regard to the assessment of hazards that can emanate from hydrogen plants. With the help of CFD simulations, it is possible to determine both the composition of such explosive mixtures and the total mass of hydrogen within this cloud. A challenge, however, is to accurately assess a possible explosion of such a mixture and its effects, as there are several approaches described in literature, but most are unvalidated or not directly applicable to hydrogen. One of the most common ways is to derive a TNT equivalent for the hydrogen-air mixture to get an idea of how severe an explosion would be. As the name suggests, the TNT equivalent expresses the energy released in the explosion in kg TNT. According to [19] one kilogram of hydrogen has corresponds to the energy of 2.41 kg TNT. This means that only the mass of hydrogen within the explosive cloud needs to be determined. The TNO Multi-Energy Method or the Baker-Strehlow-Tang (BST) methods [20] provide further possibilities for drawing conclusions about the effects of explosions of hydrogen-air mixtures. These methods can be used to derive the overpressures and impulses generated by explosions and thus the consequences for human health can be derived in the same way as for blast waves.

In addition to blast waves and explosive mixtures, the spontaneous self-ignition of hydrogen is of particular interest in the case of sudden hydrogen releases. If the auto-ignition temperature of hydrogen of 585°C is reached during the release, combustion occurs in the form of a jet flame, which in turn means risks for people and facilities, particularly in terms of thermal exposure. The CFD simulation results can be used to determine whether and, if so, where the auto-ignition temperature is reached in the event of a hydrogen discharge.

2.6 Result: Derivation of adequate safety measures

After evaluating the direct and indirect hazards that arise, appropriate safety measures must be taken to minimize the risks to people inside and around the facilities.

Typical risk reduction measures can include:

- Installation of gas detectors in combination with emergency ventilation in confined areas. This ensures the prevention or reduction of explosive gas mixtures within the area. However, in the case of sudden hydrogen discharges as described in section 2.4, the start-up time of ventilation systems may be too long to effectively prevent explosive mixtures.
- Install explosion flaps or explosion protection doors in enclosed areas to reduce overpressure and allow explosive gas mixtures to vent outside.
- Define safety distances to zones that could pose a risk. For example, around vents, as explosion zones may be located there, in the area of doors that could burst open in the event of a sudden hydrogen leak or general safety distances to areas with increased risk in order to be out of reach of pressure waves or flying debris in the event of an incident.
- Entry prohibitions for facilities in which the presence of people is not necessary during normal operation. This significantly reduces the likelihood of people being affected in the event of a hazardous situation.
- Structural or technical measures such as changing the geometry of vents, reducing the flow in vent lines, installing baffles or constructing separating walls.

The results of the procedure allow well-founded statements to be made about:

- Assessment of standard safety measures such as stationary ventilation and dilution
- Effectiveness of activated safety measures such as explosion ventilation and explosion flaps
- Assessment of the explosion effect and damage caused by detonation and blast wave
- Derivation of structural, operational and procedural safety measures as well as limitation of safety distances

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