SUPPORT SUSANA

SUpport to SAfety ANalysis of Hydrogen and Fuel Cell Technologies

Critical Analysis and Requirements to Physical and Mathematical Models

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(randomly ordered by list of partner Institutions)

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1 Releases (Authors: NCSRD / UU, Reviewer: EE)

1.1 Models (NCSRD)

The models that have been developed and used in CFD simulations of hydrogen release and dispersion were presented in the document "State of the art review concerning FCH technologies". Here, turbulence models and release models that play a key role in hydrogen safety modeling are presented briefly. The comparison and the critical analysis of these models are presented in Section 1.2.

1.1.1 Turbulence models (NCSRD, UU)

Turbulent flow is the most often encountered flow type in everyday life. Most of hydrogen safety related phenomena are characterized by turbulent flows. Turbulent flows are highly three-dimensional and stochastic, and are characterised by high diffusivity and dissipation. The stochastic behaviour of fluid properties makes the analytic expression of a turbulent flow field (as a function of time and space) impossible. Furthermore, the numerical solution of the equations that describe the fluid motion demand an extremely large number of grid points and a very small time step in order to resolve the physics of turbulent flows. A number of different approaches are currently being used by numerical modellers in order to simulate turbulence flows. These approaches can be grouped in three broad categories:

- Reynolds-Averaged Navier-Stokes (RANS). In RANS (Reynolds, 1895) simulations the instantaneous quantities are decomposed into the time-averaged and fluctuating parts. Decomposition of Navier-Stokes equations results in introduction of a number of additional variables, which means that the solution of RANS equations requires additional equations, known as turbulence closure equations. A number of RANS models have been proposed, including k-ε (B. E. Launder and Spalding, 1974), $k-\omega$ (Wilcox, 2008), Shear Stress Transport (SST, (Menter, 1994), etc.

- Large Eddy Simulation (LES). In LES, originally proposed by (Smagorinsky, 1963), the turbulent motion is divided into large and small scales, the former of which are explicitly resolved, while the later are modelled. The separation of large and small scales is achieved by filtering the governing equations (Favre averaging being the most popular form of filtering used by Computational Fluid Dynamics (CFD) researchers). Scales smaller than the filter width, known as Sub Grid Scales (SGS), are not resolved and are modelled by separate SGS models. A number of different SGS models have been proposed over the years, including Smagorinsky (Smagorinsky, 1963), Smagorinsky-Lilly (Lilly, 1992), Monotone Integrated LES (MILES, (Boris, 1990), (Germano et al., 1991), etc.

- Direct Numerical Simulation (DNS). In DNS Navier-Stokes equations are explicitly resolved on all scales without application of any special turbulence model.

The mathematical formulation of the above models is described in detail in Paragraph 1.2.3 of the "State of the art review concerning FCH technologies". The comparison and the critical analysis of turbulence models are presented in the Paragraphs 1.2.1.1 and 1.2.2.1.

1.1.2 Source models (NCSRD)

Another critical issue of hydrogen release modelling is source modelling, especially in the cases of **under-expanded jets** and **liquid spills**.

- **Under-expanded jets** occur when the ratio of hydrogen storage pressure to atmospheric pressure is more than approximately 1.9. To model an under-expanded jet the user can either use the actual nozzle or apply notional nozzle approaches. Several notional nozzle approaches have been developed over the past years. Some information can be found in Paragraph 1.1.7 of the "State of the art review concerning FCH technologies". Presentation and comparison of the notional nozzle approaches are presented in Paragraph 1.2.1.2.

- L**iquid release** occurs when hydrogen is stored in the liquid phase at very low temperatures. In the case of liquid hydrogen (LH2) release, two source modelling approaches can be used: two phase jet and evaporating pool. The details can be found in Paragraph 1.2.6 of the "State of the art review concerning FCH technologies". Comparison of LH2 source modelling follows in Paragraph 1.2.1.2.

1.2 Comparison of models and requirements (NCSRD)

1.2.1 Comparison of models

1.2.1.1 Comparison of turbulence models (NCSRD, UU)

Turbulence models can be grouped in three approaches: Reynolds-Averaged Navier-Stokes (RANS), Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS). RANS simulations are the least computationally expensive and are frequently found in simulations of practical problems, but their capability to accurately predict turbulent flow behaviour is limited to well-characterised applications where the turbulence models have been well validated against experimental data. LES is somewhat of a compromise between good predictive capability and acceptable computational resource requirements – although run times are significantly greater than RANS. DNS provides the most accurate results at the expense of very high computational resources requirements driven by the necessity to resolve the flow field down to Kolmogorov scales. This requirement usually means DNS is unsuitable for the simulation of flows of practical interest involving complex geometries and/or large scale flows.

Several numerical inter-comparison exercises have been performed with the objective of comparing predictive capabilities of various numerical codes using different turbulence models. These studies provide a set of results by which users can make an informed selection of an appropriate numerical approach and turbulence model. In the next paragraphs, some examples from the literature concerning the comparison of turbulence models are presented.

An early inter-comparison exercise was carried out by (Gallego et al., 2007) within the European Network of Excellence HySafe. Twelve partners used 8 codes with different turbulence models in order to reproduce an experiment with hydrogen release, mixing and distribution inside a closed vessel of height of 5.5 m and diameter of 2.2 m (about 20 m^3 volume). In this experiment, hydrogen was released vertically upwards at a distance of 1.4 m from the top of the vessel filled in with air at atmospheric pressure. Release continued for 1 minute with a release rate of 4.5 litres per second

through a pipe of 10 mm diameter with velocity 57.3 m/s (Re=3000). After release, sensors measured hydrogen concentration transients at different heights for a further 250 min. Non-realistically high transport of hydrogen to the bottom of the vessel was observed with practically all of the RANS models applied. The LES model gave probably the best agreement with the experiment and reproduced more closely the hydrogen concentrations at the bottom of the enclosure due to restoring the laminar viscosity when the flow becomes laminar.

In 2009 an inter-comparison of CFD models was undertaken by (Venetsanos et al., 2009) to assess the predictive capability of various CFD models to reproduce hydrogen distribution in a mock-up garage of volume 78.38 m^3 (W x L x H = 3.78 x 7.2 x 2.88 m) with 1 g/s mass flow rate release from 20 mm diameter pipe and two small vents at the bottom of one wall of 5 cm diameter located close to each other. Release Reynolds number was approximately Re=4000. The duration of the release was 240 s. A diffusion phase was followed. Partners used 10 CFD codes with 8 different turbulence models. During the release phase, the k-ε models (standard, RNG and realizable k-ε) showed a tendency to overestimate the concentrations. The SST model was in better agreement with the experiment. The Smagorinski LES model was in good agreement with the experiment using Smagorinski constant equal to 0.12. The Smagorinski VLES model with Smagorinski constant equal to 0.1 gave overestimation of concentration close to the source, while the RNG VLES model showed underestimation. During the diffusion phase, the models generally tended to overestimate turbulent mixing.

In 2010 another numerical exercise was performed between four partners (Papanikolaou et al., 2010). That study investigated passive ventilation requirements for a residential garage with hydrogen-powered vehicle. In the experiment used for comparison with simulations the garage was ventilated by two vents (one upper and one lower). Helium release of 7200 l/h was simulated for two hours as in experiment. The leak location was at the bottom of the vehicle in the front part and centred at its width. Three participants used standard k-ε model and one partner used laminar and SST models. It was concluded that the distance to the boundary of the calculation domain beyond the garage and the vent resolution affected flow behaviour in the vent, while the turbulence model selection did not drastically influenced the results.

Choice of a proper turbulence model may be not straightforward for transitional laminar-turbulent flows. Recent work by (Bernard-Michel et al., 2013) describes an inter-comparison of CFD models performance for a small helium release of 4 Nl/min in a 1 m^3 volume box (H×W×L = 1.26×0.93×0.93 m) with a 1 cm round opening (vent) at the bottom of one wall (GAMELAN experiment). It is believed that the fluid flow demonstrated partially turbulent and partially laminar character. Five partners employed four different CFD codes using both laminar and turbulent models. The maximum deviation of simulation results from experimentally measured concentrations at different times after the release start was up to 80%. Similar to previous findings it was observed that in the cases of transitional flow the RANS turbulent models gave too-diffusive results with certain under-prediction of helium concentration at the top of the enclosure and over-prediction at the bottom. It should be pointed out that the Reynolds number in the release pipe was equal Re = 41, indicating that, at least at the release point, the flow was laminar. Laminar and LES models, on the other hand, underestimated mixing and diffusion in a part of flow and provided the opposite distribution of concentrations, i.e. an over-prediction at the top and an under-prediction at the bottom. It was suggested that this result for the laminar and the LES models is probably due to geometrical

simplifications applied by one of the partners when the parallelepiped shape of the enclosure was substituted by a cylindrical shape of the same height and the base area in the simulations. Another contributing factor could be the use of 2D axisymmetric mesh for LES simulations.

In 2014 a CFD benchmark was performed (S. G. Giannissi et al., 2015b) comparing three different turbulence models (SST, k-ε and LES model) in experiment related to 60NL/min helium release (as a surrogate for hydrogen) from 20 mm diameter nozzle (Reynolds number equal to 577) in a partially closed box (Cariteau and Tkatschenko, 2013). Three different cases were tested with different vent sizes. Figure 1-1 is a comparison of the He concentrations from various turbulence models, at a time when steady state is reached. It is observed that all models perform well except for the case with vent c which has the smallest vertical extension. In this case the concentration in the lower part of the enclosure is overestimated. Possible reason for the under-prediction could be the overestimated turbulent diffusivity.

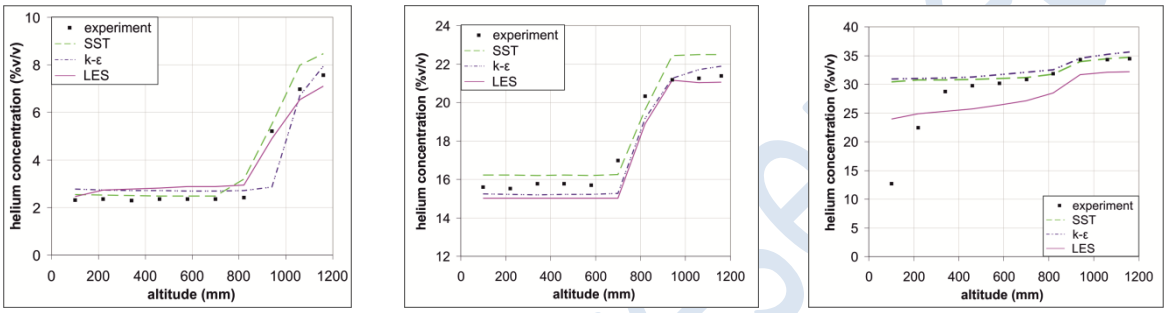

Figure 1-1 Comparison of the SST, k-ε and LES predictions with the experiment at steady state for the three different vent sizes (vent a, vent b, vent c).

A comparison of k-ε and LES models using different CFD codes was performed by (S. G. Giannissi et al., 2015a). The comparison was performed based on an experiment (test 25) carried out by HSL (Hooker et al., 2014) related to upwards hydrogen sonic release in a partially enclosed box (W x L x H = 2.5 x 5.0 x 2.5 m) with one opening and subjected to external wind. Figure 1-2 shows the predicted concentration and the experimental one. HSL used the ANSYS CFX 14.5 code and k-ε model, NCSRD used the ADREA-HF code and k-ε model and UU used the ANSYS FLUENT 14.5 and the LES model. It was concluded that both turbulence models are consistent with the experiment. However, the k- ε model predicts higher concentrations in the early build-up stage of the release, while LES tends to underestimate the concentration at latter times during the release, especially near the bottom of the enclosure. After the end of the release the LES predictions are in better agreement with the measurements. According to the average concentration time histories at three different heights during the release, the LES model predicts some stratification inside the enclosure, while both experiment and k-ε model show a homogenous mixture.

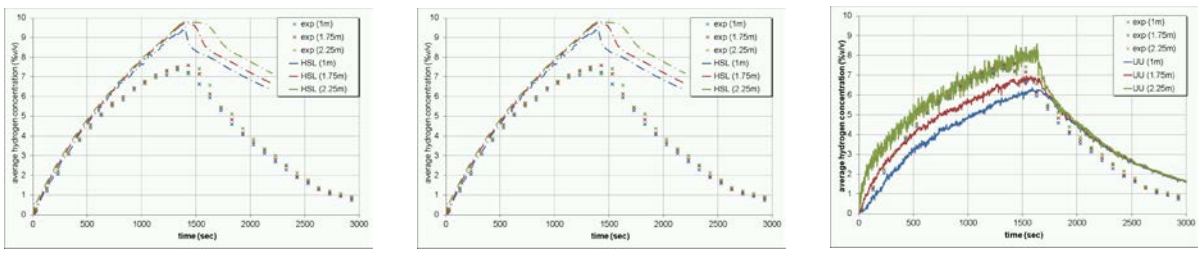

Figure 1-2 Average hydrogen concentration (% v/v) versus time at three different heights from the HSL (left), NCSRD (middle) and UU (bottom) partner

More recently, a comparative study of several models performed at University of Ulster (Molkov and Shentsov, 2014a). The aim of the study was to formulate requirements to numerical simulations of light gas release and dispersion in a vented enclosure that would provide an acceptable predictability of CFD models to be used for hydrogen safety engineering, including recommendation on selection of turbulence model. Simulation results were compared against experimental data reported by (Cariteau and Tkatschenko, 2011) covering laminar, transitional and turbulent releases with the release Reynolds number in a range from 39 to 6968 in the enclosure (W x L x H = 0.93 x 0.93 x 1.26 m) with one vent (three different vents were used, rectangular vent of sizes W x H = 90 x 18 cm, square vent of 18 x 18 cm and round vent of 1 cm diameter located 1 cm above the floor at the centre of the wall). Three physical models are applied, including laminar, standard k-ε and LES Smagorinsky-Lilly (Lilly, 1992), to establish the area of their applicability for predictive simulations. Three flow regimes in the release pipe were examined, laminar, transitional and turbulent. For every flow regime laminar, $k-\varepsilon$ and dynamic Smagorinsky-Lilly (Lilly, 1992) LES models results were compared against experimental data.

In the laminar flow release and dispersion case, helium flow was released through a 20 mm pipe with release rate of 4 Nl/min (Re=39). The laminar model provided a good prediction of concentration levels through the duration of the release except for the area close to the floor where about 50% under-prediction was observed by the end of the release. The LES model achieved an accuracy of concentration prediction similar to the laminar model, although once again the LES model under-predicted the helium concentration near the floor. Finally, the $k-\varepsilon$ model did not provide a good agreement with the experimental concentration throughout the enclosure height. The concentrations under the ceiling were under-predicted whereas the concentrations at the floor were over-predicted. The cause of poor performance of $k-\varepsilon$ model in simulation of laminar regime release can be attributed to its inability to recover molecular viscosity (i.e. to predict zero turbulent viscosity). It was concluded (Molkov and Shentsov, 2014a) that among three attempted simulations the LES approach presents the best choice, combining high accuracy with acceptable computational requirements.

In the transitional flow release and dispersion case, helium flow was released through the 20 mm pipe with a release rate of 300 Nl/min (Re = 2863). The laminar model demonstrated poor reproduction of the experimental concentration transients for the transitional flow. There was a significant delay in reaching experimentally observed concentration levels near the floor, while the concentration level near the ceiling grew excessively fast. Performance of the LES model was significantly better. There was only a small delay of about 25 s in the reproduction of the experimental concentration at the floor level (h=0.1 m) by the LES model, compared to 125 s delay by the laminar model. Concentration growth in the middle of the enclosure (h=0.7 m) was slightly too fast, by approximately 10 s (relative to experimental data). There was a slight under-prediction of concentration level at the top of enclosure (about 6%) and over-prediction at the bottom of the enclosure (maximum 20%), but overall results are much closer to experimental data than those of the laminar model. The standard $k-\varepsilon$ model demonstrated very poor performance for the transitional flow release. It exhibited early and overly fast concentration growth at all sensor locations. More importantly, experimentally measured concentrations were over predicted by 60% at the bottom and middle of the enclosure and by 9% near the top. While this result is conservative i.e. an over-prediction, the extent of concentration overestimate makes it inappropriate for application to a hydrogen safety system development. As far as the steady state solution concerns, all models

successfully reproduced two layers structure of helium concentration with the interface height matching the experiment. The laminar model under-predicted concentrations both close to the ceiling and near the bottom while $k-\varepsilon$ model grossly over predicted concentrations throughout the enclosure. The best overall performance in reproducing concentration distribution was exhibited by the LES model (Molkov and Shentsov, 2014a).

In the turbulent flow release and dispersion case, helium flow was released through a 5 mm pipe with a release rate of 180 Nl/min (Re = 6968). The laminar model did not correctly predict the steady-state concentration distribution, producing noticeably non-uniform helium distribution. The k-ε and LES models fared better, producing a reasonably close approximation to experimental data. The standard k-ε model accurately predicted helium concentration levels in the lower portion of the enclosure, but slightly over-predicts the concentration level in the upper portion of the enclosure, resulting in a helium distribution with two distinct layers (the experimental data point toward the uniform mixture). The LES model correctly predicted nearly uniform helium distribution while slightly under-predicted the concentration level. Therefore, the best performance for turbulent release simulation was ascribed to the LES model.

The overall conclusion of the above simulations (Molkov and Shentsov, 2014a) was that a dynamic LES model can be recommended as a preferable tool for simulation of the releases in the vented enclosures for all flow regimes as providing the best overall agreement with experiment.

The main characteristics (in terms of advantages and disadvantages) of the most frequently used turbulence models are presented in Table 1-1.

Table 1-1 Comparison of turbulence models

Turbulence models		
Model		Requirements
Laminar		**Advantages:** • Simple model **Disadvantages:** • For release problems, can give reasonable results only for very small Reynolds numbers.
RANS	k-ε	**Advantages:** • Extensively validated for hydrogen applications. • Robust and economical in computational cost. **Disadvantages:** • Valid only for turbulent flows. Inaccuracies in laminar and transitional flows. • The standard model over-predicts the rate of spreading for round jets. • The model performs poorly in boundary layers with strong adverse pressure gradients (Pope, Turbulent flows). • In the standard form, it is not suitable for low turbulent Reynolds number regimes, for flow separation prediction and for impinging jets.
	RNG k-ε	**Advantages:** • Can predict more accurately flows involving both laminar and turbulence regions. • Model has an additional term in its epsilon equation that significantly

	k-ω	improves the accuracy for rapidly strained flows. • The effect of swirl on turbulence is included in the model, thus enhancing accuracy for swirling flows. • The RNG theory provides an analytical formula for turbulent Prandtl numbers, while the standard k-epsilon model uses user-specified, constant values. **Advantages:** • It performs better than k-ε for boundary layers with strong adverse pressure gradients (Pope, Turbulent flows). **Disadvantages:** • It shows a strong sensitivity to freestream conditions.
LES	SST	**Advantages:** • It combines the advantages of the k-ω model in the near-wall regions and of the k-ε model in the free shear regions. • The SST model was designed to give highly accurate predictions of the onset and the amount of flow separation under adverse pressure gradient. **Disadvantages:** • The tendency of the model to generate excessive turbulence levels in flow regions with large normal strain. Examples are stagnation regions and regions with strong acceleration, where excessive turbulence is still predicted but it is much less pronounced than with a normal k-ε model.
	Smagorinsky LES	**Advantages:** • Increased level of details in flow structure compared to RANS models. • Large eddies are simulated directly. **Disadvantages:** • Computationally more expensive compared with RANS models. • Higher grid resolution required. • Valid only for transient 3D calculations. • Smagorinsky constant has to be specified. • Unsteady simulation with small time steps generates long run times and large volumes of data.
	Dynamic LES	**Advantages:** • Increased level of details in flow structure compared to RANS models. • Large eddies are simulated directly. • Self-contained; no need to specify Smagorinsky constant. • Predicts zero eddy viscosity in laminar regions of the flow. **Disadvantages:** • Computationally more expensive compared with RANS models. • Higher grid resolution required. • Valid only for transient 3D calculations. • Unsteady simulation with small time steps generates long run times and large volumes of data.
	RNG LES	**Advantages:** • Increased level of details in flow structure compared to RANS models. • Large eddies are simulated directly. • The model is capable to reproduce not only turbulent, but also transitional and laminar flows. • At low Reynolds numbers the effective viscosity becomes equal to molecular viscosity. This allows the model to perform better in the vicinity of walls.

		• In highly turbulent regions of the flow RNG model reduces to the Smagorinsky model. • In laminar flow regions the model recovers molecular viscosity. **Disadvantages:** • Computationally more expensive compared with RANS models. • Higher grid resolution required. • Valid only for transient 3D calculations. • Unsteady simulation with small time steps generates long run times and large volumes of data.

1.2.1.2 Comparison of source models (NCSRD)

1.2.1.2.1 Under-expanded jets

In order to model an **under-expanded jet** the user can either model the real nozzle or they can employ notional nozzle approaches, in order to avoid having to resolve the complex shock structure and thereby avoid the extreme computational cost.

With the notional nozzle approach, the actual nozzle is replaced by a notional nozzle with the same flow rate but which occupies a larger area at ambient pressure. The notional nozzle approach has been first developed by (Birch et al., 1984). They employed a mass balance between the actual nozzle and the notional nozzle and they assume an isentropic process from the reservoir conditions to the actual nozzle, in order to estimate the temperature and pressure at the nozzle. The pressure and the temperature at the notional nozzle are set equal to ambient conditions. Finally, they assume that the velocity at both the real nozzle and notional nozzle is the sonic velocity at the respective temperature. Later, (Birch et al., 1987) developed another approach, in which they performed a momentum balance from the real nozzle to the notional nozzle, in order to estimate the velocity at the notional nozzle instead of assuming sonic velocity. (Ewan and Moodie, 1986) introduced an approach similar to (Birch et al., 1984) approach, however, their approach assumed that the temperature at the notional nozzle is not equal to atmospheric (as Birch has assumed) but is equal to the real nozzle temperature. All three approaches make the assumption of ideal gas, and thus for very high reservoir pressures they may not work properly. (Schefer et al., 2007) proposed a similar approach to Birch 87 (Birch et al., 1987) using both mass and momentum conservation but using the Abel-Nobel equation of state.

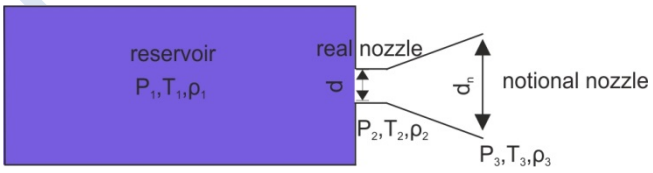

Figure 1-3 Schematic diagram of an under-expanded gas release from an infinite reservoir (level 1) through a nozzle of diameter d (level2) showing also the expansion to ambient conditions at the notional nozzle (level 3)

(Yüceil and Ötügen, 2002) and (Xiao et al., 2011) performed an energy balance to calculate the temperature at the notional nozzle assuming an ideal gas and real gas respectively. (Molkov et al., 2009a) also performed an energy balance from the actual nozzle to the notional nozzle to estimate the temperature at the latter, but did not perform a momentum balance. Instead, a sonic velocity was assumed at both the real and the notional nozzle using the Abel-Nobel equation of state for the calculation of the gas properties.

(Harstad and Bellan, 2006) developed a notional nozzle approach, in which is proposed that the location of the notional nozzle is just after the Mach disk with an area equal to that of the disk and pressure equal to atmospheric. Very recently an approach has been introduced by (S. Giannissi et al., 2015), which is similar to Ewan and Moodie (Ewan and Moodie, 1986) approach but a momentum balance is performed from the real nozzle to the notional nozzle to estimate the velocity at the latter using real gas properties. Finally, (X. Li et al., 2015) developed a two-layer partitioning model, in which mass, momentum and energy conservation equations are solved taking into account air entrainment in the slip region.

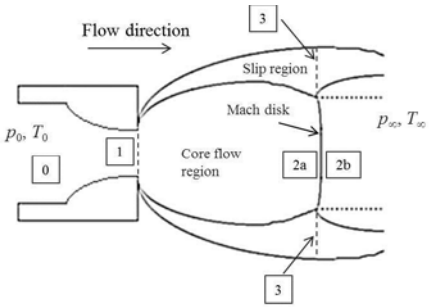

Figure 1-4 Structure of under-expanded jet (X. Li et al., 2015)

When the actual nozzle is modelled in case of under-expanded jet the numerical requirements are significantly greater compared to the case with the notional nozzle. A very fine grid near the nozzle should be used, in order to accurately capture the shock waves that occur downwind the nozzle (Shishehgaran and Paraschivoiu, 2014). Therefore, higher computational time is required which in some cases (e.g. large scale problems) is prohibitive with the available resources.

Few studies have been carried out to compare and evaluate the performance of the notional nozzle approaches (Papanikolaou and Baraldi, 2011), (Papanikolaou and Baraldi, 2012) and (X. Li et al., 2015).

In the (Papanikolaou and Baraldi, 2011) study the Birch 84 (Birch et al., 1984), Birch 87 (Birch et al., 1987), Ewan and Moodie (Ewan and Moodie, 1986) and Schefer (Schefer et al., 2007) approaches were compared based on high momentum hydrogen releases with a storage pressure 98.1 bars at a temperature of 14.5 ^{o}C and a nozzle diameter of 1 mm. Birch 84 (Birch et al., 1984) and Ewan and Moodie (Ewan and Moodie, 1986) approaches estimated a sonic velocity at the notional nozzle, while Birch 87 (Birch et al., 1987) and Schefer (Schefer et al., 2007) calculated higher velocities, since it is assumed that all of the excess pressure goes to increasing the jet's momentum. In general, Birch 87 (Birch et al., 1987) and Schefer (Schefer et al., 2007), which had higher initial momentum fluxes, performed better than the other two.

(Papanikolaou and Baraldi, 2012) compared the same notional nozzle models, and the Harstad (Harstad and Bellan, 2006) approach, against three different experimental sets with different storage pressures, nozzle diameters and flow rates. According to this study once again the Birch 87 (Birch et al., 1987) and Schefer (Schefer et al., 2007) approach performed the best overall. This was followed by Birch 84 (Birch et al., 1984) and Ewan and Moodie (Ewan and Moodie, 1986) and lastly Harstad (Harstad and Bellan, 2006) which deviated from the data the most giving the greatest underprediction of concentration. The Birch 87 (Birch et al., 1987) and Schefer (Schefer et al., 2007) approaches predict a momentum flow rate and net rate of energy flow (sum of the specific enthalpy

and specific kinetic energy) which are higher compared to the other approaches. Moreover, the Harstad (Harstad and Bellan, 2006) approach gave the lowest values with velocities far less than sonic as the conditions after the Mach disk are considered. Therefore, it seems that the approaches with the higher release velocities provide a better correlation with experimental data.

(X. Li et al., 2015) compared Birch 87 (Birch et al., 1987), Birch 84 (Birch et al., 1984), Ewan and Moodie (Ewan and Moodie, 1986), Yüceil and Ötügen (Yüceil and Ötügen, 2002) approaches along with the two-layer partitioning model, which they have developed. In two-layer partitioning model the mass, momentum and energy conservation equations from the nozzle exit to state 2b and state 3 (Figure 1-4) were performed. For more details about the model the reader can refer to (X. Li et al., 2015). They concluded that the two-layer model performed better overall than the other notional nozzle approaches, especially for higher pressure sources. In terms of prediction quality, Birch 87 followed with small differences from experimental date. Yüceil and Ötügen (Yüceil and Ötügen, 2002) approach gives results close to Birch 87 (Birch et al., 1987) and Birch 84 (Birch et al., 1984) and Ewan and Moodie (Ewan and Moodie, 1986) follow predicting incorrectly high concentrations. (X. Li et al., 2015) constructed a fully resolved (actual nozzle) simulation and compared this with the experimental data. This CFD simulation required almost 7 times more mesh elements (for the grids presented in the study) compared to the notional nozzle approaches. The results of the full CFD simulation were in good agreement with the experiment though it slightly under-predicted hydrogen concentrations. However, it is valid to note that the results of the full CFD simulation were similar to those of the two-layer partitioning model and Birch 87 (Birch et al., 1987) approach, which are much less computationally demanding.

Finally, in (S. Giannissi et al., 2015) two notional nozzle approaches were employed to model the under-expanded jets in cryogenic high pressure releases: the Ewan and Moodie (Ewan and Moodie, 1986) approach was used and a modified Ewan and Moodie approach, was introduced in that study. The difference in the modified Ewan and Moodie approach is that the velocity at the notional nozzle is calculated by performing momentum balance from the actual nozzle to the notional nozzle instead of assuming sonic velocity. Though the main scope of the study was not to evaluate the performance of the notional nozzle approaches, it was shown that for cryogenic high pressure releases Ewan and Moodie (Ewan and Moodie, 1986) performed well overall. The modified Ewan and Moodie approach was consistent with the experiment, however, the Ewan and Moodie (Ewan and Moodie, 1986) approach performed better compared with both experiments that were simulated, and especially for the one with the higher reservoir pressure. According to the statistical analysis that was carried out both approaches tend to generally under-predict (based on the value of the geometric mean bias, MG) the concentrations along the jet centerline.

In **blowdown** phenomena the volumetric source model can be employed in combination with a notional nozzle approach in case of high pressure releases. For more details about the model the reader can refer to Paragraph 1.2.4 of the “State of the art review concerning FCH technologies”. The volumetric source model has the advantage that there is no need to change the domain and the grid characteristics during the simulation. However, lower accuracy is achieved at the region near the nozzle, which may become a particular problem when the volumetric source sizes are much larger than the actual nozzle or the notional nozzle size.

1.2.1.2.2 Liquid hydrogen releases

To model **liquid hydrogen release** (LH2) two approaches can be used: two phase jet and evaporating pool. In two-phase release models the source is modelled as a homogeneous two phase jet. In the evaporating pool the source is modelled as a liquid pool along the ground that evaporates. Only the vapor phase that evaporates enters the computational domain. More details for these approaches can be found in Paragraphs 1.2.6.1 and 1.2.6.2 of the "State of the art review concerning FCH technologies".

Different data are required for each approach, in order to estimate the source characteristics. For the two-phase jet approach the primary data required (apart from the spill rate and the orifice diameter) are the hydrogen storage conditions (temperature and pressure), in order to be able to assume isenthalpic or isentropic process and estimate the flashed vapour fraction at the source (see Paragraph 1.2.6.2 of the "State of the art review concerning FCH technologies"). This information is in most cases available and measured during the experiment. Moreover, in LH2 releases the storage conditions are usually near identical: pressure slightly above atmospheric and saturation temperature at storage pressure. On the contrary, for the evaporating pool approach information about the ground heat flux is required. This information is not always available with any level of accuracy, because it is not always measured during the experiment. Furthermore, even if the substrate above which the release occurs is known, its properties are not always known accurately. Therefore, the user cannot estimate with acceptable accuracy neither the evaporation rate of the pool nor its shape and this could affect significantly the prediction. The evaporating pool is less demanding in terms of computational time, since it is a simplified model with vapour phase only in the computational domain (no multi-phase flow as in the two-phase jet approach). Therefore, there is no need to solve extra conservation equations for the liquid phase if you use the multi-fluid model (see Paragraph 1.2.6 of the "State of the art review concerning FCH technologies"). Or to calculate the liquid phase mass fraction (e.g. using the Raoult's law) in case you use the mixture model.

In (Venetsanos and Bartzis, 2007) the two models are compared with the help of a LH2 dispersion experiment. The experiment was the NASA 6 trial (Chirivella, JE, Witcogski, 1986) related to hydrogen release vertically downwards on sandy ground. The two-phase jet approach was in much better agreement with the experiment compared with the pool model. Modelling the source as a pool resulted in overestimation of the concentration levels.

The main characteristics (in terms of advantages and disadvantages) of the source models are presented in Table 1-2.

Table 1-2 Comparison of source models

Source models	
Model	Requirements
Real nozzle	**Advantages:** • Resolution of shock structures in case of under-expanded jet. • More accurate solution in near-to-nozzle area compared to effective nozzle and volumetric source models. **Disadvantages:** • Use of smaller control volume sizes and compressible flow formulation

Notional (effective) nozzle	(under-expanded flows) require qualitatively larger computational resources (RAM, CPU time). • Due to the above issue, it cannot be applied to real large scale problems. **Advantages:** • Allows the simulation of under-expanded jet flows with relatively modest computer resources. • Satisfactory accuracy for the best notional nozzle models. • Low computational cost. • Extensively validated for hydrogen applications. **Disadvantages:** • Moderate accuracy in the near nozzle region (cannot replicate the shock structure). • The accuracy depends on the specific notional nozzle model that is selected. • More suitable for constant release rate nozzles. Unsteady releases require the modification of the mesh and notional nozzle parameters (e.g. the size of the notional nozzle) or to be used combined with the volumetric source approach.
Volumetric source	**Advantages:** • Opportunity to vary nozzle parameters without changing calculation domain geometry, e.g. for blowdown processes. **Disadvantages:** • Low accuracy in near-to-nozzle area • Deteriorating accuracy when volumetric source sizes are qualitatively larger than real nozzle size (expanded flows) or effective nozzle size (under-expanded flows).
Two phase jet	**Advantages:** • Required information is the spill rate, the storage conditions and the orifice diameter, which are usually measured during the experiment. • Release conditions closer to the real case scenarios compared to the evaporating pool approach. • Capability of calculating both the vapour dispersion and the pool spreading and evaporation. **Disadvantages:** • Uncertainties in the flashed vapor fraction at the source.
Evaporating pool	**Advantages:** • Only vapour phase release, so less complicated model. **Disadvantages:** • Estimation of the evaporation rate in order to calculate the pool's surface. • Ground heat flux is required, which is usually not experimentally available data. In general, difficulties in calculating accurately the ground heat flux. • Inaccuracies due to uncertainties in the estimation of the evaporation rate and the calculation of the pool surface or shape, consequently in the source rate.

1.2.2 Critical analysis of release models (NCSRD)

1.2.2.1 Critical analysis of turbulence models (NCSRD, UU)

The choice of the appropriate turbulence model depends on the specific problem and physical phenomena to be modelled, available computational resources and required degree of accuracy. The most widely used turbulence model is the standard k-ε model. . It is a robust turbulence model with low computational cost. However, it is more appropriate for fully turbulent flows, while in complex

flows (such as involving separation regions, or severe pressure gradients) its applicability is narrowed down. Nevertheless the k-ε model has been successfully used for atmospheric flows for several years. In general, for simulations related to hydrogen release and dispersion in open environments the k-ε model performs satisfactorily. However, in these circumstances a modification which introduces extra buoyancy terms (Markatos and Pericleous, 1984) is often used and it is recommended in hydrogen applications. A model that performs better in flow separation regions is the k-ω turbulence model. This model allows for a more accurate near-wall treatment with an automatic switch from a wall function to a low-Reynolds number formulation based on grid spacing (non-dimensionalised). In addition, this model can be used for transitional flows. However, it requires high mesh resolution near the wall. SST k-ω model is a combination of the k-ε and k-ω model. It transitions from the k-ε model in the free stream to the k-ω model in the regions near walls. It makes use of the advantages of both models dependent on the flow region.

Large Eddy Simulation (LES) model resolve the unsteady fluctuations and can reproduce phenomena such as recirculation areas. For turbulent flows it can reproduce the solution more accurately, in particular the turbulent diffusion in turbulent regions. Furthermore, LES models (especially Dynamic LES and RNG LES) seem to have better behaviour in flows with transitional or laminar regions. However, LES models needs a much finer grid than RANS models, with a consequently reduced computational time step, and are unsteady (rather than steady-state) solutions, so in general it is computationally more expensive. Moreover, in geometrically symmetric problems, the symmetry assumption (which saves computational time) is not valid and it cannot be used in LES modeling.

Finally, the laminar model can give reasonable results only at low Reynolds numbers where the flow may not have strong turbulence characteristics.

1.2.2.2 Critical analysis of source models (NCSRD)

For the **under-expanded jets** although fully-resolved CFD simulation of the actual nozzle provides accurate results it requires significant grid refinement near the nozzle and thus it is has high computational cost. On the other hand the notional nozzle approach is capable of providing good results within more acceptable computational times. So, in terms of both satisfactory accuracy and low computational cost the notional nozzle approaches are almost always preferred in hydrogen safety real case scenarios. From the available studies which compare the notional nozzle approaches it is apparent that Birch 87, Schefer and the two-layer partitioning model perform better with Birch 84 and Ewan and Moodie approaches to follow, while Harstad approach seems to provide the least accurate results. Finally, the Ewan and Moodie approach provides good results in cryogenic compressed releases.

Regarding **LH2 releases** the two phase jet approach requires experimental data such as the H_2 storage conditions, which are usually experimentally available; in order to estimate the source conditions, while the evaporating pool requires additional information, such as the ground heat flux, that it is not always available. Therefore, the user will encounter more difficulties and uncertainties to estimate the source conditions in the case of the evaporating pool approach. Finally, the two-phase jet approach is more demanding in terms of computational time; however, it seems to provide more accurate predictions than the evaporating pool approach.

1.2.3 Physical and numerical requirements to models (NCSRD)

In Table 1-3 and Table 1-4, the physical and numerical requirements to turbulence and source models are presented respectively.

Table 1-3 Physical and numerical requirements to turbulence models

Turbulence models		
Model		Requirements
Laminar		**Physical requirements:** • Small Reynolds numbers: For release problems, can give reasonable results only for very small Reynolds numbers. **Numerical requirements:** • No special numerical requirements
RANS	k-ε	**Physical requirements:** • Turbulent flows: Valid only for turbulent flows. Inaccuracies in laminar and transitional flows. • Flows without strong adverse pressure gradients. **Numerical requirements:** • No special numerical requirements - Robust and economical in computational cost.
	RNG k-ε	**Physical requirements:** • No special physical requirements. **Numerical requirements:** • No special numerical requirements.
	k-ω	**Physical requirements:** • No special physical requirements. **Numerical requirements:** • No special numerical requirements.
	SST	**Physical requirements:** • No special physical requirements. **Numerical requirements:** • No special numerical requirements.
LES	Smagorinsky LES	**Physical requirements:** • No special physical requirements. **Numerical requirements:** • Higher grid resolution. • Transient 3D calculation: Valid only for transient 3D calculations. • Smagorinsky constant has to be specified. • Small time-steps: Small time-steps may be required to capture accurately transient phenomena. • High order numerical schemes.
	Dynamic LES	**Physical requirements:** • No special physical requirements. **Numerical requirements:** • Higher grid resolution. • Transient 3D calculation: Valid only for transient 3D calculations. • Small time-steps: Small time-steps maybe required to accurately capture transient phenomena.

		• High order numerical schemes.
	RNG LES	**Physical requirements:** • No special physical requirements. **Numerical requirements:** • Higher grid resolution. • Transient 3D calculation: Valid only for transient 3D calculations. • Smagorinsky constant has to be specified. • Small time-steps: Small time-steps maybe required to accurately capture transient phenomena. • High order numerical schemes.

Table 1-4 Physical and numerical requirements to source models

Source models	
Model	Requirements
Real nozzle	**Physical requirements:** • No special physical requirements. **Numerical requirements:** • Resolution of shock structures in case of under-expanded jet. • Use of small control volume sizes. • Compressible flow formulation.
Notional (effective) nozzle	**Physical requirements:** • Under-expanded jet: Storage pressure to atmospheric pressure ratio above approximately 1.9. • Constant release rate: More suitable for constant release rate nozzles. Unsteady releases require the modification of the mesh and notional nozzle parameters (e.g. the size of the notional nozzle) or to be used combined with the volumetric source approach. **Numerical requirements:** • Estimation of the notional nozzle size, exit velocity and exit temperature.
Volumetric source	**Physical requirements:** • No special physical requirements. Opportunity to vary nozzle parameters without changing calculation domain geometry, e.g. for blowdown processes. **Numerical requirements:** • Source terms: Source terms to the conservation equations need to be added at the cell where the volumetric source is applied.
Two phase jet	**Physical requirements:** • Two phase release (Storage conditions: liquid or supercritical state). **Numerical requirements:** • Estimation of the flashed vapor fraction at the source • Multiphase modelling: CFD code needs to be able to model multiphase flows. • Phase transition modelling • Accurate correlations for physical properties of both liquid and vapor phase at low temperature.
Evaporating pool	**Physical requirements:** • Two phase release (Storage at liquid phase). **Numerical requirements:**

	• Estimation of the evaporation rate in order to calculate the pool's surface.

1.3 Knowledge gaps (NCSRD)

Despite the significant levels of research concerning the study of hydrogen release and dispersion, there remain several knowledge gaps that need to be addressed. The aim of this section is to gather and identify these gaps and the key parameters that need to be improved.

In vapour hydrogen releases knowledge gaps still exist and they can be identified as follows:

- CFD validation of releases in real scale complex configurations: The majority of CFD studies concerns simplified geometries. Thorough model validation in complex geometries (e.g. with barriers, obstacles) still needs to be performed.
- Study of hydrogen release through non-circular nozzles and nozzle geometries which resemble real case accidents (e.g. cracks).
- CFD modeling of the wind direction, in order to accurately predict the wind effect on vapour dispersion.
- Further validation of the turbulence models in transitional flows.
- Further validation of more sophisticated turbulence models such as Dynamic LES and hybrid turbulence models (e.g. Detached Eddy Simulation model).
- Comparison of all the available notional nozzle approaches based on several experiments (different nozzle diameter, storage conditions etc.) is necessary to make generalised conclusions about their performance and to indicate which approach performs best under which conditions.
- Evaluation of the performance of the notional nozzle approaches in the case of non-circular nozzles.
- The non-ideal behaviour of hydrogen in CFD codes in compressed releases should be studied.

Knowledge gaps can also be identified in **cryogenic compressed releases** (where hydrogen is stored at both high pressure and low temperature). In these cases hydrogen can be in supercritical state inside the storage tank and two phase chocked flow can be achieved at the nozzle. Therefore,

- More research is required in modelling the two phase chocked releases. Although approaches (Simoneau and Hendricks, 1979), (Darby, 2004), (Travis et al., 2012) have been developed in order to estimate the mass flow rate at the nozzle based on the storage conditions, there are several problems regarding the accurate estimation of the mass flow rate. Especially when nozzle conditions are near the critical point where the mass flow rate is underestimated.
- Evaluation and comparison of the performance of the different Equation of States (EOS) in the two phase chocked flow approaches, in order to estimate the mass flow rate at the

nozzle. The NIST (Leachman et al., 2009) EOS seems to work properly, however more EOSs, like Peng-Robinson should be tested in order to evaluate their performance.

- A proper correlation for accurately calculating the specific heat capacity of hydrogen at low temperatures and high pressures should be further investigated and incorporated into CFD codes.
- Studies on humidity and air condensation during cryogenic compressed releases should be undertaken in order to inform modelling of these phenomena.

The knowledge gaps in **liquid hydrogen releases** can be identified in the following subjects:

- Further development of pool spreading and evaporation models. The coupling of these models with vapour dispersion should also be studied further.
- Comparison between the models that solve the liquid pool separately and the models that do not solve the pool separately.
- Research should be directed at improving the modelling of ground heat flux in cases where a liquid pool is formed- for both solid and liquid (usually water) substrates. The heat flux modeling from the ground to boiling pool based on the hydrogen boiling curve should be further investigated.
- The radiative heat transfer and its contribution to the total heat transfer from the air and ground to the cold cloud should also be studied.
- The source modeling is another key parameter that needs further research. A comparison between isenthalpic and isentropic assumption is required to estimate the flashed vapour fraction at the source (in the case of two-phase jet approach) can be performed to assess their effect.
- A sensitivity study regarding the turbulence intensity at the source to include turbulence effects can be performed in both source modeling approaches (two-phase jet and evaporating pool).
- Humidity and air condensation phenomena need further exploration. The effect of the size of the humid droplets on the vapor dispersion and the effect of the ice (from air and humidity freezing) that is accumulated on the ground on both heat flux and dispersion should be thoroughly investigated. In general, models to accurately predict all these complex phenomena should be incorporated in the CFD codes, which would then constitute useful and practical tools for modeling consequences in hydrogen safety applications.
- Study of the effect of non-ideal behaviour of hydrogen on CFD predictions in liquid releases.
- A proper correlation for calculating the specific heat capacity of hydrogen at low temperatures should be further investigated and incorporated in CFD codes.
- Finally, in order to close out the above knowledge issues related to liquid hydrogen releases, it is essential to carry out additional experiments under more controlled conditions, in which

all the above key parameters will be measured. Conducting experiments not only will give better insight on the physical effects but also will provide the ability to validate the CFD models.

2 Ignition (Author: UU, Reviewer: HSL)

In the majority of CFD simulations with premixed combustion the ignition is modelled in a simplistic way in which the temperature and the combustion products are patched in a region with a limited number of control volumes around the ignition point. This type of ignition model performs sufficiently well in a large number of combustion cases in which the purpose of the study is to investigate the flame propagation, overpressures and heat fluxes after the ignition. If the emphasis of the CFD investigation is to understand and predict whether and when the spontaneous ignition occurs, a more sophisticated modelling approach is required. This Section focusses on the critical analysis of models to identify the conditions and requirements under which the self-ignition occurs.

2.1 Models (UU)

There are number of experimental confirmations of spontaneous ignition by diffusion mechanism for releases from high pressure equipment to the atmosphere through a tube was obtained in "controlled laboratory environment" by (Dryer et al., 2007; Golub et al., 2008, 2007; Mogi et al., 2008; Pinto et al., 2007).

The list of models that can be used to simulate the phenomenon of spontaneous diffusion ignition is described in Deliverable 2.1 (State of the art review concerning FCH technologies) Section 2.2. These models were divided into three main categories: 1, 2 and 3 dimensional, varying by the level of complexity and capability to predict and resolve specific phenomena. The models employed Reynolds-averaged Navier-Stokes (RANS) or Large Eddy Simulation (LES) governing equations to simulate turbulence.

2.2 Comparison of models and requirements (UU)

Numerical modelling of the shock-related turbulent mixing problem is mathematically challenging due to the presence of the thin diffusion layer and strong shock waves. Direct numerical simulation (DNS) would be desirable approach, but computing power requirement are prohibitive for such tasks, prompting researchers to consider less computationally intensive methods such as large eddy simulation (LES). Many researchers considered reduction of the problem to 2D and in some cases to 1D, often taking advantage of axisymmetric geometry, in order to reduce mesh size requirements. The application of 1D models is questionable especially in complex geometries like pressure relief devices (PRD) requiring 3D simulations. Particularly, as it was suggested by (Dryer et al., 2007) complex geometry plays an important role in the "diffusion mechanism" of ignition leading to multiple reflections of shocks and an increase of hydrogen-air mixture temperature due to co-interaction of shocks.

2.2.1 Comparison of models (UU)

2.2.1.1 One-dimensional model

One-dimensional modelling described in (Maxwell and Radulescu, 2011) addressed the ignition problem of an unsteady diffusion layer of fuel and oxidizer, undergoing volumetric expansion. This model was applied to shock induced diffusion-ignition of pressurized fuel jets that are released into an oxidizing atmosphere. Upon the sudden release of a pressurized gaseous fuel into the ambient atmosphere through a hole, a strong shock wave forms, driven by rapid expansion of the forming jet.

The model applies only to evolution of the thin diffusion layer at the head of the jet in Lagrangian coordinates, with its rate of expansion dictated by the local pressure evolution of the surrounding gas flow.

The entire reactive jet expansion problem is governed by the Navier–Stokes equations for a chemically reactive fluid augmented by the evolution of each chemical reactive species. Neglecting viscous effects and spatial pressure gradients within the diffusion layer due to its dimension being very small compared to that of the jet, decouples the momentum equation from the evolution of the diffusion layers.

Mathematical model

- Combustion model: Arrhenius reaction rate.
- Discretisation scheme:
    - Central difference approximations on the diffusive terms (Anderson, 1995),
    - Explicit time stepping for the unsteady terms(Anderson, 1995).
- Initial conditions for the release problem:
    - Initial vessel pressure was ranging from 100 to 1000 atm,
    - The pressure of the ambient air is taken to be 1 atm,
    - The initial temperatures of both gasses are 300 K.
- Grid: independent solutions was found to be $\Delta x = 8.0 \times 10\text{-}6$ m.
- The only controlling parameter for the shock tube problem is the storage pressure of the fuel.
- Boundaries of the 1D problem are specified to have zero gradients i.e. inflow/outflow.

Numerical details

- The temperature at each grid point was computed using Cantera software (Goodwin, 2009) coupled to CFD solver.
- The solutions across the shock discontinuity and expansion fan were found using the numerical methods described by Browne et al., (2008) and iterated until the pressure and velocity at the hydrogen-air contact surface were matched.
- For the production rates of each chemical species the reaction mechanism chosen for this study involved 19 reversible elementary reactions and thermochemical data updated by Li et al., (2004).
- For calculating transport properties of the gasses (i.e. diffusion velocities of each specie and thermal conductivities) mixture averaged expressions described by (Coffee and Heimerl, 1983) were used.

2.2.1.2 Two-dimensional Direct Numerical Simulation (DNS) compressible axisymmetric Navier-Stokes equations by Pinto et al.

Pinto et al., (2007) utilized a two dimensional Direct Numerical Simulation (DNS) approach to study auto-ignition of high pressure hydrogen release in a tube with diameter ranging from 4.8 to 10.3 mm and length from 48 to 180 mm. They concluded that 2D numerical simulations seem to give fair comparison with experiments, but more effort would be required to better match simulation results with experimental data.

Mathematical model

- Combustion model: Arrhenius reaction rate.
    - Compressible solver with governing equations discretized using finite difference formulation.
- Discretisation scheme:
    - The convective terms: second-order Explicit Harten-Yee Non-MUSCL modified-flux type TVD scheme
    - The viscous terms: standard second-order central difference formulation.
    - The time integration method: second-order Strang-type fractional step method
    - The chemical reactions: point implicit method to avoid the stiffness.
- Initial conditions:
    - Pressure varied from 3 to 7 MPa
    - Ambient atmosphere pressure and temperature were 1 atm and 300 K respectively
- Grid: rectangular uniform grid size of $\Delta x = \Delta y = 20$ µm, giving a total of 27 million control volumes.
- Boundaries: Non-slip on the wall

Numerical details

- A chemical reaction model by Petersen & Hanson (1999) with 9 species and 18 reactions was used.
- The transport coefficients of each chemical species: viscosity, heat conductivity, and binary diffusion coefficient, were evaluated using the Lennard- Jones intermolecular potential model (Chapman and Cowling, 1970), and those of the gas mixture were calculated by Wilke's empirical rule (Wilke, 1950).
- The enthalpy of each chemical species was derived from NIST data base (National Institute of Standards and Technology, 2016).

2.2.1.3 Two-dimensional DNS compressible axisymmetric Navier-Stokes equations by Lee and Jeung

Lee & Jeung (2009) performed direct numerical simulation to analyse the processes of mixing and spontaneous ignition of hydrogen within a tube after the rupture of a disk at a bursting pressure of 86.1 atm in a domain of size 228.6 x 6.35 mm.

Mathematical model

- Combustion – Arrhenius reaction rate
- Type of solver and pressure-velocity coupling:
  - Cell-centred unsteady finite volume solver.
- Discretisation scheme:
  - The convective terms: AUSM-DV scheme (Wada and Liou, 1997),
  - The viscous terms: 2nd-order central differencing,
  - The chemical reactions: 5th-order implicit Runge–Kutta RADAU5 (Hairer and Wanner, 1996).
  - The time integration method: second-order Strang-type.
- Initial conditions:
  - Bursting pressure 86.1 atm,
  - Ambient pressure and temperature 1 atm and 300 K respectively.
- Grid: $\Delta x = \Delta y = 19$ µm, total of 4 million control volumes.
- Boundaries:
  - Adiabatic non-slip conditions for the tube wall,
  - Both ends of the computational domain were told to have transmissive boundary conditions,
  - Slip conditions for the axis of symmetry.

Numerical details

- Reaction kinetics with 9 species and 19 reactions were used for hydrogen combustion described by (Li et al., 2004).
- The evaluation of thermodynamic properties, transport properties, and chemical source terms was assisted by the Cantera library (Goodwin, 2009).
- Thermodynamic properties of the species were based on NASA polynomials (McBride et al., 1993).
- The viscosity, thermal conductivity, and binary diffusion coefficients for each species were determined using Lennard–Jones potentials (Chapman and Cowling, 1970) and kinetic theory.
- Calculation of mixture-averaged values was as described by (Mathur et al., 1967; Wilke, 1950).

2.2.1.4 Two-dimensional DNS, Golub

(Golub et al., 2008) reported numerical and experimental investigation of hydrogen self-ignition in a tube as a result of the formation of a shock wave in front of a high- pressure hydrogen gas. It was been shown that as the initial pressure in the high-pressure reservoir increases the distance from the burst location to the hydrogen flash on the hydrogen-air contact surface reduces. The 2D model with the full Navier–Stokes equations for the multicomponent mixture of gases accounted for viscous gas transport, multi-component diffusion, heat transfer, and incorporated a kinetic scheme of hydrogen oxidation with 21 reactions and 11 species.

Mathematical model

- Combustion model: physicochemical model involving gas-dynamic transport of a viscous gas.
- Turbulence mode: $k - \omega$ differential.
- Type of solver and pressure-velocity coupling:
    - Explicit scheme of the 2nd-order for both convective and diffusion terms.
- Grid: 0.05 to 0.15 mm.
- Time step requirements: Time step was determined by the CFL criterion.
- Boundaries: solid surface were assumed non-catalytic and adiabatic, with a slip boundary for the pipe walls.

Numerical details

- Model involved the gas-dynamic transport of a viscous gas and the detailed kinetics of hydrogen oxidation (21 reactions and 11 species by (Miller and Bowman, 1989).

2.2.1.5 Two-dimensional implicit LES model by Xu et al.

In study by (Xu et al., 2007) a model of spontaneous ignition utilizing Implicit Large Eddy Simulation (ILES) was developed. The simulations were performed by solving the unsteady Navier–Stokes equations of a chemically reactive multicomponent mixture of ideal gases.

Mathematical model

- Combustion model: Arrhenius reaction rate.
- Turbulence model: Implicit LES (ILES).
- An arbitrary Lagrangian and Eulerian (ALE) method (Hirt et al., 1974) for numerical implementation where convective terms are solved separately.
- Each time cycle was divided into two phases: a Lagrangian phase and a rezone phase (different numerical schemes were adopted in the two phases).
    - In the Lagrangian phase –second-order Crank-Nicolson scheme was used for the diffusion terms and the terms associated with pressure wave propagation, where the coupled semi-implicit equations were solved by a SIMPLE type algorithm with individual equations solved by a conjugate residual method (O'Rourke and Amsden, 1986).
    - In the rezone phase - two-stage, second-order MacCormack method (MacCormack, 2003) was used to solve the convective terms.

- Spatial differencing - a second-order total variation diminishing (TVD) scheme (Amsden et al., 1989) was used for the convection terms
- All the other terms the second-order central differencing scheme was used.
- Grid cell size: 15 – 30 µm.

Numerical details

- A mixture-averaged multi-component approach (Kee et al., 2000) was used for the calculation of molecular transport with consideration of thermal diffusion which is important for non-premixed hydrogen combustion. The thermodynamic data was adopted from (Kee et al., 2000).
- A detailed chemistry scheme by (Saxena and Williams, 2006) involving 8 reactive species and 21 elementary steps was used.
- The chemical kinetic equations were solved by a variable-coefficient ODE solver (Brown et al., 1989) to deal with the stiffness problem of the chemistry.

This model was subsequently improved by replacing a second-order TVD scheme for spatial differencing with high order WENO scheme (Xu et al., 2009, 2008). It was found that the second-order TVD schemes are overly dissipative to capture the mixing process and higher order weighted essentially non-oscillatory (WENO) shock-capturing schemes can better resolve the underlying physical process with the same grid resolution (Mosedale and Drikakis, 2007). Since the ILES approach uses numerical dissipation to model the unresolved small scales, the accuracy order of the numerical schemes applied to the convection terms is essential. Several high order WENO schemes had been investigated (Xu et al., 2008). It had been shown that 9^{th}-order scheme results in numerical oscillations leading to unphysical results on the hydrogen-air contact surface. Accordingly, subsequent works (Wen et al., 2009; Xu et al., 2009) used 5^{th}-order upwind WENO scheme (Balsara and Shu, 2000) for the convection terms. Furthermore, second order MacCormack method used in the rezone phase to solve the convection terms was replaced with a 3^{rd}-order TVD Runge–Kutta method (Balsara and Shu, 2000). This updated model had been used in a number of follow up works aimed at investigation of the effects of the obstacles and non-instantaneous membrane opening (Xu et al., 2011; Xu and Wen, 2014, 2011).

2.2.1.6 Other two-dimensional models

Two-dimensional (2-D) modelling of hydrogen releases through a tube were simulated in (Wen et al., 2009). It was demonstrated that spontaneous ignition is governed by focusing of reflected shocks from the tube wall. The influence of internal tube geometry had been investigated in (Xu and Wen, 2014, 2012). The simulations confirmed the experimental finding by Dryer et al. (2007) that internal geometries with a forward-facing vertical plane can significantly increase the propensity of spontaneous ignition.

A two-dimensional (2-D) simulation of spontaneous ignition of high-pressure hydrogen in a duct was conducted to explore ignition mechanisms by Terashima et al. (2014) and focused on the effects of the initial diaphragm shape on spontaneous ignition. The Navier-Stokes equations with a detailed chemical kinetics mechanism were solved using direct numerical simulation. The study demonstrated that for a straight diaphragm, ignition only occurs near the wall owing to the adiabatic wall condition, while three ignition events were identified for a greatly deformed diaphragm: ignition due to

reflection of leading shock wave at the wall, hydrogen penetration into shock-heated air near the wall, and deep penetration of hydrogen into shock-heated air behind the leading shock wave.

Rudy et al. (2014) performed 2D simulations of the spontaneous ignition of pure hydrogen with the use of 23-reaction hydrogen-air mechanism provided by (Konnov, 2000). The turbulence model used was RNG k-epsilon.

Numerical simulations were conducted by (Lee et al., 2015) for a cylindrical tube with various burst conditions. It was shown that there is a significant relevance between the ignition features and the burst conditions.

Morii et al. (2015) performed 2D numerical simulation of high-pressure hydrogen release in a duct with two obstacles on the walls to explore the spontaneous ignition mechanisms. The Navier-Stokes equations with a detailed chemical kinetic mechanism involving 9 species and 34 elementary reactions were solved by using direct numerical simulations. It was demonstrated that the presence and position of obstacles drastically change the interaction of shock waves with the hydrogen-air contact surface. For some obstacles position spontaneous ignition may take place at a relatively low pressure, which is attributed to the propagation direction and interaction timing of two reflected shock waves.

2.2.1.7 Three-dimensional LES model (UU)

A 3D model, using large eddy simulation (LES) approach was developed at Ulster University (Bragin et al., 2013) in order to model the dynamics of spontaneous ignition in the complex realistic geometries mimicking T-shaped TPRD as described in (Golub et al., 2007).

Mathematical model

- Combustion model: The Eddy Dissipation Concept (EDC) (Magnussen, 1981) with updates that incorporates detailed Arrhenius chemical kinetics in turbulent flames was applied as the combustion sub-model.
- Turbulence model: LES Renormalization group theory (RNG).
- Type of solver and pressure-velocity coupling:
    - Explicit linearisation of the governing equations with explicit method for solution of the linear equation set.
- Discretisation scheme:
    - Convection terms: AUSM flux splitting.
    - Diffusion terms: 2nd-order upwind scheme.
    - Temporal terms: the four step Runge–Kutta algorithm.
- Grid: 3D unstructured combined hexahedral-tetrahedral.
- Wall treatment: Non-slip impermeable adiabatic boundary conditions.
- Time step requirements: CFL = 0.2.

Numerical details

- The large eddy simulation (LES) model employs “coarser” 3D grids compared to 1D and 2D modelling. This “forced” increase in the mesh size is “compensated” by an advanced sub-grid scale (SGS) modelling of the combustion by the eddy dissipation concept (EDC) with a detailed chemistry.
- Use of the EDC combustion model allowed an increase in control volume size compared to 1D and 2D models, and to reproduce experimental results obtained in complex realistic geometries, where 1D and 2D simulations cannot be applied without loss of predictive accuracy.
- The burst disk opening was expected to play an important role in the process of ignition due to the effect of mixing between hydrogen and air and therefore membrane opening was simulated.
- The effective viscosity was calculated using the renormalization group (RNG) theory (Yakhot and Orszag, 1986a).
- Arrhenius kinetics were realized by 21-step chemical reaction mechanism of hydrogen combustion in air employing 37 elementary reactions (Gutheil et al., 1993). The effect of nitrogen chemistry was taken into account by considering the detailed mechanism of nitrogen oxide (NO) formation.

2.2.2 Critical Analysis (UU)

Most simulations of hydrogen spontaneous ignition by the diffusion mechanism were carried out mostly in 2D formulations, with validation only for relatively simple axisymmetric geometries and fine mesh to directly resolve the diffusion ignition phenomenon. In spite of a measure of success achieved by 2D models, capturing the physics of turbulent mixing requires implementation of a fully 3D model. Furthermore, utilization of 3D models is required in order to be able to perform simulations and reproduction of experimental results obtained in complex realistic geometries, where 2D simulations cannot be applied.

In a one dimensional model by Maxwell & Radulescu (2011), owing to the thinness of the diffusion layer, its curvature can be neglected, restricting the analysis to a single space dimension perpendicular to the diffusion layer. The model allows predicting overpressure and ignition limits for certain pipe lengths and storage pressures. However it is not capable of handling shock reflection, wall treatment and membrane opening. For complex geometries ignition may occur outside of flow centre-line. For example, as it was demonstrated in (Bragin et al., 2013) in the case of a T shaped PRD, that the highest temperature was reached on the centre-line where there was no combustible hydrogen-air mixture, ignition occurred somewhere aside of centre-line, limiting the applicability of 1D ignition models.

2.2.3 Physical and numerical requirements to models (UU)

Review of diffusion ignition models and simulations demonstrates that application of Arrhenius reaction rate for combustion modelling requires direct resolution of laminar flame and ignition phenomena. This requires a corresponding fine numerical mesh implying 1D or 2D simulations, which have limited practical applicability. Easing numerical restrictions and embarking on simulation of realistic 3D geometries required implementation and use of turbulent combustion model, e.g. (Bragin et al., 2013). At the moment of writing this document the simulation described in (Bragin et

al., 2013) remained the only one which was validated against experimental data for realistic 3D geometry.

- SGS modelling of turbulent combustion following ignition (i.e. further jet propagation from the ignition point) is required to tackle practical problems.
- Use of 2D models prevents the development of vortices and mixing of hydrogen with surrounding air in third direction while use of 3D simulations allows predicting ignition in complex confined realistic geometries. If geometry is simple, i.e. orifice, 2D could be used with caution.
- The importance of membrane opening and internal tube geometry in predicting ignition phenomena was demonstrated in the following simulations:
    - Recent numerical studies investigated modelling of non-instantaneous membrane opening time studies (Xu et al., 2009), (Wen et al., 2009);
    - The effect of burst disk shape was investigated by (Lee and Jeung, 2009);
    - The effect of burst disk opening on combustible mixture formation preceding hydrogen spontaneous ignition was investigated by (Bragin and Molkov, 2010), (Bragin et al., 2013);
    - The effect of release tube internal geometry was investigated by (Xu and Wen, 2012), (Xu and Wen, 2014) and the presence of obstacles by (Xu et al., 2011);
- Detailed or reduced chemistry is preferable to one step or two step equations.
- Ignition happens close to a wall due to flow stagnation, i.e. higher temperature. Non-slip boundary conditions at walls are therefore important for ignition prediction capability of simulations.

2.3 Knowledge gaps (UU)

The diffusion ignition of hydrogen has been a target of substantial modelling and simulation effort. However, model validation in complex 3D geometries is limited to qualitative results – observation of ignition or non-ignition phenomena. Further validation of ignition CFD simulations is hampered by lack of high-quality quantitative experimental data on:

- Ignition location and ignition time,
- Membrane or burst disk opening time and duration,
- Ignition in complex geometries and confinements.

Currently there is no experimental evidence of the possibility of direct ignition of open jets and potential for this ignition scenario remains a knowledge gap. Other phenomena which may affect diffusion ignition and which validation requires quality experimental data include heat transfer to pipe walls, effect of initial temperature, transition from diffusion ignition to jet fire and quenching of diffusion ignition.

At the time of writing the only available hydrogen ignition models are models for simulation of diffusion hydrogen ignition. Models for other ignition sources, like:

- Ignition by hot surface,

- Ignition by static electricity discharge (e.g., due to triboelectric charging by dust particles lifted by near to the ground release),
- Ignition due to shock focusing,

are not available or identified. Only limited experimental data is available and no models or simulation validation have been performed in these areas. Thus, (Merilo et al., 2012) studied potential for particulates entrained in hydrogen jets to generate electrostatic charge and induce electrostatic discharge ignitions. Hydrogen-air mixture ignition due to shock focusing with following combustion is described in the paper (Naboko et al., 2006).

3 Fires (Author: UU, Reviewer: HSL)

An unscheduled release of hydrogen followed by a jet fire is a possible incident/accident scenario for hydrogen and fuel cell systems and infrastructure. In case of spontaneous or early ignition a jet fire is less likely to develop into deflagration or even detonation with high overpressure.

Jet fires are mainly modelled as non-premixed combustion while deflagrations are treated as premixed. The critical analysis of the models to identify requirements to model hydrogen fires is a therefore the aim of this Section.

3.1 Models (UU)

The list of models that potentially can be used to simulate non-premixed combustion of hydrogen is described in Deliverable 2.1 (State of the art review concerning FCH technologies) Section 3.2. These models were divided into 3 main categories:

1. Where combustion rate is described by the Arrhenius expressions;
2. Where combustion rate is limited by the turbulent mixing rate ignoring chemical kinetics;
3. Where combustion rate includes detailed chemical mechanisms in turbulent flow combustion.

These models vary in their level of complexity and capability to predict and resolve specific phenomena e.g. flame lift-off and blow-off, fire regimes etc. For turbulence simulations the models employ time averaged Reynolds-averaged Navier-Stokes (RANS) or space-filtered Large Eddy Simulation (LES).

3.2 Comparison of models and requirements (UU)

There are various CFD models for combustion simulation ranging by the level of complexity. The popular Eddy Dissipation Concept (EDC) model (Magnussen and Hjertager, 1977) is based on the Eddy BreakUp (EBU) model originally proposed by Spalding (Spalding, 1977, 1971). Various refinements have been made to the original EDC model by (Byggstøyl and Magnussen, 1985; Ertesvåg and Magnussen, 2000; Magnussen, 1981), and it has been shown to provide a good compromise between accuracy and affordability for a number of different non-premixed flames.

3.2.1 Comparison of models (UU)

3.2.1.1 Arrhenius reaction rate model (finite rate chemistry)

The Arrhenius reaction rate model computes the chemical source terms using Arrhenius expressions. The model is exact for laminar flames, but is generally inaccurate for turbulent flames due to highly nonlinear Arrhenius chemical kinetics. Due to exponential dependence on temperature this model is mathematically stiff and typically requires very small time step resulting in high computational cost of simulation. It is therefore usually restricted to a relatively low Reynolds number small scale simulations, e.g. spontaneous ignition DNS simulations described in Deliverable 2.1 Section 2.

3.2.1.2 Eddy Break-Up model (EBU)

The Eddy Break-Up model assumes that the chemical kinetics are much faster than the turbulent timescales, and the combustion rate therefore is limited by the turbulent mixing rate only controlling delivery of fresh reactants to the reaction zone, hence unable, for example, to predict lift-off of turbulent flames. A modelling approach by (Makarov and Molkov, 2013) utilises the EBU combustion model to simulation of hydrogen plane jets. To reduce the computational effort the problem was modelled in two stages: first the compressible flow in the near-to-nozzle field was simulated, and then the results were used as boundary conditions for the far-from-nozzle field simulations where the incompressible flow approach was applied.

Mathematical model

- Combustion model: Eddy Break-Up.
- Turbulence mode: $k-\varepsilon$ standard.
- Type of solver and pressure-velocity coupling:
    - Mathematical model includes 3D Favre-averaged governing equations
    - The density-based explicit solver was applied for solving compressible part of the problem, and the pressure-based implicit solver was used for incompressible simulations
- Discretisation scheme:
    - The convective terms: MUSCL third order approximation scheme
    - The time integration method: simulations were started as transient (unsteady) using explicit time marching, and switched to the steady-state simulations later on when the shock structure was established. Simulations in the far-field were run as steady-state thus neglected the transient term.
    - The chemical reactions: 1 step “mixed-burned”.
- Initial conditions:
    - Vessel storage pressure 40 MPa
    - Ambient atmosphere pressure and temperature were 1 atm and 300 K respectively
- Grid: two grid approach (near nozzle grid (compressible stage) 530,546 mix of tetrahedral and hexahedral CVs), farfield calculation domain (incompressible stage) (868,546 hexahedral CVs)
- Boundaries: specified pressure at hydrogen inflow and non-reflecting pressure-far-field at outflow in compressible part of the problem; specified zero pressure at all inflow and outflow boundaries in incompressible part of the problem except of interface with compressible domain, where velocity, temperature and species profiles from compressible part of the problem solution were specified.

Numerical details

- Turbulence was modelled using k-ε standard model by (B.E. Launder and Spalding, 1974a).
- The EBU combustion model in (Magnussen and Hjertager, 1977) formulation was employed for combustion modelling.

- MUSCL third order approximation scheme following the study by Houf et al. (2007) was used to avoid the effect of overestimation of the spread rate of axisymmetric jet in conjunction with standard k-ε turbulent model.

3.2.1.3 Flamelet probability density function (PDF)

The effect of reaction chemistry on the modelled combustion phenomena may be accounted to some degree using flamelet PDF model. Brennan et al. (2009) employed a LES turbulence model to simulate high-pressure, under-expanded hydrogen jet flames. The model is based on the mixture fraction approach and probability density function to account for flame–turbulence interaction. A flamelet library of the relationship between the instantaneous composition of the reacting mixture and the mixture fraction was calculated in advance.

Mathematical model

- Combustion model: flamelet probability density function model
- Turbulence mode: Large Eddy Simulation (LES)
- Type of solver and pressure-velocity coupling:
    - Segregated solver
    - PISO algorithm for pressure–velocity coupling
- Discretisation scheme:
    - Implicit linearization of the governing equations
    - Bounded central-difference 2nd order accurate scheme for momentum terms
    - Upwind scheme for mixture fraction terms
- Initial conditions:
    - Vessel storage pressure 40 MPa
    - Ambient atmosphere pressure and temperature were 1 atm and 300 K respectively
- Time step requirements: time step of 0.005 s was chosen to maintain CFL number of less than 1 in the majority of the domain except of the vicinity of the jet exit.
- Grid: Two grids were considered. The finer grid with 341,160 hexahedral cells with a minimum of 8 cells across the inlet boundary. The coarser grid with 87,151 hexahedral cells and a minimum of 4 cells across the inlet boundary.
- Boundaries: velocity inlet for release, pressure outflow for domain boundary.

Numerical details

The notional nozzle approach by (Molkov et al., 2009b) was used to simulate an under-expanded jet at pressures up to 1000 bar which are realistic for hydrogen storage.

The mathematical model employed was based on the solution of conservation equations for mass, momentum and a conserved scalar. The Favre averaged equations for mass and momentum are described in (Makarov and Molkov, 2004).

Rather than solving conservation equation for each species a mixture fraction approach is used (Bilger, 1976). The approach is based on the assumption that the diffusivity of all species is equal. It

allows simplification of calculations by decoupling simulation of the flow and complex reaction chemistry.

The laminar flamelet approach by (Peters, 1988) which is well developed for application to non-premixed flames was applied. The approach assumes that the turbulent flame brush can be approximated as a system of instantaneous laminar flamelets, where species concentrations and temperature are described as a function of mixture fraction (Poinsot and Veynante, 2005).

Turbulent fluctuations at the boundary modelled using a random flow generation technique by (Smirnov et al., 2001). Different levels of maximum turbulence intensity and turbulence scale have been imposed at the jet boundary. It was concluded that the turbulence intensity of 25% and turbulence length scale equivalent to 7% the equivalent diameter provided the closest agreement with experimental observations.

3.2.1.4 Eddy Dissipation Concept model (EDC)

The EDC model is an extension of the eddy dissipation model to include chemical reaction mechanism in a turbulent flow. It assumes that reactions occur in small turbulent structures, called the fine-scales. Among the advantages of the model are the inclusion of detailed chemical mechanisms in turbulent flow combustion and capability to predict lift-off, blow-off of turbulent flames and under-ventilated fire regimes. The recent study by (Molkov and Shentsov, 2014b) builds on the initial numerical experiments performed and reported in (Molkov et al., 2013). It aims to increase understanding of phenomena related to indoor hydrogen fires in an enclosure with one horizontal or vertical vent (located at the top of one wall) and a sustained hydrogen release of constant flow rate and temperature. The study exploits the most advanced modelling and simulation techniques to gain insights into various regimes of hydrogen jet fire indoors.

Mathematical model

- Combustion model: EDC.
- Turbulence mode: The renormalization group (RNG) k-ε turbulence model.
- Type of solver and pressure-velocity coupling:
  - Pressure-based segregated solver with SIMPLE pressure-velocity coupling algorithm.
- Discretisation scheme:
  - Spatial discretization: convection terms of the 1st order, diffusion terms of the 2nd order.
  - The time integration method: 1st order implicit
  - The chemical reactions: 18 reactions with 9 species
- Initial conditions:
  - Ambient atmosphere pressure and temperature were 1 atm and 298 K respectively
- Grid: Structured hexahedral
- Boundaries: velocity inlet for release, pressure outlet for domain boundary, adiabatic walls

Numerical details

The renormalization group (RNG) k-ε turbulence model was applied that was derived from the instantaneous Navier-Stokes equations (Orszag et al., 1993; Yakhot and Orszag, 1986a).

The eddy dissipation concept model by Magnussen (1981) included the 18-step reduced chemical reaction mechanism of hydrogen combustion in air that is a subset of the (Peters and Rogg, 1993), mechanism that excludes H_2O_2 formation and consumption. For the reactants at room temperature and not very large pressures up to 4 MPa, the H_2O_2 concentration is very low and does not play an important role in the structure of the flame (Treviño and Mauss, 1993).

Reactions are governed by the Arrhenius rates, and are integrated numerically using the in-situ adaptive tabulation (ISAT) algorithm by Pope (1997) that can accelerate the chemistry calculations by two to three orders of magnitude, offering substantial reductions in run-times.

3.2.2 Critical analysis (UU)

The Arrhenius reaction rate model is precise for laminar flames, but is generally inaccurate when applied for turbulent flames modelled using time averaged (RANS models) or space-filtered (LES models) approaches, due to the non-linear dependence of the rate of reaction on temperature and the large fluctuations of temperature in turbulent flames. It could probably be applied for the microflames.

The Eddy-Break Up combustion model, with its main advantage being simplicity, has some disadvantages which may affect the simulation results:

- Combustion rate is limited by the turbulent mixing rate ignoring any effect of chemical kinetics.
- The model tends to overestimate the reaction rate in highly strained regions where the ratio k/ε is large.
- Due to its infinitely fast reaction rate assumption, EBU combustion model is unable to predict lift-off of turbulent flames and under-ventilated fire regimes.
- The model cannot describe any ignition or stabilization mechanism because fuel and oxidizer burn as soon as they get in contact like all models with infinitively fast chemistry for non-premixed flames.

The flamelet PDF model has the following advantages:

- Availability to deal with chemistry.
- Possibility of treating complex chemical sources directly (Veynante and Vervisch, 2002).
- Only two scalar equations have to be solved independent of the number of chemical species involved in the simulation.
- Inclusion of both finite-rate chemistry and the influence of the local mixture fraction gradients imposed by the flow field (Pitsch et al., 1998).

Disadvantages of the flamelet PDF model are**:**

- The model is restricted by assumptions such as fast chemistry or the neglecting of different Lewis numbers of the chemical species.

- The model does not account for the curvature effects which can change the flame structure and is more detrimental while the structure has not reached the quasi- steady state.
- The model is limited to flames with relatively fast chemistry.
- The model cannot capture deep non-equilibrium effects such as ignition, extinction, and slow chemistry (like NOx).

The EDC combustion model has the following advantages and disadvantages:

- The combustion rate includes detailed chemical mechanisms in turbulent flows.
- Capability to predict lift-off, blow-off of turbulent flames and under-ventilated fire regimes.
- The only disadvantage of the EDC model is its computational expense.

3.2.3 Physical and numerical requirements to models (UU)

The models and examples of applications for hydrogen fires described in this section refer to their 3D formulation. The requirements for the simulation of hydrogen fires outlined are outlined as follows.

Due to its infinitely fast reaction rate assumption, the EBU combustion model can be applied to cases where this phenomenon has no significance, e.g. micro flames.

For the scenario with an impingement jet as stated in (Z. Li et al., 2015) a tetrahedral mesh would not be suitable from the perspective of the gradient calculations comprising large velocity gradients. A major disadvantage of tetrahedral meshes is that tetrahedral control volumes have only four neighbours, so computing gradients can be problematic because neighbouring nodes may all lie in nearly one plane, making it impossible to evaluate the gradient in the direction normal to that plane. As a result, the calculation will have “preferential” diffusion directions. To overcome this problem, a polyhedra grid may be applied in the simulation because they have more than four neighbours, so gradients can be much better approximated.

The turbulence intensity of 25% and turbulence length scale equivalent to 7% of the equivalent diameter has been shown to provide the closest agreement with experimental observations for the hydrogen jet-flame using LES turbulence model with flamelet probability density function model for simulation of combustion.

The most promising and preferable model is the EDC model with detailed or reduced chemistry. It is able to reproduce under-ventilated fires i.e. self-extinction, external flames, re-ignition, lift-off and blow-off phenomenon.

3.3 Knowledge gaps (UU)

- Recent jet fire experiments within HyIndoor project described in deliverable D 4.4 (HyIndoor, 2014) have shown the strong influence of steam condensation. Very low under-pressures (up to -100 mbar) lead to collapse of the enclosure. Numerical simulation of hydrogen jet fires taking into account condensation effects are an important consideration in all cases, especially for indoor fires.

- All the above mentioned simulations did not account for the effect of radiation, therefore, detailed and extensive CFD validation of radiation models applied for jet fires, and accumulating combustion products is needed.

- Investigation of buoyancy effect on a flame shape and wind effect on flame parameters.
- Heat transfer during impinging reacting jets to the pipeline infrastructure and storage vessels.
- Numerical prediction of pressure effects of free jet fires (delayed ignition).
- Pressure effects of indoor jet fires – pressure peaking phenomenon for reacting jets (PPP). The key issue to be addressed is the limit of mass flow rate from a pressure relief device that will not destroy civil structures.
- Effect of jet attachment on flame length and separation distance.
- The safe design of high pressure releases through flu pipes.
- Numerical simulations and model validation of indoor fires re-ignition.
- Indoor fires in an enclosure with multiple vents, effect of vent orientation, position and shape on a fire regime.
- Very limited study on how thermally activated pressure relief device TPRD nozzle shape affects the flame length.
- Simulations to reproduce blow-off, lift-off, and blow-out phenomena to support the development of new TPRDs.

4 Deflagrations (Author: UU, Reviewer: AREVA)

4.1 Models (UU)

Turbulence and combustion models are necessary as it is currently unfeasible to directly capture every scale of motion. Therefore, as there are unsteady (turbulent) motions which affect the flow that cannot be resolved directly, such motions must be modelled. In some cases, the turbulence model selected can have a huge effect on the results obtained from CFD. This disparity in results is due to the various strengths and weaknesses of the models which can be applied. Depending on the scenario under investigation, different models are more appropriate than others, with each model having different applicability windows and limitations for use.

As introduced in Section 4.2 of Deliverable 2.1 (State of the art review concerning FCH technologies) there are different major classes of models that can be applied, each with different levels of complexity. Turbulence models are generally classified according to which governing equations they apply to, for example to Reynolds-averaged Navier-Stokes (RANS) or Large Eddy Simulation (LES) equation sets. Furthermore, within these rather broad categories, turbulence models can be additionally broken down by the number of additional transport equations that are solved in order to compute the model contributions. Various combustion models are commonly implemented, alongside these turbulence models, in order to simulate hydrogen deflagrations. A selection of the most widely used models to solve deflagration problems are outlined below in Section 4.2. It should be noted that the models described below are tailored to be used on large scale real-world scenarios.

4.2 Comparison of models and requirements (UU)

4.2.1 Modified Eddy Dissipation combustion model

- Combustion model: Eddy dissipation concept model
- Turbulence model: $k - \varepsilon$ (standard):
    - Only one turbulent and one combustion model available
- Type of solver and pressure-velocity coupling:
    - Finite volume solver, Roe's approximate Riemann Solver (Roe, 1981)– Flux-vector splitting type solver
- Discretisation scheme:
    - Convection terms: 2nd order Roe solver
    - Diffusion terms: 2nd order central difference
    - Temporal terms: 1st order Euler explicit method
- Grid: 3D unstructured tetrahedral, adaptive grid
    - For example in the simulations performed in Makarov et al. (Makarov et al., 2009) the initial computational mesh varied between 0.05 and 1 m within and around the structure of the refuelling station explosion being simulated. Grid refinement criteria based on a designated temperature and pressure range, with the average mesh resolution within the refinement regions being about $\Delta x \approx 0.12\ m$.
    - Parallelisable

- Time step requirements: CFL<1

4.2.2 Multi-phenomena deflagration model

- Combustion model: Customised premixed combustion model
    - Multi-phenomena turbulent burning velocity model (Molkov, 2009)
- Turbulence model: LES
- Type of solver and pressure-velocity coupling:
    - Finite volume explicit coupled solver, density-based pressure-velocity coupling
    - Density is determined based on the continuity equation
    - Pressure field is calculated from the equation of state
- Discretisation scheme:
    - Convection terms: 2nd order upwind
    - Diffusion terms: 2nd order central difference
    - Temporal terms: 1st order explicit linearisation
- Grid: 3D unstructured tetrahedral grid
- Time step requirements: CFL = 0.8

4.2.3 COM3D model

- COM3D similar to CREBCOM (Efimenko and Dorofeev, 2001)
    - COM3D multi-component chemical model with enthalpies and heat capacities as polynomial fits of JANF tables
- Combustion model:
    - CREBCOM model for flame tracking
        - Contains adjustable parameter C_f, governing the rate of chemical interaction and therefore visible flame speed
    - KYLCOM model (Yanez et al., 2010)
        - Model is based on the combination of “phenomenological” equations providing the flame velocity as a function of some characteristics of the reactive mixture and a “forest fire” algorithm
- Turbulence model:
    - $k-\varepsilon$ (standard) (B.E. Launder and Spalding, 1974b)
    - Eddy Viscosity LES
- Type of solver and pressure-velocity coupling:
    - Finite differences
    - Fully compressible solver
    - SIMPLE
    - Hydrodynamic solver coupled with the turbulence and chemical kinetics models

  - Euler equations used to model the process
- Discretisation scheme:
  - Convection terms: Ami Haarten, TVD 2nd order, non-oscillative
  - Diffusion terms: 2nd order central difference
  - Temporal terms: 1st order explicit
- Grid: Cubic structured
- Time step requirements: CFL < 1 (≈ 0.9)
- Turbulent burning velocity:
  - Constant when using Standard $k - \varepsilon$ model
  - S_t calculated using Kawanabe correlation (Lipatnikov and Chomiak, 2002) when using Eddy Viscosity LES

4.2.4 "b0b" model

- Combustion model: "Forest fire" model
  - CREBCOM model for flame tracking (Efimenko and Dorofeev, 2001)
  - Constant turbulent burning velocity
- Turbulence model: Inviscid fluid
- Type of solver and pressure-velocity coupling:
  - 3D Eulerian explicit solver
- Discretisation scheme:
  - Convection terms: 1st order upwind
  - Diffusion terms: 2nd order central difference
  - Temporal terms: 1st order
  - Pressure gradients: Central difference
- Grid: Cartesian structured
- Time step requirements: CFL < 1

4.2.5 Equilibrium combustion model

- Combustion model: Equilibrium combustion model
- Turbulence model: Empirical
- Type of solver and pressure-velocity coupling:
  - Numerical integration of the set of four nonlinear ODE using 4th order Runge-Kutta method
- Discretisation scheme:
  - No discretisation scheme
  - Quasi-dimensional flame propagation
- Quasi-dimensional model, spherical flame propagation from the ignitor

- Time step requirements: Time step control by truncation error

4.2.6 "β-transformed" gradient method

- Combustion model: "β-transformed" gradient method for flame tracking (Arntzen, 1998)
    - β-flame model solves a linear differential equation to control the flame thickness (3-5 grid cells).
    - Reacting rate is based on one step model with burning velocity from flame-library.
- Turbulence model:
    - $k-\varepsilon$ (standard) (B.E. Launder and Spalding, 1974b)
    - Additionally, with turbulence generation terms from subgrid geometry (Arntzen, 1998), also can include porosity terms for sub-grid obstacles
- Type of solver and pressure-velocity coupling:
    - Finite volume solver,
    - SIMPLE pressure correction (pressure-velocity coupling)
- Discretisation scheme:
    - Convection terms:
        - 1st order Power law
        - 2nd order mixed (weighting between upwind and central difference)
    - Diffusion terms: 2nd order central difference
    - Temporal terms: 1st order / backward Euler
- Grid: Cartesian structured
- Turbulent burning velocity based on:
    - Bray's correlation (Bray, 1990)
    - Gülder (Gülder, 1991)
- Solves the Reynolds Averaged Navier-Stokes (RANS) equations
- Time step requirements:
    - CFLC = 5 (uses local speed of sound as a characteristic velocity), CFLV = 0.5 (uses local gas velocity)
    - "Adaptive to solution" approach has also been implemented, meaning the user has no access to settings

4.2.7 OpenFOAM: XiFOAM based vented deflagration model

- Numerical simulations performed using a custom solver built using the OpenFOAM CFD toolbox (Weller et al., 1998b)
- Combustion model:
    - Based on a modified form of the Weller Flamelet Combustion model (Weller et al., 1998a), which solves a transport equation for a regress combustion variable, b
- Turbulence model:

- One-equation eddy viscosity model was used for sub-grid scale turbulence (Fureby et al., 1997)

- Type of solver and pressure-velocity coupling:
  - Fully compressible Pressure-Implicit Splitting of Operators (PISO) solution method (Issa, 1986)

- Discretisation scheme:
  - Second order discretisation schemes were used
  - Central differencing for velocity
  - Bounded TVD scheme for scalars
  - Backward differencing scheme in time

- Grid: Solver uses finite volume numeric to solve systems of partial differential equations built on 3D unstructured meshes of polyhedral cells. Model can also be used on a structured grid.
- Code is based on a Large Eddy Simulation (LES) solver of the Navier-Stokes conservation equations for mass, momentum and energy

4.3 Critical Analysis (UU)

The key advantage of the Modified Eddy Dissipation combustion model is it's extreme simplicity (Wilkening and Huld, 1999). However when using this model it must be considered that many important physical effects are left out. For example, as the chemical source terms depend on the turbulence quantities they are undefined in the limit of laminar flow. Additionally, combustion rate is limited by the turbulent mixing rate, ignoring any effect of chemical kinetics. At the other end of the combustion spectrum, detonations are not well modelled as they depend strongly on adiabatic compression at the detonation front, where the rate of combustion rises rapidly due to the increase in temperature and pressure. This model is not able to take this into account (Wilkening and Huld, 1999).

This modelling approach does not include any heat transfer modelling in the computations. Since the combustion process is slow, this can affect the behaviour of the flame and pressure, leading to over-prediction of the highest overpressures and also to not showing the typical decrease of pressure with time after the end of the combustion process (Breitung et al., 2005). In this study (Breitung et al., 2005) the highest overpressures were calculated by models that did not include any heat transfer modelling. Using this model however, dissociation effects can be included using an approximate approach that accounts for not all the chemical energy available in the mixture being converted into an increase in temperature. For example to obtain the correct adiabatic temperature, the calorific value can be decreased. Such a procedure was implemented in Baraldi et al. (Baraldi et al., 2009) during the simulation of hydrogen deflagrations involving pressure relief vents. Finally, a key objective of applied modelling approaches is to use the same model, without the need for additional changes or 'tuning', to reproduce and predict different scenarios. In using this modelling approach, during the simulation of hydrogen deflagrations including pressure relief vents (Baraldi et al., 2010) it was not possible to achieve the same level of accuracy of results for the two vented cases, keeping constant the initial parameters of the code for both simulations.

As stated in Section 4.2.1, the Modified Eddy Dissipation combustion model utilises the standard $k-\varepsilon$ model therefore the strengths and weaknesses of this model must also be taken into account.

The $k-\varepsilon$ model is relatively simple to implement, leads to stable calculations that converge relatively easily and provides reasonable predictions for a wide variety of flows. However due to the Reynolds hypothesis, the $k-\varepsilon$ model has some deficiencies (Mohammadi and Pironneau, 1993). There is an inaccurate prediction of normal Reynolds stress anisotropies. The model is not able to distinguish between strain and shear, meaning that the turbulence in flows against a perpendicular wall (such as an upstream obstacle) can be overestimated. Additionally, there is poor prediction of swirling and rotating flows, flows with strong separation, axisymmetric flows, certain unconfined flows, and fully developed flows in non-circular ducts. As the reacting rate is strongly dependent on the ratio of the turbulence quantities ε/κ, any deficiency of the turbulent model has a direct impact on the reaction rate, leading to inaccurate simulation results. For example in simulations undertaken in (Makarov et al., 2009) a large discrepancy with the experimental data was recorded in regions where combustion was affected by flow around and underneath the car in the calculation domain of this particular experimental analysis. For this particular case the model over-predicted the maximum pressure behind the car, particularly when compared to models that did not utilise the $k-\varepsilon$ model. The standard $k-\varepsilon$ model is realistically only valid for fully turbulent flows, thereby meaning it has problems with transient flows. For example in (Baraldi et al., 2009), involving the simulation of hydrogen deflagrations in a tunnel, this modelling approach wasn't successful in modelling the initial laminar regime of the propagation of the flame.

Considering the multi-phenomena deflagration model, by using the gradient method the integral of the source term through the numerical flame front thickness gives the same mass burning rate per unit flame surface area, $\rho_u S_t$, independent of the number and size of cells in the numerical front. This means that the calculation of the turbulent burning velocity can be decoupled from the numerical mesh. The numerical flame thickness typically spreads through three to five cells. As this model has been designed to tackle real-world problems with scales of tens to hundreds of metres, there is clearly no chance of resolving the whole structure of the real turbulent flame front (scales of the order of millimetre). However, this model is still able to reasonably reproduce the hydrodynamics of flows ahead of and behind the numerical front, and also capture overall flame propagation and explosion pressure dynamics. This is due to the energy release in the flame front being kept physically correct. This combustion model uses an adapted form of Yakhot's formula for turbulent burning velocity to compute the mass burning rate, meaning at the laminar limit ($u'=0$), the equation yields: $S_T = S_u$. Therefore it accounts for the transition from laminar to fully turbulent flow, meaning the model can be used to accurately predict flows involving both laminar and turbulent regions. Additionally the value of u' in RNG increases with mesh size. This can compensate for the increase in unresolved fraction of flow turbulence. However it must be considered that flow anisotropy can strongly affect the SGS flame front area. The larger the mesh size the stronger the anisotropy effect on the modelling of turbulent burning velocity. The model also assumes that the mixture is initially quiescent, meaning larger scales and lower turbulence intensities. Currently the model, which is under continuous development, does not account for heat transfer.

This model accounts for the increase in the flame front area due to the turbulence generated by the flame front itself, Ξ_K, following the analysis by Karlovitz (Karlovitz et al., 1951). The equation, contained in the model, which accounts for this phenomenon contains two changeable parameters, R_0 (characteristic flame radius for transition from laminar to fully turbulent flame) and ψ (empirical coefficient indicating how closely to the maximum value of the Karlovitz wrinkling factor, Ξ_K is allowed to reach). Recent efforts have been made to make the selection of these values automatic

within the model. Correlations describing how these parameters change with hydrogen mole fraction have been recently published (Molkov and Bragin, 2015).

The multi-phenomena deflagration model is designed to run on LES, therefore depending on computational power, simulations may take a substantial amount of time to run. As stated in Section 4.2.2, the multi-phenomena deflagration model utilises the RNG LES model therefore the strengths and weaknesses of this model must also be taken into account. As stated above this model is capable of reproducing not only turbulent, but also transitional and laminar flows. At low Reynolds numbers the effective viscosity becomes equal to the molecular viscosity. This therefore allows the model to perform better in the vicinity of walls. In highly turbulent regions of flow the RNG model reduces to the Smagorinsky model and in laminar flow regions the model is able to recover molecular viscosity. However, as it is an LES model it is more computationally expensive than RANS models. Additionally if considering unsteady simulations, small time steps will be required, this will result in long run times and large volumes of data. A higher grid resolution is commonly required and the approach is only suitable to transient 3D calculations.

The COM3D code is a 3D CFD code to describe turbulent combustion phenomena in complex geometries. At the initial stage of simulations the combustion model omits variations in burning rate and uses its maximum value achievable throughout the combustion process. This can result in a conservative estimate of pressures and pressure loads. Using $k-\varepsilon$ (standard) burning velocity is fixed. Using the LES approach the burning velocity is calculated by firstly considering it to be constant (to avoid flame acceleration) and then it is calculated according to the Kawanabe experimental correlation: $S_t = S_u(1 + 1.25(u'/S_u)^{0.7})$. Finally, this modelling approach includes heat losses; however accuracy is dependent on the quality of the mesh. If the mesh is too course the model may underestimate the heat losses (Baraldi et al., 2009). When implementing this model it must be considered that the applicability of the KYLCOM model (Yanez et al., 2010) is restricted to structured cubic grids. The model is limited by the assumptions made in the turbulent flame speed correlation employed and does not allow for the effects of flame wrinkling due to instabilities. Additionally, the capabilities of the KYLCOM model to correctly predict the transition from laminar to the turbulent regime is dependent on the ability of the turbulence model employed.

Considering the in-house code b0b, the Euler equations are solved (rather than the Navier-Stokes equation set) and therefore no viscous effects are modelled. Only the large turbulence scales can be captured by the mesh while the sub-grid turbulence scales are neglected. Turbulence is not included explicitly in the combustion model. Using this model, burning rate may be defined explicitly on the basis of appropriate experimental data, or using a model, which requires additional assumptions and is therefore less accurate. If this modelling approach is implemented, the combustion front propagates with maximum velocity from the moment of ignition. Therefore flame propagation velocity is overestimated at the early stages of combustion as the flame is unobstructed and should propagate in a quasi-laminar regime. This approach is therefore not designed to predict the correct pressure dynamics with time. However, if the maximum burning velocity is estimated properly, this method can provide the correct maximum overpressure and pressure loads. A unique feature of this combustion model is that the flame speed, and therefore the hydrogen consumption rate, does not depend on turbulence. Finally, heat losses are taken into account, by means of a simple empirical expression, as a function of local flow velocity and temperature in each control volume. This approach does not require a finer mesh at the walls.

The Equilibrium model contains a number of assumptions:

- The combustible mixture of ideal gases is premixed, quiescent and uniform,
- Ignition occurs at a point source of negligible energy and volume,
- The burned gas behaves as an ideal gas,
- The flow field is divided into two zones:
    - A burned zone with combustion products
    - An unburned zone with fresh mixture,
- The two zones are separated by an infinitely thin, smooth flame of spherical symmetry that propagates outwards from the point of ignition,
- The flame speed is low (relative to sound speed),
- All compression and expansion processes of unburned and burned gases are isentropic,
- The properties of burned and unburned gases are spatially uniform,
- The burned gas mixture is at chemical equilibrium,
- The influence of turbulence on combustion is included by the use of empirical relations (Maisey, 1965),
- Heat transfer to the wall is included following Tanaka (Tanaka, 1986)

Additionally, this model is highly sensitive to one input parameter, namely the turbulence intensification coefficient. This coefficient takes into account the effect of turbulence on flame speed. For example during the simulation of hydrogen deflagrations with pressure relief vents (Baraldi et al., 2010) increasing this parameter by about 10% produced an approximately 25% increase in the maximum pressure peak.

Using the "β-transformed" gradient method to simulate a vehicle refuelling environment (Makarov et al., 2009) consistently led to over-prediction of the maximum overpressure and pressure rise rate. It was concluded that the major reason for this over-prediction was the numerical grid. This over-prediction was increased when considering a mesh in which the dispensers were fitted between CVs and only partially occupied them. This was due to the code introducing porosity to those particular CVs, leading to additional turbulence. When the input flame thickness is smaller than the minimum reacting zone, the burning velocities from simulations will be overestimated, since the burning velocity is proportional with the reaction zone thickness. For flame thicknesses less than about 3Δ the flame is not properly resolved and the burning velocity increases, since the flame is thicker than what is assumed by the resolved β-model. If the flame becomes thicker the burning velocity will be too large and if it becomes thinner it will be too small. The ability of the β-flame to propagate with any given burning velocity has been investigated. It has been shown to perform well as long as the time steps were not too long, compared with the ratio flow velocity to grid size. The β-flame needs a resolution in both time and space to keep the numerical diffusion under control and keep the flame thickness constant. The β-flame responds well to transient burning velocities in a transient turbulence field (Popat et al., 1996). Another advantage of this model is that both laminar and turbulent burning can be modelled within the same model, when the burning velocity is a function of known variables. In flame propagation towards walls, the flame becomes thinner until it is one grid cell thick. A compensation model near walls is needed to keep the burning velocity high enough.

Flame propagation is affected by the curvature of the flame. The reaction zone is located around one grid cell behind the centre of the flame. For small flame radii the reaction zone area is therefore much smaller than the flame area. This can be compensated when the flame radius is known.

4.4 Physical and numerical requirements to models (UU)

Considering the Modified Eddy Dissipation combustion model this model is based on an Eddy-Dissipation Concept (EDC) model (Hjertager, 1982) (Hjertager, 1993a) (Hjertager, 1993b) (Magnussen and Hjertager, 1976). The model returns values of the mass burning rate, which is considered as a function of the inverse of the integral turbulent time scale. It was developed in order to capture the propagation of the flame in the turbulent combustion regime, assuming fast chemistry the burning rate is controlled mainly by the turbulent motion. The basis of this model is the assumption that chemical time scales are much smaller than the time scales for the turbulence, i.e. $\tau_{ch} \ll \tau_{tu}$. In regions where this is the case, the chemical reaction rate is governed only by the rate of mixing of the chemical reactions (Wilkening and Huld, 1999).

As the name suggests a number of modifications have been to the Modified Eddy Dissipation combustion model, the first of which accounts for the possibility of flame extinction in cases where the chemical time scale is much larger than the turbulent time scale (Hjertager, 1993b). Additionally, multiplication of the original expression of the burning rate by the Said-Borghi factor (Saïd and Borghi, 1989) has been added. This factor takes into account the influence of the non-dimensional quantity $k^{0.5}/S_{lam}$, which plays a role in what is called the "wrinkled flame" regime only. The laminar flame speed S_{lam} depends on the local hydrogen concentration. In calculations it has been assumed to vary with concentration using a polynomial equation fitted from published data (Koroll et al., 1993). The RANS equations are solved and the turbulence closure is achieved using the standard $k-\varepsilon$ model (B.E. Launder and Spalding, 1974b). The turbulent timescale is estimated as $\tau_{tu} = \kappa/\varepsilon$ and the chemical timescale τ_{ch} is described by the Arrhenius-based expression (Hjertager, 1993b). Finally, validation of the model has been performed by Hjertager and co-workers (Hjertager, 1993b) (Hjertager and Solberg, 1999). Numerous examples of how the model performed against different experimental scenarios have been undertaken including: (Makarov et al., 2009) (Baraldi et al., 2009) (Breitung et al., 2005) (Wilkening and Huld, 1999) (Troyer et al., 2005a) (Bielert et al., 2001) (Baraldi et al., 2003) (Gallego et al., 2005) (Huld et al., 1996) (Baraldi et al., 2010) (Garcia et al., 2010) (Makarov et al., 2010) (Venetsanos et al., 2007) (Baraldi et al., 2007) (Troyer et al., 2005b).

Considering the multi-phenomena deflagration model the turbulence model implemented is based on the Renormalisation Group Analysis (RNG) sub-grid scale turbulence model (Yakhot and Orszag, 1986b). Flame propagation is modelled using the progress variable equation. The source term in the energy equation is the heat release rate due to combustion. The mass burning rate (i.e. the source term in the progress variable equation) is calculated using the gradient method: $\dot{m} = \rho_u \times S_T \times \nabla c$, where $\rho_u =$ density of the combustible mixture, $S_T =$ turbulent burning velocity and $c =$ progress variable. The combustion model implemented is adopted from Yakhot's formula for turbulence burning velocity to compute the mass burning rate (Yakhot, 1988): $S_T = S_u \times exp(u'/S_T)^2, u' =$ sub-grid scale velocity (Pope, 2000) and $S_u =$ laminar burning velocity. At the laminar limit ($u' = 0$), the equation yields: $S_T = S_u$.

The multi-phenomena deflagration model accounts for the increase in the flame front area due to the turbulence generated by the flame front itself, Ξ_K, following the analysis by Karlovitz (Karlovitz et

al., 1951). For a particular mixture composition, there is a curvature radius with maximum burning rate, meaning flamelets with such curvature will lead the propagation of the turbulent flame. Zimont and Lipatnikov (Zimont and Lipatnikov, 1995) proposed a leading point coefficient, Ξ_{lp}, associated with this mechanism, by determining the hydrogen concentration at the leading points and using linear interpolation of the experimental data published by Kuznetsov and Sabel'nikov (Kuznetsov and Sabel'nikov, 1990) to calculate the corresponding values of burning velocity. According to the observation reported by Gostintsev et al. (Gostintsev et al., 1988) the transition to fully, developed, or self-similar, turbulent regime of flame propagation for stoichiometric hydrogen-air mixture is accomplished at a radius of $R = 1.0 - 1.2\,m$. Beyond this critical radius, chosen as $R = 1.2\,m$, the growth of the unresolved SGS flame surface area is based on the fractals theory. To account for the increase if the turbulent flame surface area due to Fractals, Ξ_f, as outlined by Gouldin (Gouldin, 1987) the flame surface area of an outwardly propagating turbulent flame will grow faster than a spherical flame. The equation describing this growth can be written as: $A_T \approx \varepsilon^{2-D} \times R^D$, $A_T =$ turbulent surface area, $\varepsilon =$ one length scale (inner cut-off), $\mathrm{R} =$ another length scale (outer cut-off), $\mathrm{D} =$ fractal dimension, defined as a measure of the degree of wrinkling and fragmentation of then flame front (Mantzaras, 1992). The equation describing the change in D was formalised by North and Santivicca (North and Santivicca, 1990). Following the inclusion of these different phenomena the equation for turbulent burning velocity is written as: $S_T = \left[S_u \times \Xi_K \times \Xi_{lp} \times \Xi_f\right] \times exp(u'/S_T)^2$. This model has recently been extended to account for Rayleigh-Taylor (RT) instability (Keenan et al., 2014). Numerous examples of how the model performed against different experimental scenarios have been undertaken including: (Makarov et al., 2009) (Gallego et al., 2005) (Molkov et al., 2006) (Molkov et al., 2007) (Baraldi et al., 2009) (Molkov et al., 2008) (Baraldi et al., 2010) (Keenan et al., 2014) (Xiao et al., 2012) (Makarov et al., 2010) (Verbecke et al., 2009) (Makarov et al., 2007). Finally, this modelling approach has proved to be readily transferrable between different codes and solvers. It is currently used by NCSR Demokritos, within their in-house CFD code 'ADREA-HF'. Comparisons of this version of the model with experimental results can be found in: (HyIndoor, 2013), (Tolias et al., 2015b), (Tolias et al., 2015a). It has been adapted for use with the OpenFOAM CFD toolbox. It is also used by Keio University in Japan (Tsujii et al., 2015). This emphasises the adaptability and versatility of this modelling approach.

Considering the XiFOAM based vented deflagration model, the transport of the regress variable is governed by a laminar burning velocity, S_L and a flame surface wrinkling factor, Ξ. In this model turbulent burning velocity is modelled as a product of the laminar burning velocity and the surface wrinkling factor. The calculation of turbulent burning velocity is based on the correlation by Bradley (Bradley et al., 1996). The coefficient used in the correlation was determined from (Bauwens et al., 2008). As it is unfeasible to resolve flame instabilities on large grids, a sub-grid model is implemented. This model includes a surface wrinkling factor due to turbulence and for vented deflagrations, that this model is primarily used to analyse, the model also includes the addition of Rayleigh-Taylor and Darrieus-Landau (hydrodynamic) instability. More detailed data on the basic properties of lean hydrogen flames is required for the development and validation of this modelling approach.

It should be noted that the developers of the XiFOAM based vented deflagration model have also developed their own in-house CFD model to account for RT instability. The models contained in both the multi-phenomena deflagration model and the XiFOAM based model solve an additional transport equation for the flame surface wrinkling due to RT instability and both utilise the same equation

describing amplitude growth, as defined in Zeldovich (Zeldovich et al., 1985). These models differ when considering the amplitude of the wrinkling, the XiFOAM based model, as described in (Bauwens et al., 2011), assumes that the amplitude of the wrinkling, A is much smaller than a quarter wavelength. Additionally, the initial estimates for the model constant, k_{RT} is obtained using high-resolution 2D simulations. In the XiFOAM based model the parameters G_{RT} and R_{RT} are therefore considered to be constant. The values of these parameters are calibrated using a subset of experimental data (Bauwens and Dorofeev, 2010). In the RT model added into the multi-phenomena deflagration model the amplitude of RT wrinkling is based on the experimental observations outlined in (Tsuruda and Hirano, 1987), leading to wavelength, and subsequently amplitude, being calculated depending on acceleration.

The COM3D code is a 3D CFD code to describe turbulent combustion phenomena in complex geometries. It uses a TVD-solver, two turbulence models (standard $k-\varepsilon$ and RNG $k-\varepsilon$), two chemistry models (Arrhenius for laminar and Eddy-Dissipation for turbulent combustion) and a multicomponent thermodynamic model which includes H2, O2, N2 and steam (Breitung et al., 1999). The hydrodynamic model considers mass, momentum and energy conservation (Breitung et al., 1999). The flame propagation algorithm assumes that combustion in a particular CV takes place when the neighbouring CV has burned out to some explicitly defined extent. This allows for the introduction of a user defined flame propagation speed. Burning rate is defined as: $\partial Y_f/\partial t = K_0/\Delta x$; where $Y_f =$ fuel mass fraction, $K_0 =$ burning rate constant, $t =$ time and $\Delta x =$ CV size. The combustion rate constant is a function of the turbulent burning velocity, S_t; $K_0 = S_t(E_i + 1)/4$ where $E_i =$ Expansion ratio of combustion products. The structure of the CREBCOM combustion model (Efimenko and Dorofeev, 2001) can be summarised as follows: for slow deflagrations, the selected criteria are the flammability limits as they can be used to determine mixture compositions that are able to support flame propagation. For fast deflagrations, the flame acceleration criteria are selected based on the mixture expansion ratio, σ. The CREBCOM model uses a simplified thermodynamic model in which the equation of state of an ideal gas is applied to the mixture of gases with constant heat capacities. The KYLCOM model (Yanez et al., 2010) is based on the solution of a transport equation for the progress variable f, a normalised burned out mixture fraction.

It should be noted that the in-house code b0b (Efimenko and Dorofeev, 2001) is based on the same flame propagation and combustion models as implemented by the COM3D model. To supplement this model, empirical correlations over a wide range of mixture compositions and scales are provided in (Efimenko and Dorofeev, 2001).

The Equilibrium combustion model is based on a simple two-zone mathematical model for the prediction of the pressure and temperature changes during a totally confined or vented gaseous explosion. The model is based on conservation equations of mass, momentum and energy with equilibrium calculations of the physical and chemical properties of combustion products.

The "β-transformed" gradient method is based on finite-volume discretisation and the SIMPLE-similar method for pressure-velocity coupling. This code suggests a time step dependent on problem formulation and laminar burning velocity for a chosen mixture. The user can also decrease the suggested time step further. It uses a standard $k-\varepsilon$ model (B.E. Launder and Spalding, 1974b) for modelling turbulence. Turbulence generation terms from subgrid geometry and the "β-transformed" gradient method for flame tracking are adopted (Arntzen, 1998). The burning velocity of the flame relative to the premixed reactants (S_u) is calculated as the maximum value between the turbulent

burning velocity and the quasi-laminar burning velocity, S_L. This calculation takes into account the effects of flame radius and flame wrinkling as a function of fuel type and fuel concentration. An expression for the turbulent burning velocity based on Bray's correlation (Bray, 1990) or Gulder (Gülder, 1991) has been implemented. The transition between quasi-laminar and turbulent flame regime is based on the local conditions of the flow and mixture. It does not depend on space or time. The mass burning rate is found from the expression based on the one-dimensional analytical solution for flame front propagation.

4.5 Knowledge gaps (UU)

As described previously in Section 4 there are so many different models to choose from that no single code can fulfil all requirements. As a result, when choosing a model for a particular application, the user will be constrained by the particular solver being implemented. Therefore it is essential to match up the physics of the particular application under consideration with the available models. For example, what flow features are likely to be present? What will have the most impact on the scenario? Etc. The SUSANA consortium will produce a CFD model evaluation protocol to aid users to make the most suitable choice.

However, a number of knowledge gaps must still be addressed when considering deflagration scenarios, these include:

- Currently a single physical model and numerical tool that can cover the entire range of phenomena, accounting for flame acceleration and propagation does not yet exist. In the majority of cases the range of applicability of many models is limited to or geared towards a specific flow phenomenon or scenario.

- Experimentally a number of parameters require further investigated, including laminar burning velocities for all ranges of pressure, temperature and equivalence ratio. Additionally more detailed experimental data on the basic properties of lean hydrogen flames is required.

- The effect of thermos-diffusive instabilities, flame stretch and curvature on flame speed is not completely understood, including how these interact with and influence other mechanisms which affect burning rate.

- Using physical models to represent unresolved small-scale geometries, without for example introducing porosity which leads to additional turbulence and therefore simulation over-prediction.

- The multi-phenomena combustion models under development must also take into account mechanisms beyond the interaction between flow turbulence and combustion. For example, they must be further developed to include anisotropic effects, flame instabilities (i.e. acoustics, Rayleigh-Taylor instability, Kelvin-Helmholtz instability, Richtmyer-Meshkow instability, Landau-Darrius instability, etc.), as well as their effect on flame dynamics.

- Dynamics and physical models which allow for the capture of coherent deflagrations (i.e. the parallel development of internal and external deflagrations).

- The effect of inertial vent covers on explosion dynamics, including the simulation of Deflagration-To-Detonation Transition (DDT).
- Modelling partially premixed flames in hydrogen-air layers and their pressure effects in enclosed spaces. Additionally, understanding the influence of ignition time and location on the resulting overpressures.
- Capturing deflagration strength mitigation measures using CFD, e.g. water mitigation systems such as water spray or mist.
- Undertaking simulations and validations in real-scale configurations containing real and varied objects and obstacles, and considering complex geometries.
- The full disclosure and scientific explanation of any model coefficients that must be changed depending on the scenario under investigation. Such 'tuning' parameters are often contained in models, and not fully explained, in order to artificially increase the applicability window of a given model.
- Large scale deflagration scenarios are often undertaken using Large Eddy Simulations (LES) or Very Large Eddy Simulations (VLES). Such simulations are computationally exhaustive. Such modelling approaches must be made practically useable when considering the availability of only limited computational resources.

5 Detonations (Author: KIT, Reviewer: JRC)

5.1 Introduction

Among all accident scenarios detonation is considered often as the 'worst case' scenario, therefore, in safety analysis detonation modelling should be considered as a 'must have' model.

The mechanisms for the detonation onset are multiple, but in principle they could be classified into two major groups: a) Direct initiation trough an ignition with a high energy source (spark, explosive); b) Deflagration-to-Detonation Transition (DDT) process.

The mathematical description of the detonation should include the propagation mechanism which consists of a shock wave plus a chemical reaction complex resulting in the temperature rise needed for the reaction initiation. The temperature increase is purely due to pressure compression, unlike in the deflagration process where the heat and species transfer play the main role. This results in a super-sonic combustion wave characterized by the propagation velocity of the detonation D_{CJ}.

The detonation modelling includes distinct and multidisciplinary topics such a fluid mechanics modelling, chemical modelling, numerics, etc. We devote the following sections to this differentiate topics.

5.2 Comparison of models and requirements

5.2.1 Comparison of models

Modern *Detonation Modelling* starts in late 70's and 80's with the seminal works by Oran & Boris (e.g. (Oran and Boris, 1987)) and Fujiwara (e.g. (Taki and Fujiwara, 1978)) and it has been continued by many other authors in the following years.

Detonation modelling should not be interpreted in a restrictive manner, reducing the topic to the selection of a more or less accurate expression for the chemical consumption rate. Other topics of significant importance should be discussed in a more global interpretation, as discussed below

One of the first choices that should be selected is whether the full Navier-Stokes equations or just the Euler equations will be utilized for the modelling. Euler equations are the governing equations for inviscid flows. They correspond to the Navier–Stokes equations (Landau and Lifshitz, 1987) without the viscosity and heat conduction terms. Based on the conservation of mass, momentum, energy and species, the equations are:

$$(\rho)_t + (\rho u_j)_{x_j} = 0 \qquad \text{Equ 5-1}$$

$$(\rho u_j)_t + (\rho u_i u_j)_{x_j} = \rho g_j - p_{x_j} \qquad \text{Equ 5-2}$$

$$(\rho e)_t + ((\rho e + p)u_j)_{x_j} = \rho g_j u_j \qquad \text{Equ 5-3}$$

$$(\rho Y_\alpha)_t + (\rho Y_\alpha u_j)_{x_j} = \omega_\alpha \qquad \text{Equ 5-4}$$

Certainly, the different timescales between the propagation of the detonation wave and the diffusion process suggest the use of the Euler equations exclusively (Oran et al., 1998). Other authors consider the detonation process as a part of the flame acceleration process, and try to simulate the whole physical process, including the *Deflagration to Detonation Transition*, and thus utilize the same model for the deflagration and the detonation propagation. Certainly, this will require the use of the Navier–Stokes equations (e.g. (Zbikowski et al., 2008) utilizes the Zimont model (Zimont, 1977) for the detonation with the corresponding detonation velocity for the propagation of the combustion wave inside of frames of Navier–Stokes equations modeling).

The selection of the numerical scheme is also relevant for the positive outcome of the simulations. A very significant amount of literature has been dedicated to this topic, e.g. (Hussaini et al., 1997) or the very classic (Oran and Boris, 1987). During the last decades the schemes, TVD (Harten, 1997), Godunov (Quirk, 1994), ENO (Harten et al., 1987), have been mostly used e.g. (Uemura et al., 2013) (Bédard-Tremblay et al., 2009).

We focus hereafter mainly on the modelling of the chemical consumption rate ω_α. Models for this variable should provide the correct pressure, the correct speed, the correct wave structure, and thus impulse independent on time and space stepping. The selection of the chemical reaction model should also consider when necessary the stiffness of the chemical reaction equations (Westbrook, 1982) (Young and Boris, 1977). Several possibilities appear as feasible (Kuo, 2005) depending of the required level of details, the goals of the simulation, etc.

Those possibilities are:

- Single step chemical reaction (Williams et al., 1996);
- A reduced mechanisms: multi-step approximation with different degree of accuracy, e.g. (Boivin et al., 2011);
- Intrinsic Low-Dimensional Manifolds (ILDM) method (Maas and Pope, 1994);
- Detailed chemical scheme (Oran et al., 1998).

In this document, we separate Detonation from Deflagration to Detonation Transition (DDT). The study of DDT is an active field of scientific research and as such will not be addressed within the scope of this document. For an interesting review of Deflagration to Detonation Transition the reader is directed to Ciccarelli and Dorofeev (Ciccarelli and Dorofeev, 2008).

In this document, we describe the following models for the fuel consumption rate that appear to be especially suited for our purposes: the one-step Arrhenius chemistry and the Heaviside model.

5.2.1.1 One-step Arrhenius law

The Arrhenius Detonation model (W. Breitung, 1999) is based on the formulation:

$$k = K_{ch} e^{-\frac{E_{ch}}{T}} \qquad \text{Equ 5-5}$$

in which *k* is the rate of chemical reactions constant, K_{ch} is the pre-exponential factor, E_{ch} is energy of activation in divided by universal gas constant R. With this assumption, the consumption of the species, i.e. fuel, could be specified as:

$$\Delta y_{H_2} = \Delta t \cdot y_{H_2} K_{ch} \cdot e^{-\frac{E_{ch}}{T}} \qquad \text{Equ 5-6}$$

Note that, with the utilization of this model, the reaction zone must be resolved. That means that several cells must be placed inside of it. This is a limitation of the Arrhenius formula for the numerical simulation of detonation, because, if the cell size of the domain is not small enough, the reaction zone may not be well resolved and the results become invalid.

Nevertheless it is possible to use this model for low resolution simulations by the simple means of modifying the values of the activation energy and the pre-exponential factor. The calibration of those values should be carried out, e.g. with a trial and error procedure mimicking the size of the detonation cell size. Information regarding activation energy could also be obtained from the experimental data, referring to ignition delay and the experimental conditions encountered e.g. reflected shock. The procedure is described in detail in (Zeldovich et al., 1985). In general it should be taken into account that an increase of activation energy would mean an increase in the irregularity of the pattern to the structure of cells that the simulation will deliver. With an increase of the pre-exponential factor the size of the cell size of the simulation becomes smaller and vice versa.

A modification of the model to take into account different reaction orders and e.g. dependence on the pressure could be also taken into account, implying a new tuning of the factors.

It must be underlined that the values of the activation energy and the pre-exponential factor obtained will be valid in a very limited range of the conditions (concentration, temperature, pressure) considered.

5.2.1.2 'Heaviside' detonation

The Heaviside Detonation model (J. Yáñez, 2011) is based on the fact that the Chapman-Jouguet parameters are independent of the chemical kinetics. By doing this it is assumed that chemical reaction is infinitively fast.

The Heaviside detonation model is a simplified model, specially designed for problems in which geometrical or computational constraints force the use of coarse grids and thus it is especially suited for worst-case scenario studies. Inspired by the Heaviside function, it is possible to define the consumption of fuel as:

$$\Delta y_{H_2} = 100 \cdot C_f \frac{\Delta t}{\Delta x} y_{H_2} \cdot R_r \qquad \text{Equ 5-7}$$

where C_f is a constant inside of this model that for H2-Air mixtures has been calibrated to be approximately. The model shows almost no influence of the C_f constant as the R_r factor works as a shocking capturing algorithm, defined as:

$$R_r = \begin{cases} 0 & T < T_0 \\ \dfrac{T - T_1}{T_1 - T_0} & T_0 < T < T_1 \\ 1 & T > T_1 \end{cases} \qquad \text{Equ 5-8}$$

where T_0 is the auto-ignition temperature (T_0=800 K) and T_1 is a temperature high enough to be representative of the products. After some trial an error, the value of T_1 for this model has been established at T_1=1700 K.

The consumption formula of this model has no real physical interpretation, it is just a mechanism to provide enough variation of the species and heat release to generate and maintain the detonation.

T_0 is supposed to simulate the auto-ignition temperature and it is set to a constant value, almost independent for all concentrations. Following the references in the literature, e.g. (Zabetakis, 1965), this temperature is almost independent of the chemical composition of the unburned gas for a given pressure and temperature. Data for the lower flammability limit (LFL), upper flammability limit (UFL) and self-ignition limit are shown in the figure below (M. Kuznetsov, 2008).

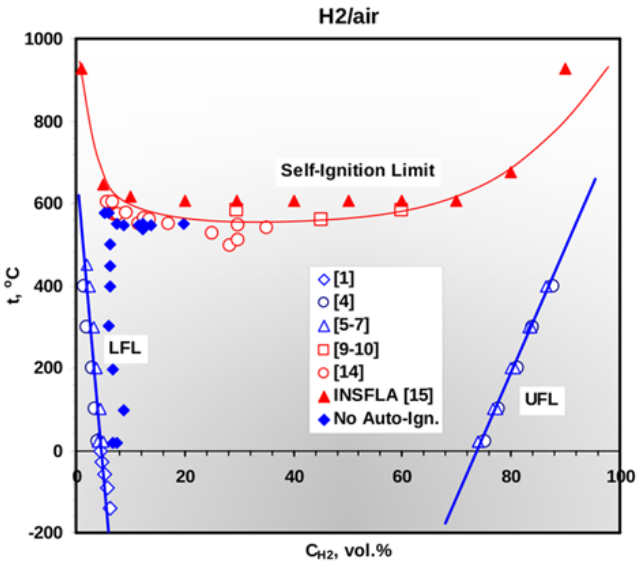

Figure 5-1 Low and upper flammability limits and auto-ignitions temperatures (M. Kuznetsov, 2008)

5.2.2 Physical and numerical requirements to models

The simplest theory to predict the behaviour of detonations in gases is known as Chapman-Jouguet (CJ) theory (Fickett and Davis, 2000), developed around the turn of the 20th century. This theory, described by a relatively simple set of algebraic equations, models the detonation as a propagating shock wave accompanied by exothermic heat release. Such a theory confines the chemistry and diffusive transport processes to an infinitely thin zone.

A more complex theory was advanced during World War II independently by Zel'dovich, von Neumann, and W. Doering. This theory, now known as ZND theory, admits finite-rate chemical reactions and thus describes a detonation as an infinitely thin shock wave followed by a zone of exothermic chemical reactions.

In the reference frame of the leading shock, the flow following behind the shock wave is subsonic, so that an acoustic reaction zone follows immediately behind the leading front until the Chapman-Jouguet conditions are reached. The ZND theory has been the object of numerous scientific publications where its detailed description, characteristics and limitations have been methodically discussed, e.g. (Fickett and Davis, 2000) (Schneider, 1977). A schematic comparison between S*imple* and ZND theory can be seen in Figure 5-2:

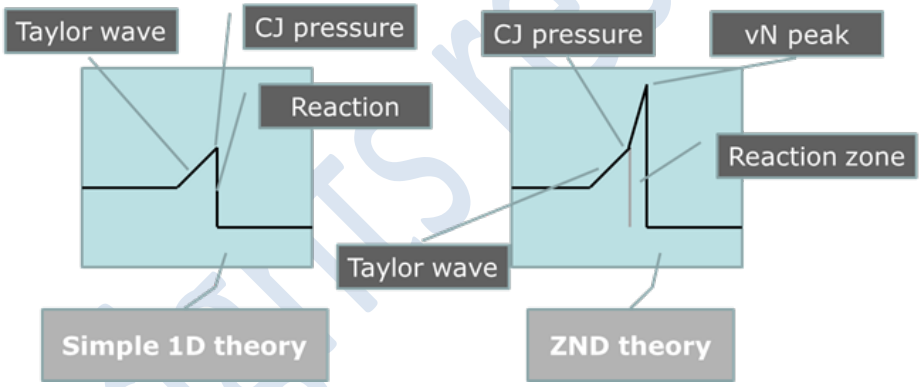

Figure 5-2 Schematic comparison of the Simple and ZND theory, CJ: Chapman-Jouet; vN: von Neumann peak

Most notably, these theories have allowed for the determination of the velocity and conditions of the von Neumann peak (Fickett and Davis, 2000). Those are:

$$D_{CJ} = \sqrt{0.5(\gamma_p - 1)\left((\gamma_p + 1)Q_{chem} + (\gamma_p + \gamma_r)T_0 C_v^r \mu_r\right)} + \sqrt{0.5(\gamma_p + 1)\left((\gamma_p - 1)Q_{chem} + (\gamma_p - \gamma_r)T_0 C_v^r \mu_r\right)} \approx \sqrt{2(\gamma_p^2 - 1)Q_{chem}} \quad \text{Equ 5-9}$$

$$P_{CJ} = P_0 \frac{(D^2 + (\gamma_r - 1)T_0 C_v^r \mu_r)}{(\gamma_p + 1)(\gamma_r - 1)T_0 C_v^r \mu_r} \quad \text{Equ 5-10}$$

$$P_{vN} = P_0\left(\frac{4(\gamma_p\gamma_r - 1)Q_{chem}}{(\gamma_p\gamma_r - 1)T_0 C_v^r \mu_r} - \frac{\gamma_r - 1}{\gamma_p - 1}\right)$$ Equ 5-11

$$\rho_{vN} = \rho_0 \frac{(\gamma_r - 1)p_0 + (\gamma_r + 1)P_{vN}}{(\gamma_r + 1)p_0 + (\gamma_r - 1)P_{vN}}$$ Equ 5-12

Both theories describe one-dimensional and steady wave fronts. However, in the 1960s, experiments (see Figure 5-3) revealed that gas-phase detonations were most often characterized by unsteady, three-dimensional structures, as illustrated in Figure 5-4. Only averaged global values can be predicted by one-dimensional steady theories, according to the mathematical expressions in Equ 5-9 to Equ 5-12.

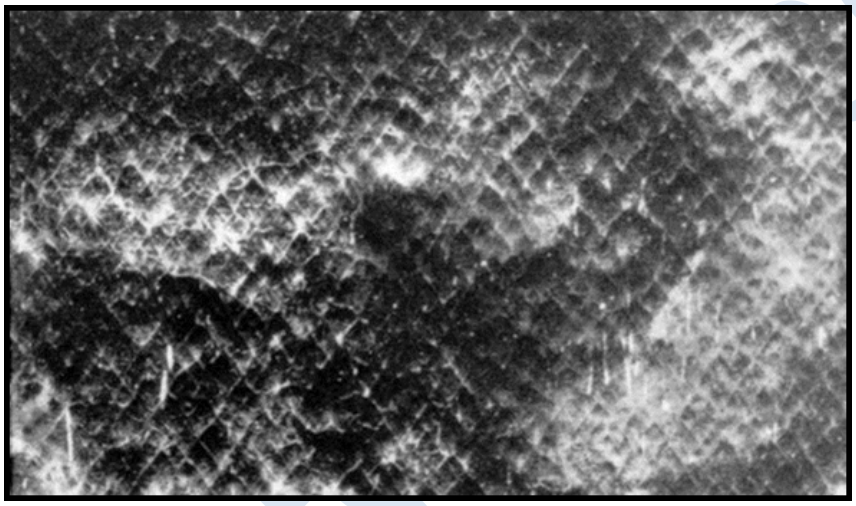

Figure 5-3 Typical *Fish Scales* structure generated by the detonation (M.S. Kuznetsov, 2000)

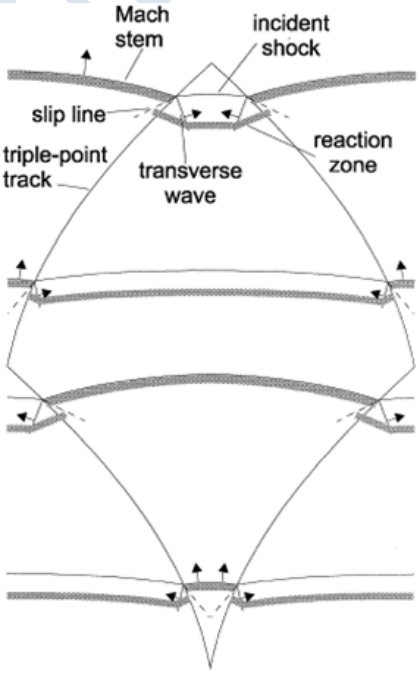

Figure 5-4 Three-dimensional structure of the detonation

The cells in the fish scale structure in Figure 5-3 are characterized by a typical length scale, the detonation cell size λ, which is one of the representative parameters of the detonation process. The detonation cell can be experimentally measured (Gavrikov et al., 2000) and its value is utilized to characterize the gaseous mixture.

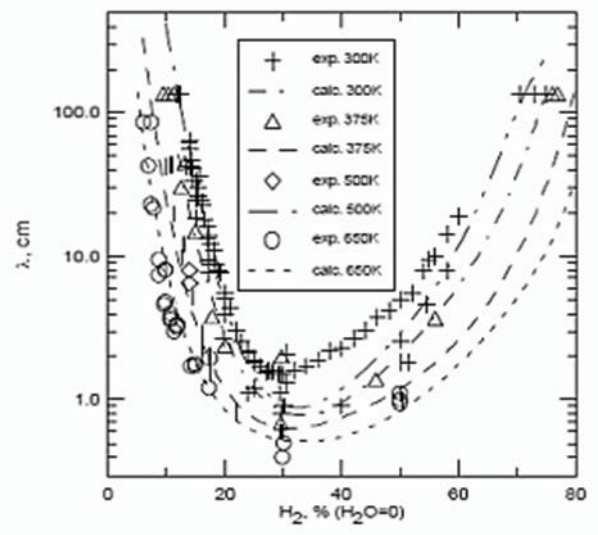

Figure 5-5 H2-air typical cell sizes for different temperatures (G. Ciccarelli, 1994)

The reproduction of the fish-scale structure has certain requirements in terms of mesh resolution. It is possible to illustrate this constrains better with an example. For the stoichiometric H2-air mixture at 300 K, the transverse size of the detonation cell is around 1.5 cm as shown in Figure 5-6. To reproduce the fish-scales structure in a three dimensional calculations, a grid resolution of around 50 control volumes inside the detonation cell is required as shown in Figure 5-6 bringing the computational cell size to 0.3 mm.

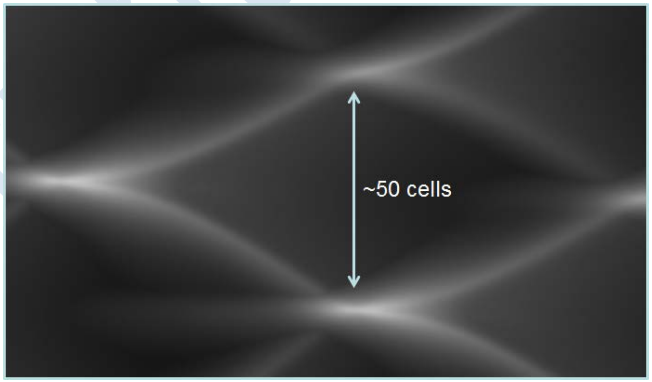

Figure 5-6 Resolution requirements (Kotchourko, 2012)

The performance of realistic calculations in industrial scales (in the order of hundreds of metres) is certainly constrained by this severe requirement for the mesh resolution. Therefore, Local Mesh Refinement (LMR) (Ren et al., 2012) for detonation modelling appears as a natural solution that provides both the necessary resolution in the detonation front and an affordable computational cost. In Figure 5-7, the typical fish-scale structure of the detonation is reproduced in the simulation results for a stoichiometric hydrogen air mixture. Two levels of mesh refinement are applied, with

four time's additional resolution in each level. In spite of a light degradation of the cellular structure by mesh coarsening, the method is successful in resolving the detonation structure (Ren, 2014).

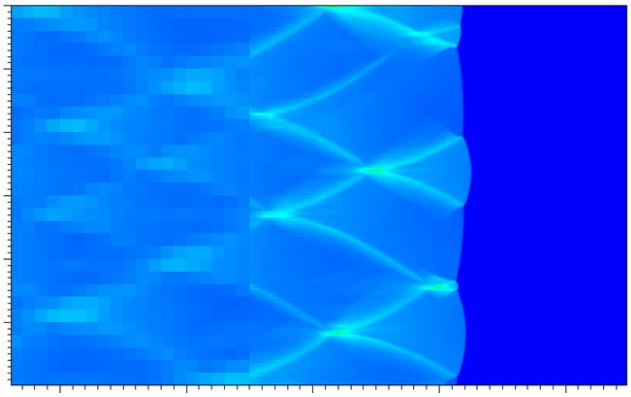

Figure 5-7 LMR calculation of a H2-air stoichiometric mixture with two levels of refinement taking four times more resolution in each step. Note that in spite of a light degradation of cellular structure by mesh coarsening, the method is successful in resolving the detonation structure (Ren, 2014)

Often, the lack of mesh resolution has another undesirable effect. In general, numerical schemes are created for non-reactive media. In the first stage of the solution method of reactive problems, an accurate non-reactive solution is achieved and subsequently in the second stage the required heat release is added. In this context, the chemical interaction could be then interpreted as a kind of perturbation of the non-reactive solution.

For those simulations in which the computational cell size is very large, the reaction zone length is small in comparison with the cell size. Due to CFL stability condition, the time step is also large and that causes too large perturbations of the non-reactive solution, leading to unrecoverable errors in the numerical solution. This kind of behaviour is illustrated in Figure 5-8, where the mesh resolution is adequate for a 1D calculation, however as shown in Figure 5-9 the resolution is too coarse. In the first case the detonation wave travels with the correct propagation velocity D_{CJ}, while in the second case, the correct detonation features are not reproduced both from the qualitative and quantitative point of view.

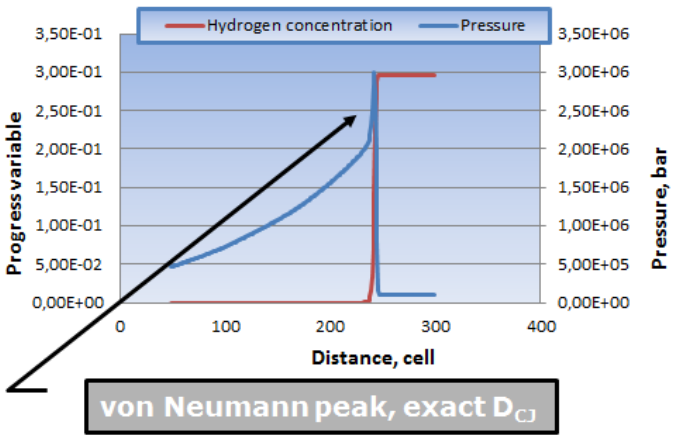

Figure 5-8 One dimensional calculation carried out with a resolution of 3 cm. The detonation exhibits an adequate propagation velocity

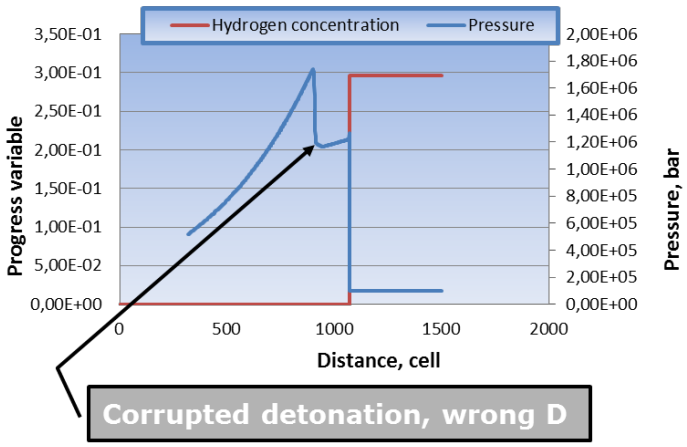

Figure 5-9 One dimensional calculation carried out with a resolution of 10 cm. The simulation exhibits a wrong reproduction, both qualitative and quantitative, of the detonation phenomena

5.3 Knowledge gaps

In the opinion of the authors, the main research topic in the field of detonations is Deflagration to Detonation transition (DDT).

In the actual status of development of the knowledge, DDT is a phenomenon still under investigation at the research level and its modelling is known to be difficult.

Conceptually DDT consists of the change of the combustion regime of a fast turbulent flame into a detonation. That is, the transition from a propagation regime based on the diffusion of species and heat to another one based on the compression of the mixture.

Until now, three main modes of DDT have been identified, namely, DDT due to shock focusing, DDT due to jet ignition and DDT due to flame acceleration and triggered by a local explosion due to different mechanisms, including instability in the flame brush, flame-shock interaction with obstacles, etc.

The identification of the mechanisms and the increase of the insight on the DDT process are some of the main topics which are still open and require further investigation.

The predictive capability of the DDT numerical modelling is still very low and its improvement is certainly necessary.

In the next generation of simulations, to gain an enhanced insight of the process it would be necessary to utilize detailed chemical reaction mechanism.

The role of turbulence in the detonation onset and the most adequate turbulence modelling strategy must be also identified.

The role of the confinement and congestion in the propagation regime has been identified as a crucial one, e.g. (Dorofeev et al., 2001). The extension of the findings to open or semi-confined spaces is necessary to identify what kind of configurations can trigger a DDT process, clarifying the role of obstacles, and the role of flame instabilities.

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7 Contributing partner acronyms

Number:	Name:	Acronym:	Country:
1	AREVA	AREVA	France
2	Element Energy Limited	EE	United Kingdom
3	Health and Safety Laboratory	HSL	United Kingdom
4	JRC – Joint Research Centre – European Commission	JRC	Belgium
5	Karlsruher Institut fuer Technologie	KIT	Germany
6	National Centre for Scientific Research Demokritos	NCSRD	Greece
7	Ulster University	UU	United Kingdom