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Support to Safety Analysis of Hydrogen and Fuel Cell Technologies

Report on Verification and Validation Procedures

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Contents

1. Introduction

1.1 Purpose of this document

As simulation tools have become more advanced and as computers have become more powerful, modelling and simulation have become a very important part of the decision making process in engineering. In application areas where fundamental physics are complex, such as is often the case with hydrogen safety related challenges, generic design *rules and codes* – often used in more mature areas of engineering such as hydrogen in industrial and chemical processes - may have limited applicability to the problem at hand. Equally, experimental data may not full reflect the physics or geometric design parameters that may be part of a specific design challenge. In these circumstances, increasingly *simulation* is used to provide a *performance based assessment* of the quality of a design, for example in evaluating if a hydrogen refuelling station design is capable of mitigating hazards as a result of an unintended hydrogen release.

As computers become more powerful, often the outputs of a simulation can seem more realistic – an example being the use of Large Eddy models of turbulence – resolving fine temporal and length scale phenomena results in realistic looking behaviour. The simulation result may have high fidelity to the activity being researched, or it may be complete nonsense. However, all models (and their resulting simulation outputs) are abstractions from reality and are based on a series of approximations. In all cases, practitioners will:

- create an abstract model which they believe reflects the physical phenomena that pertain
- programme that model into a computer and solve it in an iterative simulation

During either of these steps errors can be introduced or arise which cause the computational outputs to deviate – often significantly – from reality. In the case of high-consequence applications (nuclear energy, nuclear weapons, natural gas or hydrogen release) significant deviations could misdiagnose an unsafe design as one that is safe, and this cannot be tolerated. In relatively mature, high-consequence application areas (nuclear energy), procedures have been developed to identify and improve the fidelity and quality of their modelling and simulation processes. The purpose of this document is to help practitioners in the hydrogen safety CFD area to determine the fidelity of modelling and simulation processes. It does this by providing structure, guidelines and examples for relevant applications. The procedures in this document are described as Verification and Validation. The expected outcome is an improvement in the quality of hydrogen safety CFD simulations.

1.2 Who is this document for

Ensuring the fidelity of modelling and simulation processes is ultimately the responsibility of the **practitioner** generating simulation outputs to guide engineering design. Practitioners may be working in academia or industry but their main interest is using simulation to support performance based assessments of designs. Therefore they are the primary audience for this report and much of the guidance given relates to what can and should be undertaken by practitioners.

In the process of generating those outputs, the practitioner will often use a software programme that was developed by 3rd party **code developers**. The practitioner may not have access to the source

code or to sufficiently clear description of code development and implementation that would allow them to undertake extensive verification that could fix coding implementation errors. Code developers both industry and academia) have the responsibility of undertaking extensive test procedures on the code they are developing, and record the results for practitioners to see and reference. Unfortunately, code developers rarely undertake and publish tests of the extensive nature required; a notable exception is Fire Dynamics Simulator with extensive Verification and Validation Guides[1].

We acknowledge that practitioners are usually under time pressure to deliver outputs within a fixed time/cost, and this limits the time that will be spent on ensuring the fidelity of results. Acknowledging this, the document provides a brief overview of the subjects of simulation fidelity, verification and validation –many in depth texts are widely available.

1.3 Definitions

Verification and validation are distinct and complimentary procedures that are both required to determine the fidelity of simulation outputs. In certain safety-critical fields (nuclear energy) they are widely used and their distinct application here is understood, however this clear distinction is not upheld in all fields of application[2]. A number of definitions are available and the SUSANA project has adopted those below[3]:

Verification:

The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model

Validation:

The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.

From a practical perspective, the purpose of Verification is:

- To identify and reduce numerical errors
- Prove the numerical equations are solved correctly.
- This means that as a measure of discretisation goes to zero, the solution tends to that of the continuum equations.
- Verification is "solving the equations right"
- Assessing the numerical accuracy of a solution, compared to the conceptual model
- Association or relation to the real world is not an issue.

[1] https://firemodels.github.io/fds-smv/manuals.html
[2] For example: page 23 from "Verification and Validation in Scientific Computing", Oberkampf and Roy; and page 1 of the Fire Dynamics Simulator Technical Reference Guide Volume 2: Verification.
[3] Oberkampf et al, Verification, validation and predictive capability in computational engineering and physics Foundations for V&V in the 21st century, 2002

On the other hand, the objective of Validation is:

- To identify and reduce conceptual modelling errors
- Determines whether or not the solution has any relationship to the physical problem
- Validation is "solving the right equations"
- Addresses the physics modelling accuracy by comparing computational results with experimental data.

The figure below shows the link between Models, Simulations and V&V processes. A critical distinction is that between a conceptual model and a computerised model. A *conceptual model* represents the practitioner's representation of reality, and comprises all of the mathematical equations and modelling assumptions judged to be required to do this. The conceptual model may be incomplete, for example important physical phenomena may be represented too simply, or omitted completely in error (an example would be assuming a turbulent flow can be modelled as a laminar flow). Validation is understanding the extent to which the conceptual model is "an accurate representation of the real world from the perspective of the intended uses of the calculation method"[4].

The *computerised model* is an implementation of the conceptual model, using computer programming. At this stage errors may be introduced, from coding errors, to discretisation and iteration errors to incorrect use of material constants. Verification is "the process of determining that the implementation of a calculation method accurately represents the practitioner's conceptual description of the calculation method and the solution to the calculation"

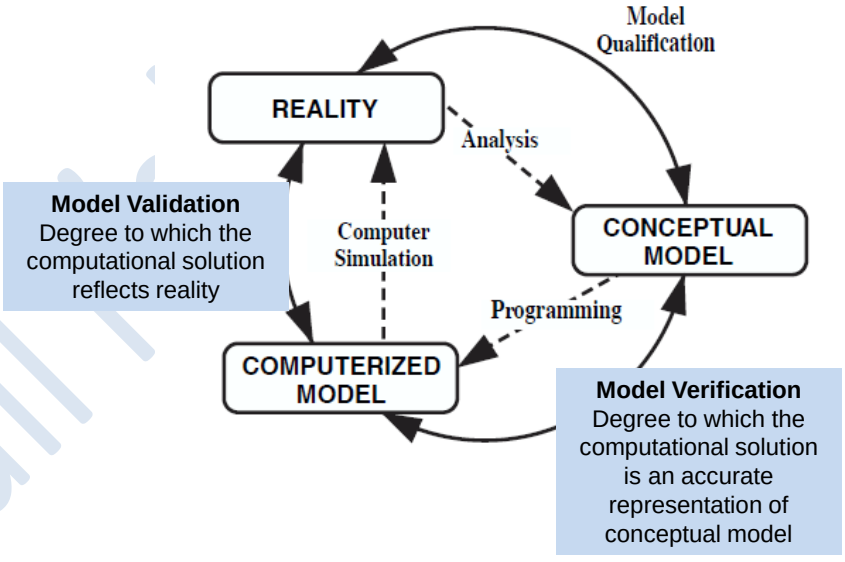


Figure 1. Phases of Modelling and Simulation and the role of Verification and Validation (adapted from Schlesinger, 1979)

[4] ASTM E 1355 "Standard Guide for Evaluating the Predictive Capability of Deterministic Fire Models,"

In practice Verification primarily involves comparing the numerical outputs from the computer model with those from a direct solution of the conceptual model. This often limits practical verification to a subset of cases where the conceptual model equations can be solved directly i.e. where an analytical solution is available – for example Couette flow. More information on verification tests is provided below. In contrast, Validation involves comparing numerical outputs with real world or experimental data.

Verification is sometimes divided into code verification – assessing that the computer implementation of the conceptual model is correct; and solution verification – assessing that the computational output has sufficient fidelity with respect to the intended conceptual model. This reflects the different nature of the errors than can be introduced as show in the figure below.

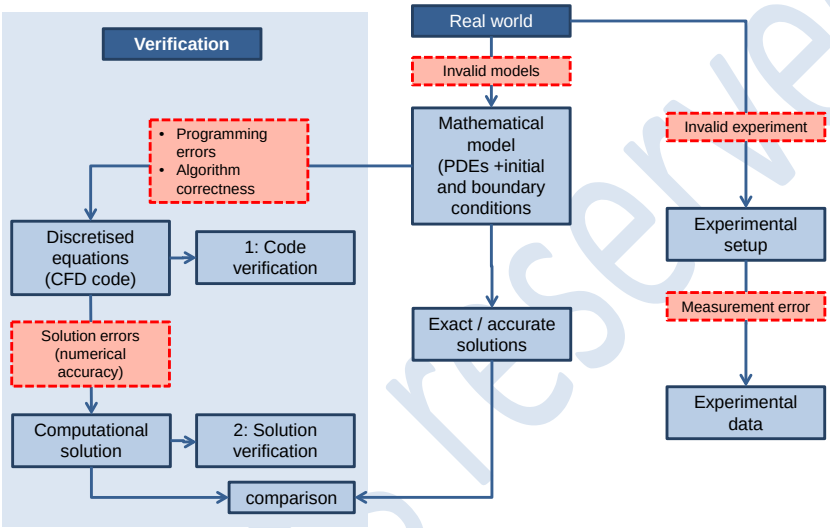


Figure 2. Sources of errors when undertaking Verification and Validation.

2. Verification

2.1 Why undertake verification?

In the time-pressured environment that most practitioners experience, it is correct to challenge the need for verification. Why not just skip straight to validation, given that validation is also required and the relevant experimental dataset for validation may be more easily obtained? The reason is that rarely do model and measurement agree so well in all applications that a practitioner would unquestioningly accept the results of a simulation. As there are always differences between model and experiment, we need to determine if those differences are due to errors or limitations in the (implementation and solution of the) numerical procedure, or within the physical sub-models that form the conceptual model.

The risk of not undertaking verification can be seen in the example on the right. The chart compares predictions and experimental data for flow over a tube bundle[5]. Sensitivity to a numerical parameter (temporal convergence) is shown. At an intermediate level of this parameter (1e-4) comparison is excellent, and the practitioner might be tempted from this simulation alone to declare both the model and the numerical predictions of high fidelity. In reality, errors in physical sub-models (conceptual models) were balanced by the numerical errors (lack of iterative convergence). Reducing the impact of this value increases the fidelity of the numerical outputs to the conceptual model, but in doing so shows that the *conceptual model is not a good reflection of physics*.

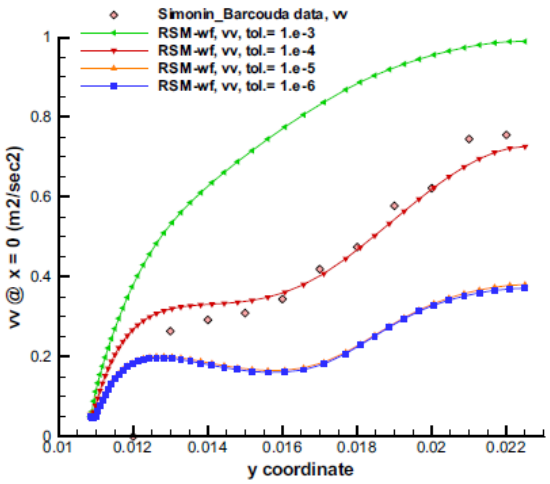


Figure 3. Comparison of predictions and experiment (transverse normal stresses) for flow over a staggered tube bundle, indicating where less strict temporal convergence criteria results in better agreement with experiment.

Whereas validation consists mainly of comparing predictions with measurement, model verification consists of a much broader range of activities, including code checking, comparison of outputs to analytical solutions, and checking sensitivity of outputs to numerical parameters. The literature reflects the preference (or certainly the dominance) of validation, where validation papers outnumber verification papers perhaps by 10-1.

[5] Johnson et al; "Processes and Procedures for Application of CFD to Nuclear Reactor Safety Analysis". Idaho National Laboratory, 2006.

2.2 Overview of verification procedures

The objective of this section is to describe in general terms each of the types of verification tests that may be undertaken. The presentation of these tests and processes follows the logical sequence of figure 2 i.e. Code Verification and Solution Verification. While practitioners may have limited access to source code and so are somewhat restricted in the code verification they can and should undertake, their ultimate responsibility for signing off the fidelity of their simulations means that practitioners should understand what is required under Code Verification. Clearly Code Verification is very relevant to those developing and running their own codes, as is often the case in University departments.

2.3 Code Verification

Code verification ensures that the computer program is a faithful representation of the original mathematical model. In figure 2 above, we showed that errors can be introduced when implementing the conceptual models on a computer, via coding mistakes. Practitioners cannot fix errors in coding but by they need to understand the processes involved in this stage of verification.

2.3.1 Software engineering

It is extremely difficult to estimate the effect of unknown software defects on computational predictions[6], therefore it is prudent to minimise the introduction of defects through good software engineering practices. Essentially this entails monitoring and controlling the software development processes and software products to ensure reliability. A practitioner cannot control this directly, but can do so indirectly, by choosing to use software where there is evidence of this good practice.

Commercial software providers should provide a description of the verification processes they have undertaken. While a formal quality procedure such as ISO 9001 is a positive indication of good practices, best practice is the publishing of a comprehensive set of verification tests such as those provided by CFX and FDS[7] [8].

The practitioner should ensure that the verification tests undertaken reflect as closely as possible the case under study, for example the terms in the governing equations, application of boundary conditions, grid topology etc, as this increases confidence that the practitioner is using the code within its verified application domain.

2.3.2 Invariance: Symmetry, Translation, Rotation, Scaling

These tests ensure equations are implemented correctly, by testing invariance of solutions under the above transformations. For example, checking the correct implementation of buoyancy terms can be achieved by rotating the domain 180degrees, and changing the direction of the gravity vector.

[6] Knupp et al. 2007
[7] Ansys Verification manual available at http://148.204.81.206/Ansys/150/Fluid%20Dynamics%20Verification%20Manual.pdf
[8] NIST Special Publication 1018-2 Sixth Edition Fire Dynamics Simulator Technical Reference Guide Volume 2: Verification

2.3.3 Conservation

Another simple test is to check that the computer model correctly reproduces conservation for mass, momentum or energy. For example, SUSANA T5.3 examines conservation of mass in four different CFD codes each modelling the same helium release – after a fixed time, the mass of helium in the domain is the sum of helium released less helium which leaves the domain. Similarly the FDS verification tests (reference provided above) include conservation of energy which are relevant to combustion.

2.3.4 Order of accuracy verification

This is a rigorous test of verification, and examines the convergence of the numerical solution and whether the discretization error reduces at the theoretical rate expected as the mesh and/or time step are refined. Most practitioners will assume that in choosing e.g. 2nd order accurate difference operators the differential equations will actually reflect this – if they do not then there may be a coding problem that should be corrected by the developers. In practice, the user will often need to undertake a grid refinement study to prove the solutions are grid independent. That means separating those errors due to poorly resolved flow features (which the user can change by local refinement) from the errors arising from the discretization of the equations.

The truncation error (difference between the discretized equations and the original partial differential equations) is the metric used to determine formal order of accuracy. For example, the discrete L1 Norm of the solution error over the domain may be used:

$$\|u - u_{ref}\|_1 = \frac{1}{N}\sum_{n=1}^{N}|u_n - u_{ref,n}|$$

The L1 norm provide a measure of the average absolute error over the domain (in the above example for constant cell spacing). Alternatively the L2 norm can be used, which is the root mean square of the error:

$$\|u - u_{ref}\|_2 = \left(\frac{1}{N}\sum_{n=1}^{N}|u_n - u_{ref,n}|^2\right)^{1/2}$$

The above error terms can be used to compare the observed order of accuracy with the formal order of accuracy.

It is important to note that these formal order of accuracy assessments require uniform grid refinement. Local refinement is often used to resolve flow features in selected regions of interest, but is not appropriate for assessing the asymptotic behaviour of discrete solutions.

2.3.5 Convergence and Discretization tests

In the example above (Figure 3) it was shown that insufficient iterative convergence introduces numerical errors which may offset (mask) more fundamental modelling errors. A general recommendation is that iterative convergence is demonstrated by showing at least 3 orders of magnitude degrease in the normalized residuals for each equation solved (Johnson et al). Roy (2005) suggests that iterative error should be no more than 1% of the discretization error on the finest mesh employed.

For time dependent problems, iterative convergence at each time step should be checked, and convergence trends should be shown on selected variables. An example might be the evaluation of the global mass error at each timestep in a domain[9].

Systematic mesh refinement

The asymptotic behavior of the discretized equations would be observed in the limit by taking the discretization parameters to zero. In practice a realistic and pragmatic evaluation of discretization error is required.

Generally, the discretization error is evaluated by computing solutions on a number of systematically refined grids. Comparing an appropriate error norm (L1, L2 etc) as a function of the discretization parameter, one can evaluate whether this relationship reflects the expected (formal) order of accuracy). At least three meshes are typically required, this is to demonstrate that the solutions are in the asymptotic part of the domain

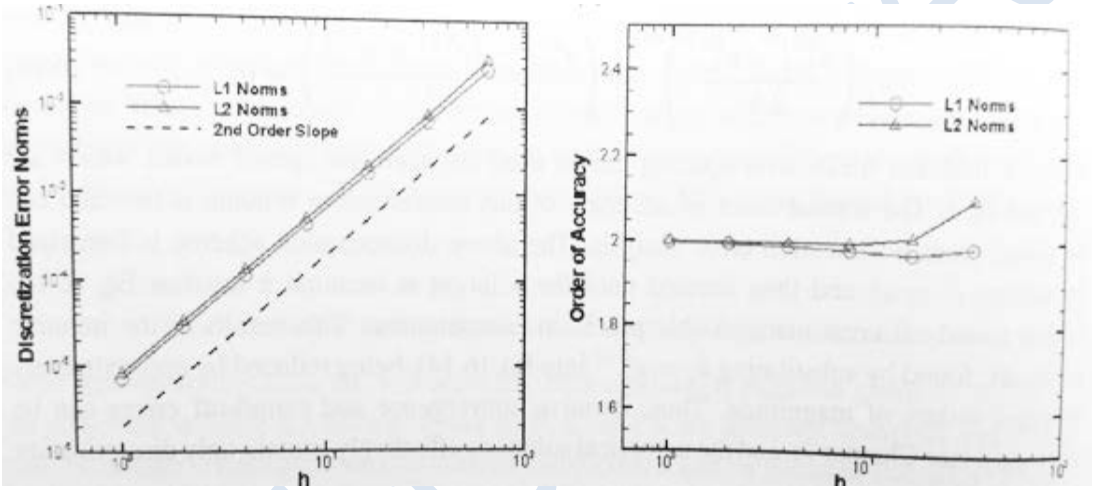


Figure 1. Error norms (left) and observed order of accuracy (right) as a function of systematic grid refinement (Oberkampf and Roy, 2010).

Local versus systematic global refinement

In many practical CFD simulations, local refinement is undertaken to improve spatial resolution of high gradient phenomena in particular volumes in a domain. However, this is not equivalent to the systematic uniform grid refinement that is required to evaluate discretization error.

Grid dependent model terms

Care is required that the refinement does not inadvertently change the governing equations being solved. This can be the case when sub-models are incorporated which have thresholds/switches/filters which are dependent on grid size. An example would be LES modelling. In such circumstances the practitioner should identify these models which are grid/discretization scale dependent, and if possible fix these to be constant in all verification tests.

[9] Johnson et al; "Processes and Procedures for Application of CFD to Nuclear Reactor Safety Analysis". Idaho National Laboratory, 2006.

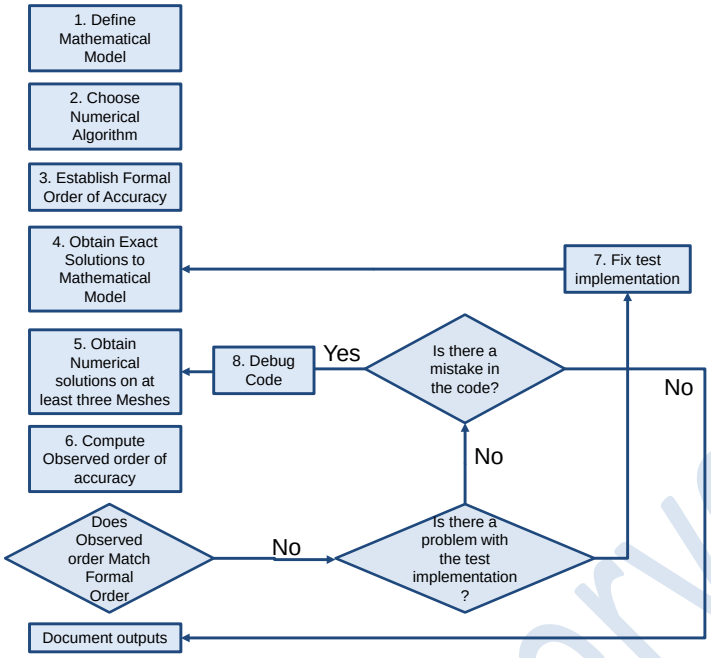


Figure 1. Flowchart showing order verification procedure (Oberkampf and Roy, 2010).

2.3.6 Method of Manufactured Solutions

The Method of Manufactured Solutions is a general and very powerful method for verification. However, immediately it must be acknowledged that implementing MMS requires access to source code, and is time intensive, and so is unlikely to be used by practitioners, the key audience for this document. So its description here is relatively high level, and those wishing to pursue this technique may follow the many references available.

MMS is a response to the challenge of finding an exact solution to the complete partial differential equations in many fields of simulation, particularly fluid dynamics. As will be shown below, only the simplest equations and geometrical domains permit e.g. analytical (exact) solutions against which the outputs of the numerical scheme can be compared.

MMS works the problem the other way around. The method proposes a form of a solution (which might be given by analytical sine/cosine/exponential terms) and then works out how to modify the equations to produce that solution. The modification is done by adding source terms to the governing equations; these can be thought of as "pushing" the solution towards the desired form.

The benefits of MMS is that it can provide solutions to governing equations of high complexity, allowing all terms to be fully exercised (tested for correct implementation). However this does come at a cost. The approach of working the "reverse problem" is non-intuitive, and some may object to the lack of any clear physical analogue in the results (even though there is no requirement for any verification solution to be related to a physically realistic problem[10]). Perhaps the greatest barrier is the implementation of the source terms, which not only requires access to source code, but great care must be taken when implementing the many terms in the resulting (modified) equations. An extensive discussion on the use of MMS for code verification is presented by Knupp and Salari (2003).

[10] Oberkamp and Roy; "Verification and Validation in Scientific Computing", Cambridge University Press, 2010

2.4 Solution Verification

The objective of solution verification is to improve confidence in the fidelity of numerical simulations in relation to a particular case or application problem at hand. As stated above, it is a pre-requisite that the code being used will have undertaken code verification to identify and remove errors in the coded implementation of the conceptual model.

It is not the case that verification procedures can prove absolutely that the numerical model exactly match the conceptual model. Rather, verification procedures improve confidence that the code has been implemented correctly and the simulation has been constructed in a way that provides confidence in the results. Solution verification commonly takes the form of a series of test cases, each focussing on part of the code features or governing terms, each adding to the evidence that the implementation and use is correct. Taken together, the set of test cases would ideally cover the main features of the computation (physical terms, grid topology, discretisation etc), providing confidence that its use is verified for the case under study.

2.4.1 Analytical Solutions

For comparison with numerical solutions, an exact solution may be available in the form of an Analytical Solution to the governing equations. A typical limitation of analytical solutions is that they are available only for physical problems much simpler than the situation of interest; and also terms/physical phenomena may be left uncoupled

A key requirement of the test is that it is able to exercise all the relevant terms in the governing equations. For example, running a viscous code at very high Reynolds number means that the viscous terms will be swamped by the inertia terms; any errors in the implementation of the viscous terms will be severely diluted and may remain unobserved. Identifying a test where (in this case) the Re ≈1 is more appropriate for exercising the main terms.

The choice of an appropriate analytical solution will depend on the nature of the physical terms being verified. For example, verification of a compressible flow solver (relevant for H2 detonation) may be undertaken with a Sod Shock tube / Riemann problem, where spatial discontinuities in the flow are a strong test of spatial discretisation accuracy[11]. Many examples are given in the literature, and worked examples are provided below.

2.4.2 Numerical and Benchmark Solutions

In this approach, the need to identify an exact solution is avoided, by instead using an approximate solution which is the output from another numerical procedure. This “benchmark” case should be from a code which has been well tested and where the solutions are of known high quality. Proving this is difficult; two basic criteria for a benchmark solution are:

- The asymptotic convergence range is shown to have been achieved for the benchmark solution

[11] See ref. ANA-1 from the SUSANA verification database. The database provides 6 references using analytical solutions for verification on applications of relevance to H2 safety flows.

- The code used to generate the benchmark solution has passed the order of accuracy code verification test for the terms exercised in the benchmark problem[12].

Benchmark solutions which meet the above criteria are rare, as each one is case and physics specific. A notable exception is the NASA turbulence modelling verification database, which relies on benchmark solutions[13].

The use of numerical solution comparisons is relatively common in the literature as identical problems may be run by two or more codes and then compared relatively easily. Such verification tests are weaker than Benchmark solution verification, because in comparing two or more "peer" codes, none has the status of a high quality benchmark solution. Numerical solution verification does build the evidence that the chosen scheme is implemented correctly, particularly if more than two schemes are compared.

2.4.3 Parameter Sensitivity Studies

The above sets of solution verification tests improve the confidence that the solutions are a faithful reproduction of the intended conceptual model, but each test is specific to the parameters which define it. It may be that an analytical or numerical solution is available but the geometry is less complex than the case in hand, or temperatures/environmental conditions deviate from the case in hand. How can the practitioner be sure that when the actual test case in hand is run, that the successful verification remains true?

Extrapolating the conclusions of a successful solution verification to more general cases can only be supported if sensitivity studies are undertaken. A careful evaluation of the impact of changing one parameter at a time – and ensuring that the expected results occur, improves confidence that the application domain is within that of the verified domain. These include physical properties, initial conditions, boundary conditions, and numerical parameters such as relaxation, artificial viscosity, solution parameters etc.

We note that practitioners will often vary physical modelling parameters in order to improve the agreement between numerical output and experimental data. This is called:

Calibration: the process of adjusting physical modelling parameters in the computational model to improve agreement with experimental data[14]*.*

The purpose of calibration is very different from a sensitivity study, because in a sensitivity study we are trying to assess whether the numerical scheme is being used within acceptable boundaries, and whether the verification undertaken to date is robust, or in contrast whether its verification status is sensitive to changes in key parameters.

[12] Oberkampf and Roy, 2010
[13] http://turbmodels.larc.nasa.gov/
[14] ASME Guide 2006

2.5 Verification examples

2.5.1 Release and Dispersion

Laminar Two-Dimensional Jet

Using boundary layer theory analysis and similarity assumptions it is possible to derive analytical expression for velocity evolution for the laminar jets issued from the infinitely thin two-dimensional slit and from the circular nozzle:

$$u = \left(\frac{3}{32}\right)^{1/3}\left(\frac{K^2}{\nu x}\right)^{1/3}\left(1-\tanh^2\xi\right), \tag{2.5.1}$$

$$v = \left(\frac{1}{6}\right)^{1/3}\left(\frac{K\nu}{x^2}\right)^{1/3}\left[2\xi\cdot\left(1-\tanh^2\xi\right)-\tanh\xi\right], \tag{2.5.12}$$

$$\xi = \left(\frac{1}{48}\right)^{1/3}\left(\frac{K}{\nu^2}\right)^{1/3}\left(\frac{y}{x^{2/3}}\right), \tag{2.5.13}$$

for the slit nozzle and

$$u = \frac{3}{8\pi}\cdot\frac{K}{\nu x}\cdot\frac{1}{\left(1+\frac{1}{4}\xi^2\right)^2}, \tag{2.5.14}$$

$$v = \frac{1}{4}\cdot\sqrt{\frac{3}{\pi}}\cdot\frac{\sqrt{K}}{x}\cdot\frac{\xi-\frac{1}{4}\xi^3}{\left(1+\frac{1}{4}\xi^2\right)^2} \tag{2.5.15}$$

$$\xi = \sqrt{\frac{3}{16\pi}}\frac{\sqrt{K}}{\nu}\cdot\frac{y}{x} \tag{2.5.16}$$

for round nozzle. Here *x* is the distance from the nozzle along the jet axis, *y* is the distance from the jet axis, *u* is the velocity along the jet, *v* is tangential velocity, ν is the kinematic viscosity, *K* is the kinematic momentum $K = J/\rho$, where *J* is the jet momentum, $J = \dot{m}\cdot u_{nozzle}$, $\dot{m}$ is mass flow rate through the nozzle, u_{nozzle} is fluid velocity in the nozzle, and ρ is the density, $\pi = 3.1416$ and ξ is a similarity variable.

Note that these solutions are applicable in the similarity region and should not be applied to the area of immediate vicinity of release origin.

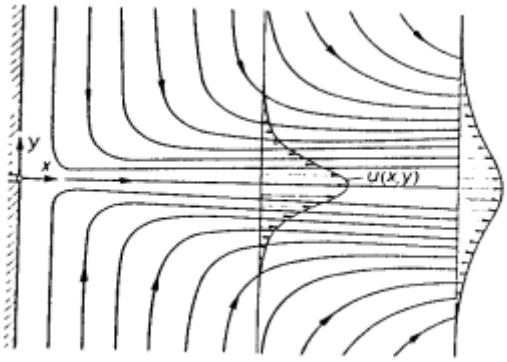


Figure 1. Schematic of streamline pattern for the jet (Schlichting, 1979).

Derivation

Let us consider jet issuing from the infinitely thin slit. Emerging jet entrains part of surrounding fluid due to the viscous friction. This results in jet spreading outwards, while its axial velocity decreases. The resulting pattern of streamlines is shown in Fig. 1. Let us set a coordinate system with the origin at the slit and *x* axis coinciding with the axis of the jet.

Boundary layer equations for two-dimensional motion (for zero pressure gradient since the ambient fluid is stationary) can be written as

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0, \tag{2.5.17}$$

$$u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}=\nu\frac{\partial^2 u}{\partial y^2}, \tag{2.5.18}$$

where *u* and *v* are the velocities in *x* and *y* directions and ν is the viscosity, with boundary conditions $y=0: \quad \frac{\partial u}{\partial y}=0;$ $y=\infty: \quad u=0$. In order to integrate continuity equation, let us introduce stream function $\psi(x,y)$ defined in such a way that $u=\frac{\partial \psi}{\partial y}; \quad v=-\frac{\partial \psi}{\partial x}$. Stream function must thus satisfy equation

$$\frac{\partial \psi}{\partial y}\frac{\partial^2 \psi}{\partial x \partial y}-\frac{\partial \psi}{\partial x}\frac{\partial^2 \psi}{\partial y^2}=\nu\frac{\partial^3 \psi}{\partial y^3}, \tag{2.5.19}$$

with boundary conditions $\frac{\partial^2 \psi}{\partial y^2} = 0$ at *y*=0 and $\frac{\partial \psi}{\partial y} = 0$ at $y = \infty$.

Let us assume that the slit is infinitely small. In order to retain final volume of the flow and finite momentum, it is necessary to assume infinite fluid velocity at the slit. The pressure gradient in the axial direction $\frac{\partial p}{\partial x}$ can be neglected due to the constant pressure exerted on a jet by the surrounding fluid. The total momentum in the *x*- direction, must, therefore, be remain constant and independent from the distance from the origin *x*, and can be expressed as $J = \rho \int_{-\infty}^{+\infty} u^2 dy = const$.

Since the problem has no characteristic linear dimension, we can assume that the velocity profiles *u*(*x*,*y*) are similar, and $u \sim y / b$, where *b* is the jet width, suitably defined. We can further assume that $b \sim x^q$. Stream function can then be expressed in the form (Schlichting, 1979)

$$\psi \sim x^p \cdot f\left(\frac{y}{b}\right) = x^p f\left(\frac{y}{x^q}\right). \tag{2.5.110}$$

Variables *p* and *q* in eq. (1.1.10) can be determined from the following assumptions:

- The flux of momentum in the *x* direction is independent of *x*;
- The acceleration and friction terms are of the same magnitude.

These assumptions lead to two equations for *p* and *q*:

$$2p - q = 0, \tag{2.5.111}$$

$$2p - 2q - 1 = p - 3q, \tag{2.5.112}$$

Resulting a solution *p*=1/3, *q*=2/3.

Stream function and independent variable can then be expressed as

$$\eta = \frac{1}{3\nu^{1/2}} \cdot \frac{y}{x^{2/3}}, \tag{2.5.113}$$

$$\psi = \nu^{1/2} x^{1/3} f(\eta). \tag{2.5.114}$$

The velocity components can be expressed as

$$u = \frac{1}{3x^{1/3}} \cdot f'(\eta), \tag{2.5.115}$$

$$v = -\frac{1}{3} \nu^{1/2} x^{-2/3} (f - 2\eta f') . \quad (2.5.116)$$

From here, it is possible to obtain differential equation for the stream function *f*

$$f'^2 + f \cdot f'' + f''' = 0 , \quad (2.5.117)$$

with boundary conditions

$$\eta = 0 \qquad \begin{cases} f = 0 \\ f'' = 0 \end{cases}, \quad (2.5.118)$$

$$\eta = \infty \qquad f' = 0 . \quad (2.5.119)$$

Integration of this equation with these boundaries provides

$$f \cdot f' + f'' = 0 . \quad (2.5.120)$$

Eq. (1.1.20) can be integrated once more by replacing variables η and *f* with ξ and *F*:

$$\xi = \alpha \cdot \eta , \quad (2.5.121)$$

$$f = 2\alpha \cdot F(\xi) . \quad (2.5.122)$$

Eq. (1.1.20) thus transforms into

$$F'' + 2F \cdot F' = 0 . \quad (2.5.123)$$

with boundary conditions

$$\xi = 0 \qquad F = 0 , \quad (2.5.124)$$

$$\xi = \infty \qquad F' = 0 . \quad (2.5.125)$$

Equation (1.1.23) can be integrated once more, resulting in

$$F' + F^2 = 1, \quad (2.5.126)$$

which solution can be obtained in a closed form as

$$\xi = \tanh^{-1} F\,. \tag{2.5.127}$$

Constant α can be obtained from the condition of conservation of the momentum in *x* direction, from which can it can be derived that

$$J = \frac{16}{9}\rho\alpha^3\nu^{1/2}. \tag{2.5.128}$$

Substituting expressions for ξ and α into eqs. (1.1.15) – (1.1.16) , one can obtained the final solution (1.1.1) - (1.1.3).

The derivation of the equations (1.1.4) – (1.1.6) is similar in the assumption of round nozzle. In this case variable *y* would correspond to the radial direction and with *u* and *v* denoting, respectively, axial and radial components of velocity. The pressure gradient is once again assumed to be negligible, and the momentum flux in the direction *x* can be expressed as

$$J = 2\pi\rho\int_0^\infty u^2 y dy = const\,. \tag{2.5.129}$$

Boundary layer simplification and equation of motion can be expressed as

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = \nu\frac{1}{y}\frac{\partial}{\partial y}\left(y\frac{\partial u}{\partial y}\right), \tag{2.5.130}$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{v}{y} = 0\,, \tag{2.5.131}$$

with boundary conditions $y = 0: v = 0, \dfrac{\partial u}{\partial y} = 0; \quad y = \infty: u = 0$. Once again, profiles *u*(*x*,*y*) can be assumed to be similar. The width of the jet is proportional to x^n and $\psi \sim x^p F(\eta)$ with $\eta = \dfrac{y}{x^n}$. Exponents *n* and *p* can be determined in the same way as for the two-dimensional jet. Assuming that the momentum is independent of *x* and inertial and frictional terms in eq. (1.1.30) are of the same order of magnitude,

$$u \sim x^{p-2n}, \frac{\partial u}{\partial x} \sim x^{p-2n-1}, \frac{\partial u}{\partial y} \sim x^{p-3n}, \frac{1}{y}\frac{\partial}{\partial y}\left(y\frac{\partial u}{\partial y}\right) \sim x^{p-4n}. \tag{2.5.132}$$

From (1.1.32) we can obtain two equations for *p* and *n*:

$$2p - 4n + 2n = 0; \quad 2p - 4n - 1 = p - 4n\,. \tag{2.5.133}$$

So that *p*=*n*=1. Consequently,

$$\psi = \nu x F(\eta); \qquad \eta = \frac{y}{x}, \tag{2.5.134}$$

from where the velocity components can be expressed as

$$u = \frac{\nu}{x}\frac{F'}{\eta}; \qquad v = \frac{\nu}{x}\left(F' - \frac{F}{\eta}\right). \tag{2.5.135}$$

Substituting these values in eq. (1.1.30) we can obtain the following equation for the stream function:

$$\frac{FF'}{\eta^2} - \frac{F'^2}{\eta} - \frac{FF''}{\eta} = \frac{d}{d\eta}\left(F'' - \frac{F'}{\eta}\right), \tag{2.5.136}$$

which after integration transforms into

$$FF' = F' - \eta F'' \tag{2.5.137}$$

with boundary conditions $u = u_{in}$ and $v = 0$ for $y = 0$, or $F = 0$ and $F' = 0$ for $\eta = 0$.

Since *u* is an even function of η, F'/η must be even, F' - odd and *F* even. Since $F(0) = 0$, the constant term in the expansion of *F* in powers of η must vanish, which determines one integration constant. The other constant, denoted as γ, can be evaluated as follows: if $F(\eta)$ is the solution of eq. (1.1.37), then $F(\gamma\eta) = F(\xi)$ is also a solution. A particular solution of the equation

$$F\frac{dF}{d\xi} = \frac{dF}{d\xi} - \xi\frac{d^2F}{d\xi^2}, \tag{2.5.138}$$

which satisfies the boundary conditions $\xi = 0 : F = 0, F' = 0$ is given by

$$F = \frac{\xi^2}{1 + \frac{1}{4}\xi^2}. \tag{2.5.139}$$

From eq. (1.1.35), it is now possible to obtain

$$u = \frac{\nu}{x}\gamma^2 \frac{1}{\xi}\frac{dF}{d\xi} = \frac{\nu}{x}\frac{2\gamma^2}{\left(1+\frac{1}{4}\xi^2\right)^2}, \tag{2.5.140}$$

$$v = \frac{\nu}{x}\gamma\left(\frac{dF}{d\xi} - \frac{F}{\xi}\right) = \frac{\nu}{x}\gamma\frac{\xi - \frac{1}{4}\xi^3}{\left(1+\frac{1}{4}\xi^2\right)^2}. \tag{2.5.141}$$

Here $\xi = \gamma\frac{y}{x}$ and the constant of integration γ can now be determined from the given value of momentum (Schlichting, 1979). From eq. (1.1.29), momentum *J* can be expressed as

$$J = 2\pi\rho\int_0^\infty u^2 y dy = \frac{16}{3}\pi\rho\gamma^2\nu^2, \tag{2.5.142}$$

from where γ can be found. Finally, by introducing kinematic momentum $K = J/\rho$, we can transform eqs. (1.1.40-1.1.41) into (1.1.4-1.1.6).

2.5.2 Release and dispersion examples

In Figure 1 a case of one dimensional release and dispersion problem is presented. Initially, the domain contains air at atmospheric pressure and temperature. At the left side of the domain inlet boundary conditions are applied: hydrogen is injected with velocity u, temperature T and liquid volume fraction α_1.

The one-dimensional continuity, momentum, mass fraction of hydrogen and energy equation along with the equation of state are solved:

$$\begin{gathered}
\frac{\partial\rho}{\partial t} + \frac{\partial\rho u}{\partial x} = 0 \\
\frac{\partial\rho u}{\partial t} + \frac{\partial\rho uu}{\partial x} = -\frac{\partial p}{\partial x} + \frac{\partial\tau_{xx}}{\partial x} \\
\frac{\partial\rho q_{H_2}}{\partial t} + \frac{\partial\rho u q_{H_2}}{\partial x} = \frac{\partial}{\partial x}\left(\rho D\frac{\partial q_{H_2}}{\partial x}\right) \\
\frac{\partial\rho h}{\partial t} + \frac{\partial\rho uh}{\partial x} = \frac{Dp}{Dt} + \frac{\partial}{\partial x}\left(\lambda\frac{\partial \mathrm{T}}{\partial x}\right) + \frac{\partial}{\partial x}\left(\rho D h_{H_2}\frac{\partial q_{H_2}}{\partial x}\right) \\
p = p\left(\rho, T\right)
\end{gathered} \tag{2.5.1}$$

where ρ is the mixture density, u the mixture velocity, p the mixture pressure, τ_{xx} the viscous stress, T the mixture temperature, q_{H_2} hydrogen mass fraction, D the diffusion coefficient, λ the thermal conductivity and h the static enthalpy. At the steady state solution of the problem the velocity, the temperature and the liquid mass fraction should have a value equal to the inlet value in the entire domain.

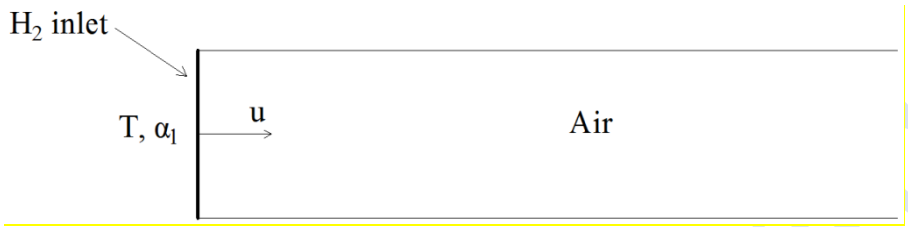


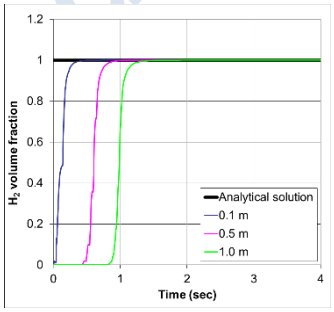
Figure 1: One dimensional release and dispersion problem

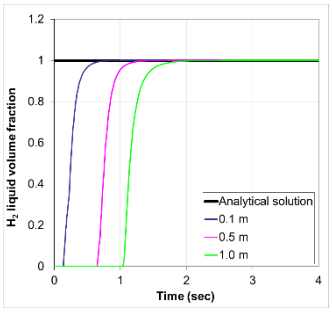
This is a very good verification case regarding two phase releases. The part of the code that calculates the phase distribution is effectively verified. The temperature and the vapor and liquid mass fractions of hydrogen are calculated by an algorithm (PH-Flasher) with given pressure, enthalpy and hydrogen total mass fraction. The algorithm uses the Raoult's law for the estimation of the phase distribution. Pressure is obtained by a SIMPLER type algorithm involving also solution of velocity. This verification case can also be used in the case of one phase release (only gaseous hydrogen) if we set $a_l = 0$.

In Figure 2, the hydrogen total volume fraction, hydrogen liquid volume fraction, and temperature time series are presented for the above verification case. The length of the domain is 1 m and the inlet velocity 1 m/s. The temperature at the inlet is set equal to 20K. This results in liquid hydrogen, $a_l = 1$ at the inlet. Constant pressure boundary condition is applied at the end of the domain. We observe that the steady state is obtained after 2 s.

In Figure 3 a similar case is presented. The differences are that hydrogen volume fraction at the inlet is equal to $a_l = 0.5$ and the temperature is the saturation temperature at ambient pressure (approximately 20.35K). We observe that the code predicts correctly the phase distribution in this case too.

The simulations were performed using the CFD code ADREA-HF. It should be noted that under-relaxation in pressure was required in order to obtain convergence.





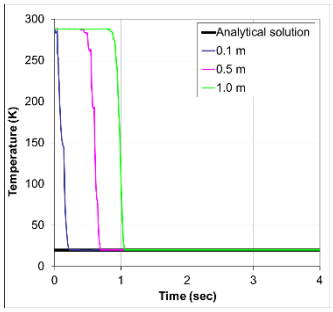


Figure 2: Hydrogen total volume fraction, hydrogen liquid volume fraction, and temperature time series for the case with inlet $a_l = 1$.

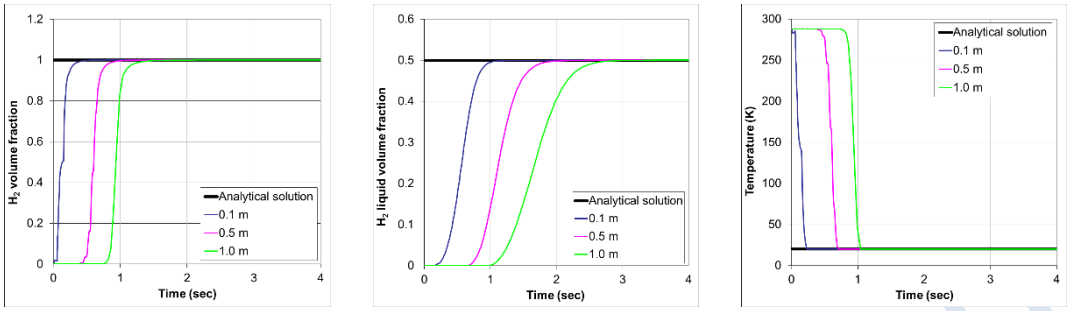


Figure 3: Hydrogen total volume fraction, hydrogen liquid volume fraction, and temperature time series for the case with inlet $a_l = 0.5$.

2.5.3 Mass balance

In the case of hydrogen CFD simulations, it is significant to verify that hydrogen mass balance is satisfied. The absolute and the relative hydrogen mass balance is defined by the equations

$$\text{mass\_bal}(t) = m_{accum} - \left(m_{released\_tot} - m_{outflow\_tot}\right) \quad (2.5.2)$$

$$\text{mass\_error}(t) = \frac{m_{accum} - \left(m_{released\_tot} - m_{outflow\_tot}\right)}{m_{released\_tot}} \quad (2.5.3)$$

where m_{accum} is the hydrogen mass inside the whole domain at time t, $m_{released\_tot}$ is the total helium released mass from t=0 to t and $m_{outflow\_tot}$ the total helium mass that flew out the domain from t=0 to t. Maximum value of the mass error equal to 0.01 is usually an acceptable limit.

2.5.4 Combustion

Premixed flame propagation velocity

Consider deflagration of hydrogen-air mixture in the tube closed at one end. Depending on the direction of the flame front propagation, flame front velocity can be expressed as:

- If the ignition occurred near the open end of the tube (Fig 2a) and the deflagration front propagates inside the tube toward the sealed-off end, the velocity of flame front relative to the tube can be estimated as S_u, where S_u is the laminar burning velocity.

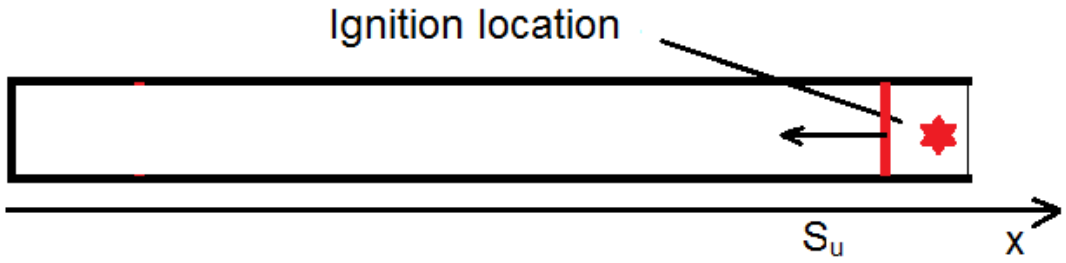


Figure 2a. Deflagration in a tube filled with hydrogen-air mixture with ignition source near the open end and deflagration wave propagating inside the tube.

- If the ignition occurred near the sealed end of the tube (Fig 2b) and the flame propagates toward the open end of the tube, the velocity of flame front relative to the tube can be expressed as $S_u \cdot E_i$, where S_u is the laminar burning velocity and E_i is the expansion factor, defined as a ration of densities of unburned and burned mixtures $E_i = \rho_u / \rho_b$. Flame propagation velocity in this case can be presented as a sum of a proper burning velocity relative to stationary mixture S_u, and the velocity due to the expansion of the burned mixture, pushing unburned mixture and the flame front toward the open end of the tube. The velocity due to expansion can be expressed as $\Delta x/\Delta t = \Delta V/(A\Delta t)$ where *A* is the tube cross-section area, $\Delta V = V_b - V_u$, V_u is volume of fresh unburnt mixture consumed by the propagating flame front in time Δt, and V_b is volume of the burnt mixture formed after the flame front consumed fresh unburnt mixture volume V_u. Since the volume of the burned mixture can be expressed as $V_b = m/\rho_b = (m/\rho_u)E_i = V_u E_i$, $\Delta V = V_u (E_i - 1)$. Then burning velocity can be expressed as a velocity of the flame front in the unburned mixture $S_u = V_u/(A\Delta t)$, the flame propagation velocity can then be expressed as $S_u + \frac{V_u (E_i - 1)}{A\Delta t} = S_u + S_u \cdot (E_i - 1) = S_u \cdot E_i$.

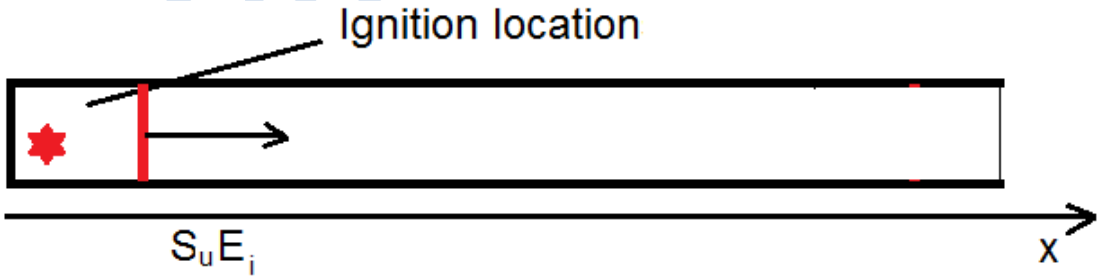


Figure 2b. Deflagration in a tube filled with hydrogen-air mixture with ignition source near the closed-off end and deflagration wave propagating toward the exit from the tube.

This solution is correct in the assumptions:

- The vessel is considered effectively one-dimensional.
- Flame front is assumed flat. Curvature of the flame front will increase combustion area and affect the result.

2.5.5 Adiabatic flame temperature

Analytical solution for adiabatic flame temperature

Calculation of adiabatic flame temperature for a given composition of reactants and combustion products may be used as a relatively simple verification problem for combustion modelling.

Calculation of adiabatic flame temperature is based on the energy conservation law for the closed system. Assuming constant pressure process the enthalpy conserves:

$$h_{reactants}(T_0, 1\text{atm}) = h_{products}(T_{ad}, 1\text{atm}), \tag{2.5.4}$$

where $h_{reactants}(T_0, 1\text{atm})$ is enthalpy of reactants at the standard state, T_0 is initial temperature (usually taken as standard state temperature T_0=25^{0}C), p is standard state pressure (p=1 atm), $h_{products}(T_{ad}, 1\text{atm})$ is enthalpy of combustion products at the sought adiabatic flame temperature T_{ad} and the same pressure 1 atm.

Adiabatic flame temperature T_{ad} may be found using expression for enthalpy of species i as function of temperature:

$$h = h_{f_i}^0 + \int_{T_0}^{T} c_{p_i}(T)dT = h_{f_i}^0 + \bar{c}_{p_i}(T - T_0), \tag{2.5.5}$$

where $h_{f_i}^0$ is i-th species enthalpy of formation (enthalpy at standard state), $c_{p_i}(T)$ is i-th species specific heat as a function of temperature, $\bar{c}_{p_i}$ is average specific heat of i-th species in the considered temperature range.

Example of analytical solution for adiabatic flame temperature

Let's consider combustion of 10% hydrogen-air mixture with water vapour as the only combustion product with left unreacted oxygen and inert nitrogen assuming the process is at constant pressure, adiabatic (no heat exchange with environment) and the reaction system is closed (no mass exchange with surroundings):

$$0.1H_2 + 0.9\cdot(0.21O_2 + 0.79N_2) \Rightarrow 0.1H_2O + 0.139O_2 + 0.711N_2. \tag{2.5.6}$$

For such a reaction the enthalpy balance is

$$0.1h_{H_2} + 0.189h_{O_2} + 0.711h_{N_2} = 0.1h_{H_2O} + 0.139h_{O_2} + 0.711h_{N_2}. \tag{2.5.7}$$

Using expression (2.5.5) the enthalpy balance may be re-written:

$$\begin{aligned} &0.1\left(h_{H_2}^0\right) + 0.189\left(h_{O_2}^0\right) + 0.711\left(h_{N_2}^0\right) = \\ &= 0.1\cdot\left[h_{H_2O}^0 + \bar{c}_{pH_2O}(T_{ad} - T_0)\right] + 0.139\left[h_{O_2}^0 + \bar{c}_{pO_2}(T_{ad} - T_0)\right] + 0.711\left[h_{N_2}^0 + \bar{c}_{pN_2}(T_{ad} - T_0)\right]. \end{aligned} \tag{2.5.8}$$

Enthalpies of formation of stable species at standard state are equal to zero: $h^0_{f_{N_2}} = 0$, $h^0_{f_{O_2}} = 0$, $h^0_{f_{N_2}} = 0$, hence:

$$0.1 \cdot \left[h^0_{f_{H_2O}} + \bar{c}_{p\,H_2O}(T_{ad} - T_0)\right] + 0.139\left[\bar{c}_{p\,O_2}(T_{ad} - T_0)\right] + 0.711\left[\bar{c}_{p\,N_2}(T_{ad} - T_0)\right] = 0. \quad (2.5.9)$$

Adiabatic flame temperature T_{ad} is the only unknown in the above equation. Isolating T_{ad}, the analytical solution becomes:

$$T_{ad} = T_0 - \frac{0.1 \cdot h^0_{f_{H_2O}}}{0.1 \cdot \bar{c}_{p_{H_2O}} + 0.139 \cdot \bar{c}_{p_{O_2}} + 0.711 \cdot \bar{c}_{p_{N_2}}}. \quad (2.5.10)$$

Numerical values of parameters in the above equation are given in Table 2.5-1, values are given both per mole for analytical solution (2.5.10) and per kg for use in numerical codes. Specific heat values are evaluated at constant temperature T=900K.

Table 2.5-1. Numerical values for analytical T_{ad} solution.

	Values per mole	Values per kg
Enthalpy of formation for water vapour $h^0_{f_{H_2O}}$	- 241838 J/mol	120.919 MJ/kg
Hydrogen specific heat $\bar{c}_{p_{H_2}}$	29.66 J/mol/K	14830 J/kg/K
Oxygen specific heat $\bar{c}_{p_{O_2}}$	34.368 J/mol/K	1074 J/kg/K
Nitrogen specific heat $\bar{c}_{p_{N_2}}$	32.088 J/mol/K	1146 J/kg/K
Water vapour specific heat $\bar{c}_{p_{H_2O}}$	39.906 J/mol/K	2217 J/kg/K

Substitution of values in solution (2.5.10) results in temperature:

$$T_{ad} = T_0 - \frac{0.1 \cdot h^0_{f_{H_2O}}}{0.1 \cdot \bar{c}_{p_{H_2O}} + 0.139 \cdot \bar{c}_{p_{O_2}} + 0.711 \cdot \bar{c}_{p_{N_2}}} =$$

$$= 298(K) - \frac{-0.1 \cdot 241838\left(\frac{J}{mol}\right)}{0.1 \cdot 39.906\left(\frac{J}{K\,mol}\right) + 0.139 \cdot 34.368\left(\frac{J}{K\,mol}\right) + 0.711 \cdot 32.088\left(\frac{J}{K\,mol}\right)} = 1063.7\,K. \quad (2.5.11)$$

Practical considerations

Above solution is for the closed, adiabatic system, which means that combustion products composition should not mix with ambient air and radiation heat exchange is ignored. Example of such reactive system may be, e.g. premixed hydrogen-air mixture deflagration in open atmosphere.

Diffusive burners and fires usually provide intensive entrainment of fresh air into reaction area resulting in temperatures significantly lower than adiabatic one.

Choice of combustion model for numerical simulations is not significant as long as it allows to specify composition of combustion products, specific heats and heat of reaction (i.e. enthalpy of water vapour formation) as per analytical solution.

If numerical simulations were conducted using compressible solver it is worth to analyse pressure to make sure that it does not deviate significantly from absolute value 1 atm and combustion products expansion or compression is not affecting adiabatic flame temperature.

2.5.6 Detonation

Key parameters for 1D detonation:

Detonation is the most violent combustion mode, through analysis of the 1D conservation law of detonation, it was identified that the chemical reaction is the key to the propagation of the detonation wave. During the analysis of a detonation wave using the 1D model, the propagation speed of the shock front can be derived in a simple form. Following such analysis the speed of detonation wave depends on the chemical energy released by the reactants:

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

In upper equation, γ_p and γ_r are the specific heat ratio of the products and the reactants, Q_{chem} is the energy released per mass through reactants, T_0 is the temperature of the reactants, C_v^r is the heat capacity of the reactants and the μ_r is the mass per mole of reactants. Based on the speed of the detonation wave important parameters such as the von Neumann pressure, CJ pressure and von Neumann density can be estimated (Zeldovich et al., 1985).

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

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

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

As shown by upper equations, energy released through chemical reaction (thermo dynamics) is the key parameter of interest. In these equations all parameters, apart from chemical energy (or the speed which is determined by the chemical energy), can be considered as constants. Therefore, if the

calculation can match the propagation speed, pressure of von Neumann peak, pressure of CJ point or density of von Neumann peak, then the chemical reaction of the detonation in the calculation will reflect reality. In most situations, the speed of the detonation wave and the peak pressure value of the detonation are the most general outputs of the calculation.

Parameters of CJ detonation in stoichiometric H_2/air mixture:

Detonation velocity	2029.058304 m/s
Chapmen-Juge pressure	16.167181 atm
Peak pressure (Energy)	28.542605 atm
Peak pressure (Mach OK)	28.775075 atm
Peak mass velocity	1622.721024 m/s
Peak density	4.261325 kg/cub.m
Initial density	0.854528 kg/cub.m
Initial pressure	1.000000 atm.
Initial temperature	298.149994 K
Reactants gamma	1.400000
Products gamma	1.210000
Reactants mol. weight	0.020911 kg/mole
Products mol. weight	0.024530 kg/mole
Combustion heat	4400000.000000 J/kg

2.6 Verification Worked Example: Molecular Diffusion

2.6.1 Introduction

This Section describes work carried out by HSL to compare ANSYS CFX predictions of molecular diffusion to an analytical solution. The work considers an 8 m high geometry initially filled with a mixture of helium and air in its upper half and pure air its lower half.

The analytical solution is described in Section 2.6.2, the CFD modelling approach is described in Section 2.6.3, the results are presented and discussed in Section 2.6.4 and finally, conclusions are drawn in Section 2.6.5.

2.6.2 Analytical Solution

Molecular diffusion in a two-component variable density mixture can be described using Fick's law of diffusion (Bird *et al.,* 1960):

$$J = -cD\nabla x_{he} \tag{2.12}$$

where J is the molar flux, c is the molar concentration, D is the molecular diffusivity coefficient and x_{he} is the helium molar fraction.

The molar concentration and molecular diffusivity coefficient can be assumed to be constant such that for a one-dimensional problem Equation (2.12) leads to the unsteady, one-dimensional diffusion equation:

$$\frac{\partial x_{he}}{\partial t} = D\frac{\partial^2 x_{he}}{\partial y^2} \tag{2.13}$$

where t is time and y is the vertical coordinate.

Equation (2.13) can be solved using the method of separation of variables to obtain (Crank, 1975):

$$x_{he} = x_{he,0}\left\{\frac{h}{l} + \frac{2}{\pi}\sum_{n=1}^{\infty}\sin\left(\frac{n\pi h}{l}\right)\exp\left(-\frac{n^2\pi^2}{l^2}Dt\right)\cos\left(\frac{n\pi y}{l}\right)\right\} \tag{2.14}$$

where h is the initial height of the helium stratification and l is the height of the geometry. For a vertically symmetrical system with $h = l/2$, Equation (2.14) can be simplified to obtain (Taylor and Krishna, 1993):

$$x_{he} = x_{he,0}\left\{\frac{1}{2} + \frac{1}{\pi}\sum_{k=0}^{\infty}\frac{1}{m}\sin\left(\frac{m\pi y}{l}\right)\exp\left(-\frac{m^2\pi^2}{l^2}Dt\right)\right\} \tag{2.15}$$

where $m = k + 1/2$.

Although Equation (2.15) is referred to as analytical solution it is usually evaluated numerically. Figure 4 shows solutions to Equation (2.15) calculated using Matlab for $D = 7.35\times10^{-5}$ m^2/s (Bird *et al.,* 1960), $l = 8$ m, $t = 1800$ s and $x_{he,0} = 0.4$ v/v.

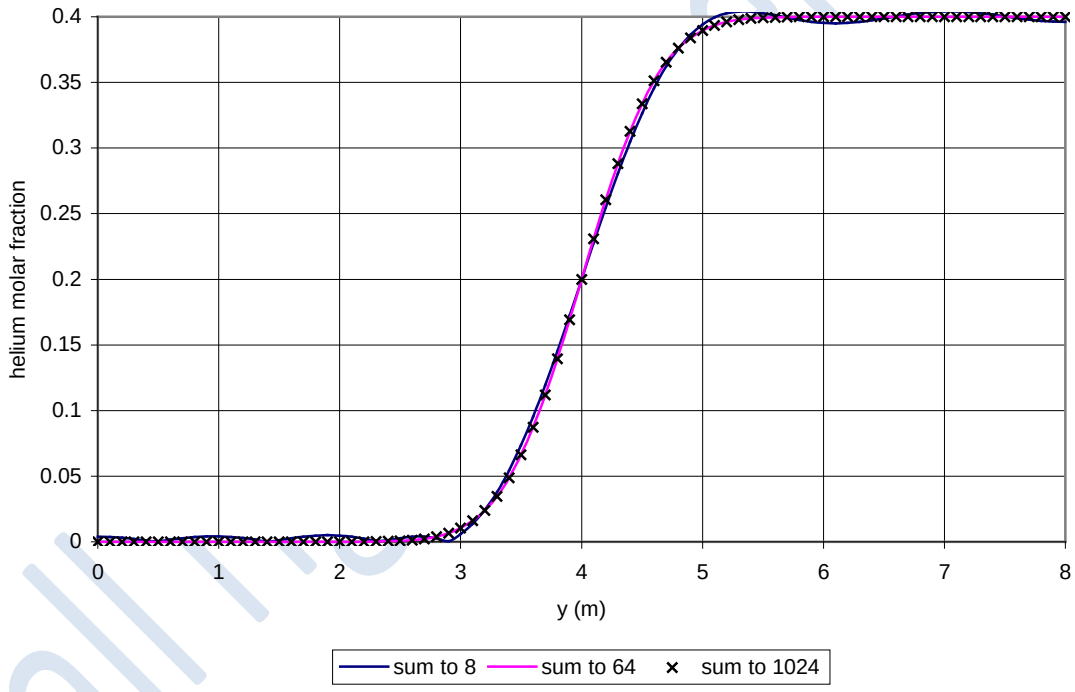


Figure 4 Solutions to Equation (2.15) with infinity replaced by 8, 64 and 1024 for $D = 7.35\times10^{-5}$ m^2/s, $l = 8$ m, $t = 1800$ s and $x_{he,0} = 0.4$ v/v.

Figure 4 shows that good accuracy can be achieved by replacing infinity with 64. As the computations are quick to run the analytical solutions presented in the following Section were calculated using 1024 in place of infinity.

2.6.3 CFD Modelling Approach

This Section describes the CFD modelling approach including the geometry, initial and boundary conditions, mesh and choice of sub-models. Note that some model settings (e.g. the sub-models for turbulence and buoyancy) were chosen on the basis of the model being used (after the verification study) for another more complicated problem involving both molecular and turbulent mixing.

The geometry is a 1 m diameter, 8 m high cylinder initially filled with a helium molar fraction of 0.4 v/v in its upper half, as shown in Figure 5. The velocity was initially set to zero and the turbulence to a low intensity. The boundaries of the cylinder were modelled as hydraulically smooth, no-slip walls.

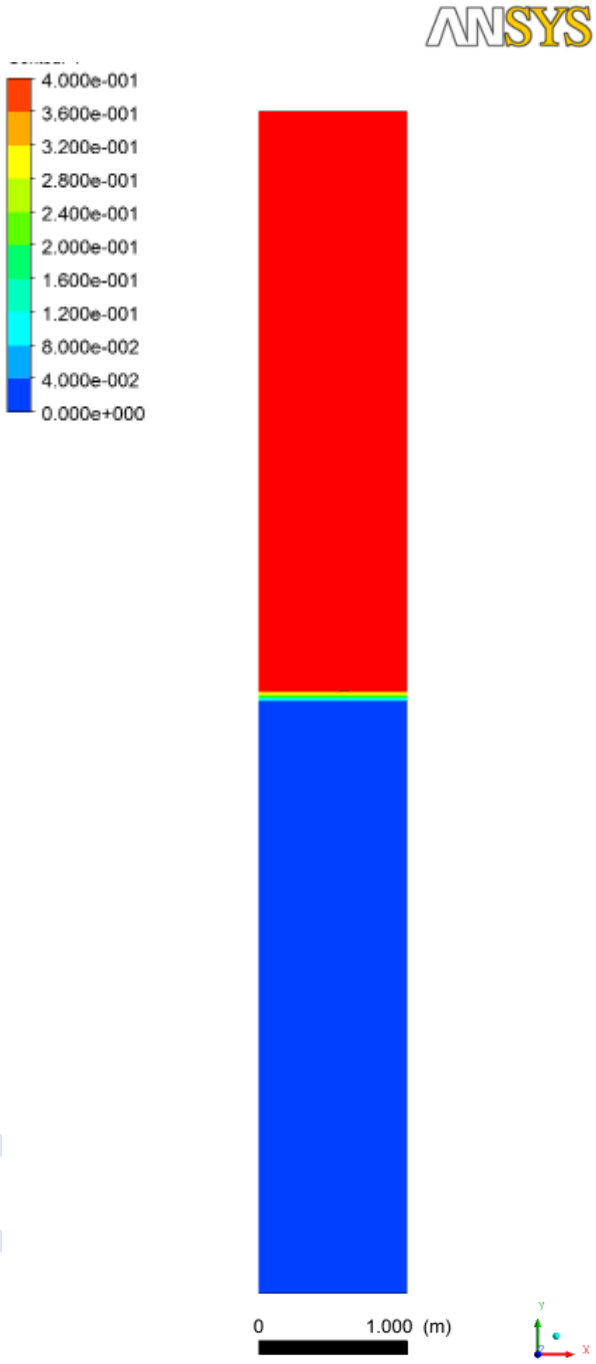


Figure 5 Initial helium molar fraction distribution used for the molecular diffusion simulations.

Six meshes were used for the simulations, namely coarse, medium and fine resolution tetrahedral and prism meshes, as shown in Figure 6.

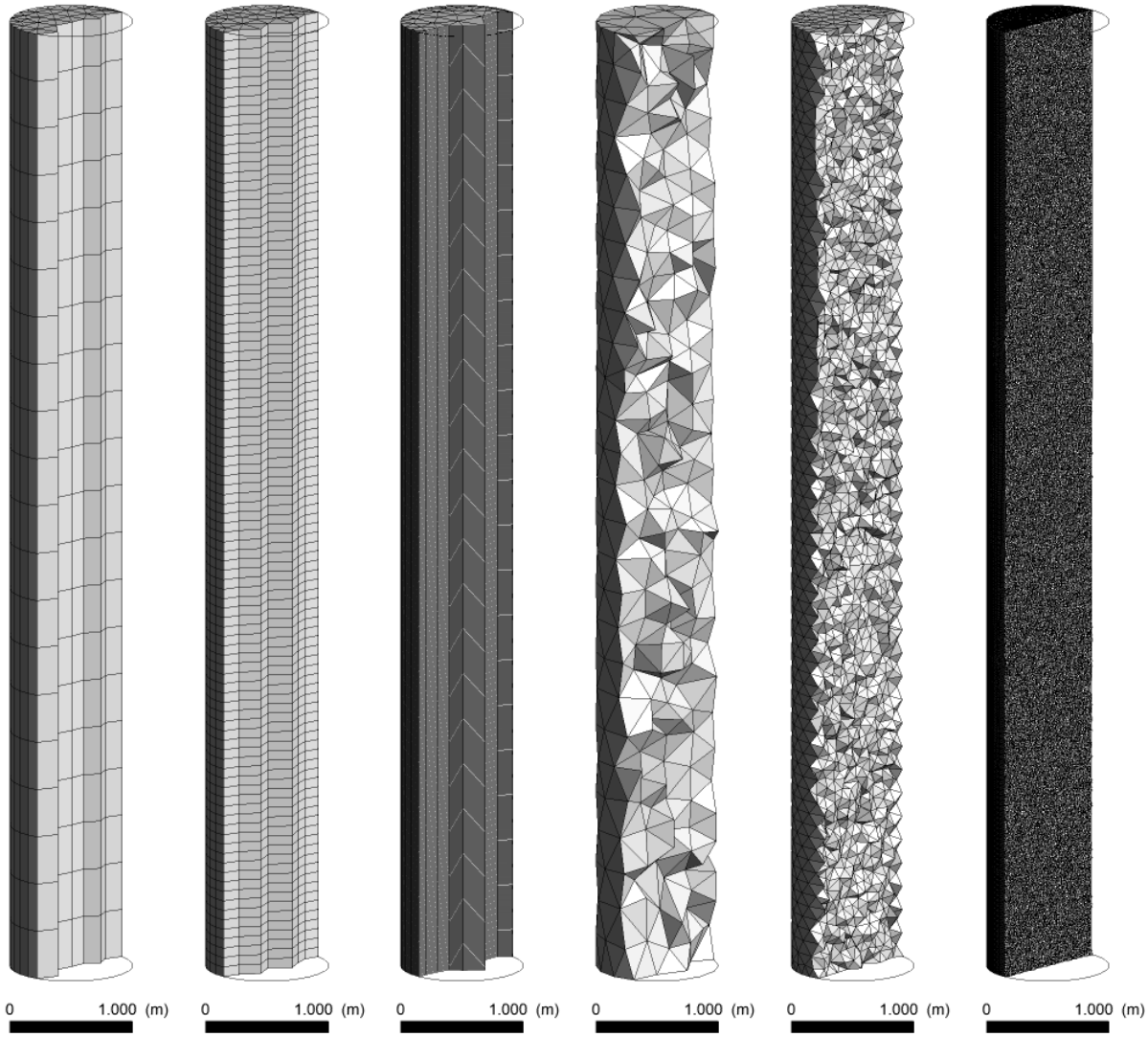


Figure 6 Coarse, medium and fine resolution tetrahedral and prism meshes used for the molecular diffusion simulations.

The helium distribution was modelled using a multi-component flow approach, which assumes that helium and air mix at the molecular level and that they share the same mean velocity, pressure and temperature fields (ANSYS, 2010a). This approach solves a scalar transport equation for the helium mass fraction (ANSYS, 2010b):

$$\frac{\partial(\rho\omega_{he})}{\partial t} + \nabla\cdot(\rho U\omega_{he}) = \nabla\cdot(\rho D\nabla\omega_{he}) \tag{2.16}$$

where ρ is the fluid density, ω_{he} is the helium mass fraction and U is the fluid velocity. The molecular diffusivity coefficient was set to D = 7.35×10^{-5} m^2/s (Bird *et al.,* 1960).

The simulations presented here were carried out using the k–ε turbulence model and included the effects of buoyancy on turbulence production and dissipation (ANSYS, 2010b). The effects of buoyancy on the velocity field are modelled using a source term in the momentum equation (ANSYS, 2010b):

$$S_{buoy} = (\rho - \rho_{ref})g \tag{2.17}$$

where ρ_{ref} is a reference fluid density and g is gravitational acceleration. Typically, the local instantaneous fluid density, ρ, depends on the temperature and is calculated using the ideal gas law or another equation of state. However, to reduce the potential for errors in the velocity field the simulations were carried out as isothermal simulations and with helium and air represented as constant density fluids (ANSYS, 2011c).

To further reduce the possibility of errors in the velocity field the simulations were carried out using the double precision solver and linearly exact numerics (ANSYS, 2011a and 2011c).

Six simulations are presented here, one simulation for each mesh, as shown in Table 2. Additional simulations were carried out to assess the sensitivity of the predictions to the choice of turbulence model and equation of state, the choice of time step and RMS convergence criteria, and the use of the double precision solver and linearly exact numerics. Whilst these additional simulations are not described here they helped inform and provide confidence in the set of analyses presented.

Table 2 Overview of the molecular diffusion simulations.

Simulation	Mesh type	Mesh resolution
S1	prism	medium
S2	prism	coarse
S3	prism	fine
S4	tetrahedral	medium
S5	tetrahedral	coarse
S6	tetrahedral	fine

2.6.4 Results and Discussion

Figure 7 shows helium molar fraction predictions at time t = 1800 s from Simulations S1, S2 and S3, which were carried out using different resolution prism meshes. The predictions are insensitive to the mesh resolution and in good agreement with the analytical solution (note that in Figure 7 the analytical solution is obscured by the predictions from Simulation S2).

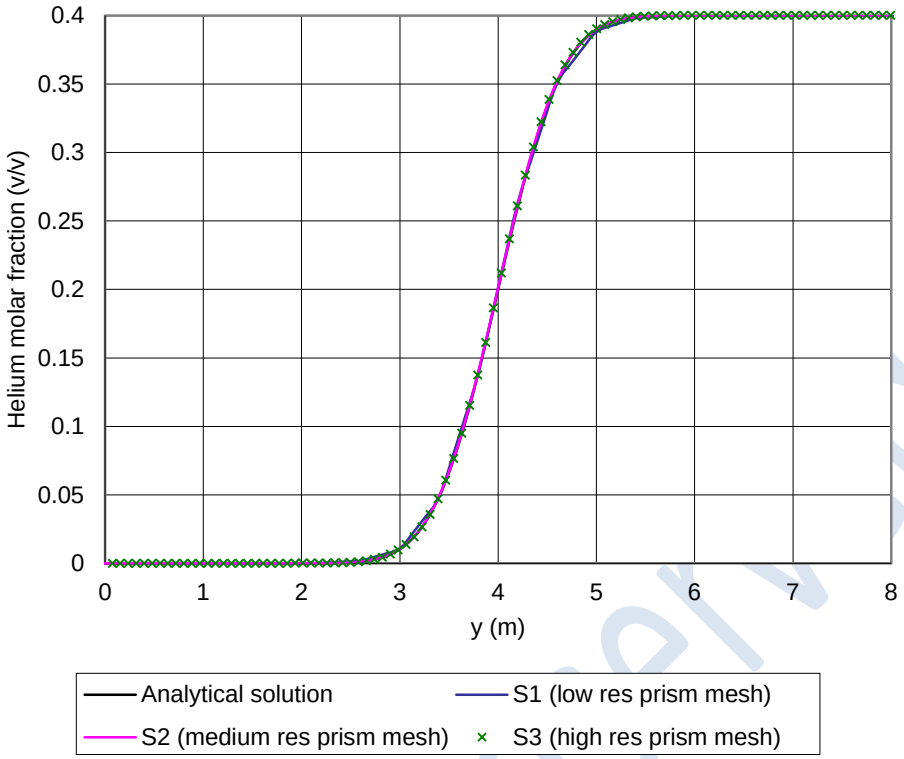


Figure 7 Analytical solution and CFD predictions of helium molar fraction at t = 1800 s from simulations on prism meshes.

Contour plots of helium molar fraction from Simulation S2 at times t = 0, 600, 1200 and 1800 s are shown in Figure 8. The helium distribution is characterised by an initially sharp interface that becomes progressively more diffuse.

Corresponding predictions from Simulations S4, S5 and S6 carried out using different resolution tetrahedral meshes are shown in Figure 9. These predictions are sensitive to the mesh resolution and not always in agreement with the analytical solution.

After some investigation it was found that the use of a tetrahedral mesh can induce small, unphysical, buoyancy-driven convection currents and that these can counteract molecular diffusion. Correspondence with ANSYS revealed that this unphysical behaviour is not unique to the version of CFX used here and that it could occur in simulations run on other non-aligned meshes (meshes that are not aligned perpendicular to gravity), including non-aligned structured meshes.

Contour plots of the helium molar fraction from Simulation S5 at times t = 0, 600, 1200 and 1800 s are shown in Figure 10. The contour plots show that the helium distribution is characterised by an initially sharp interface, which then remains sharp. A close up of the interface at t = 1800 s is presented in Figure 11, together with corresponding velocity vectors, which illustrate the small, unphysical, buoyancy driven convection currents.

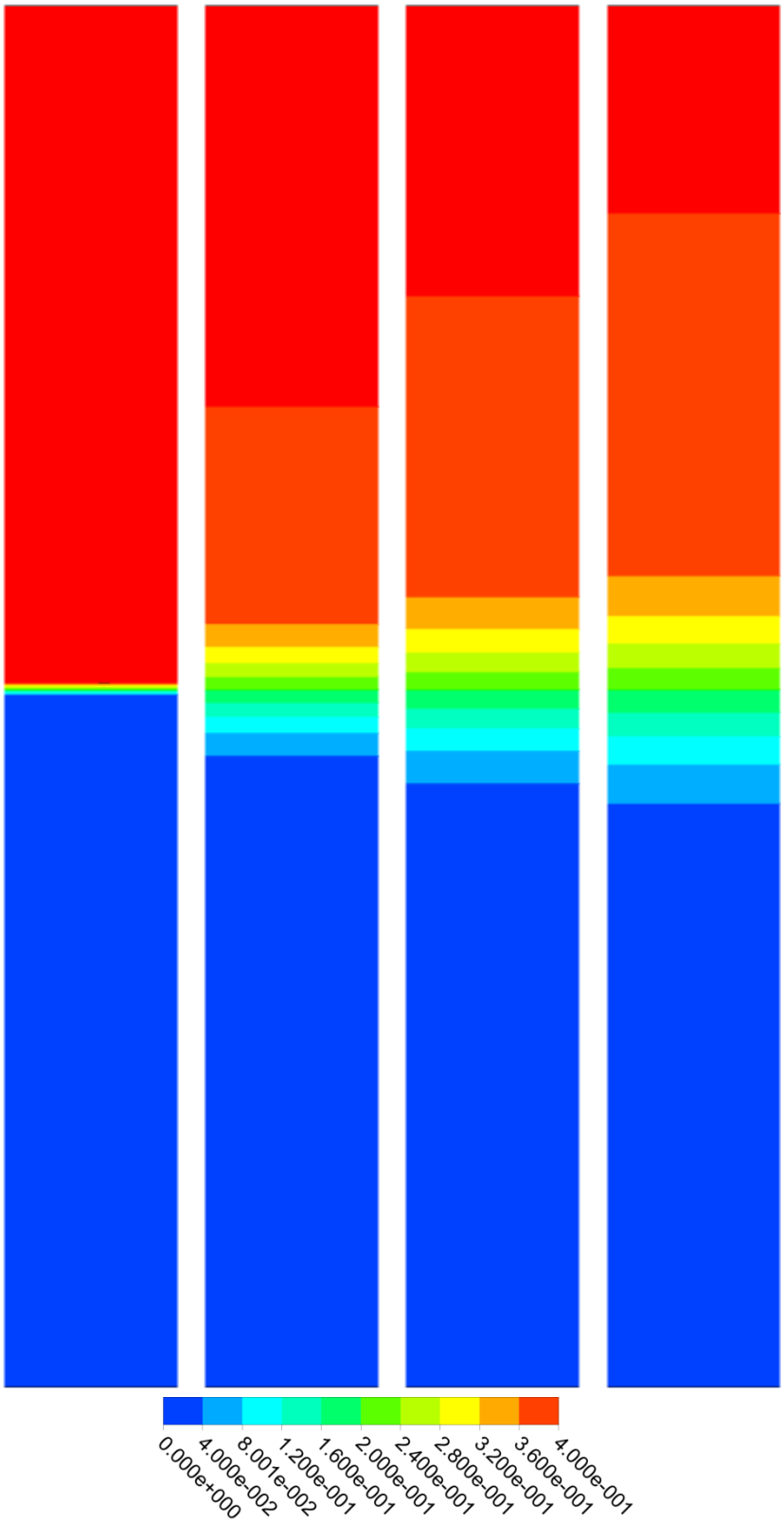


Figure 8 Helium molar fraction predictions from Simulation S2 on a prism mesh at (from left to right) t = 0, 600, 1200 and 1800 s.

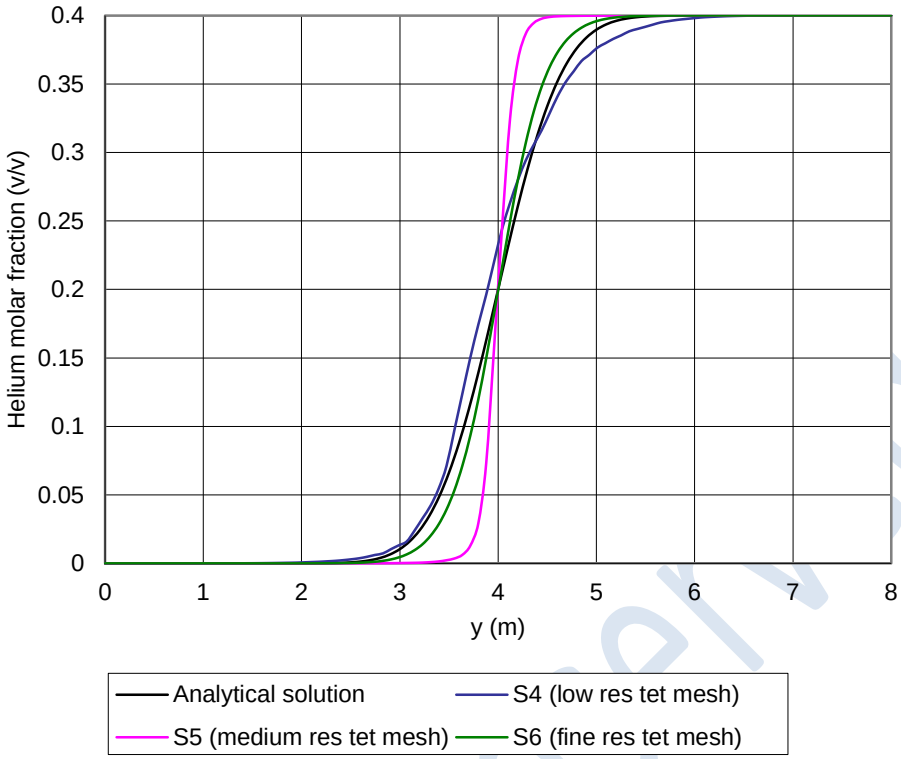


Figure 9 Analytical solution and CFD predictions of helium molar fraction at t = 1800 s from simulations on tetrahedral meshes.

2.6.5 Conclusions

This simple case study highlights the need to carry out model verification. The verification study found that while CFX simulations on gravity-aligned meshes provide accurate predictions of molecular diffusion, corresponding simulations on non-aligned meshes can lead to unphysical results.

In more complex flows this effect may be relatively subtle and therefore more difficult to spot. By considering physical processes such as molecular diffusion in isolation issues such as this can be easier to identify.

Finally, it is noted that in addition to being in poor agreement with the analytical solution, the tetrahedral mesh predictions are sensitive to the mesh resolution. Carrying out a thorough mesh sensitivity analysis as recommended in SUSANA D3.2 or existing best practice guidelines (e.g. NEA, 2015) could also help to identify this unphysical effect.

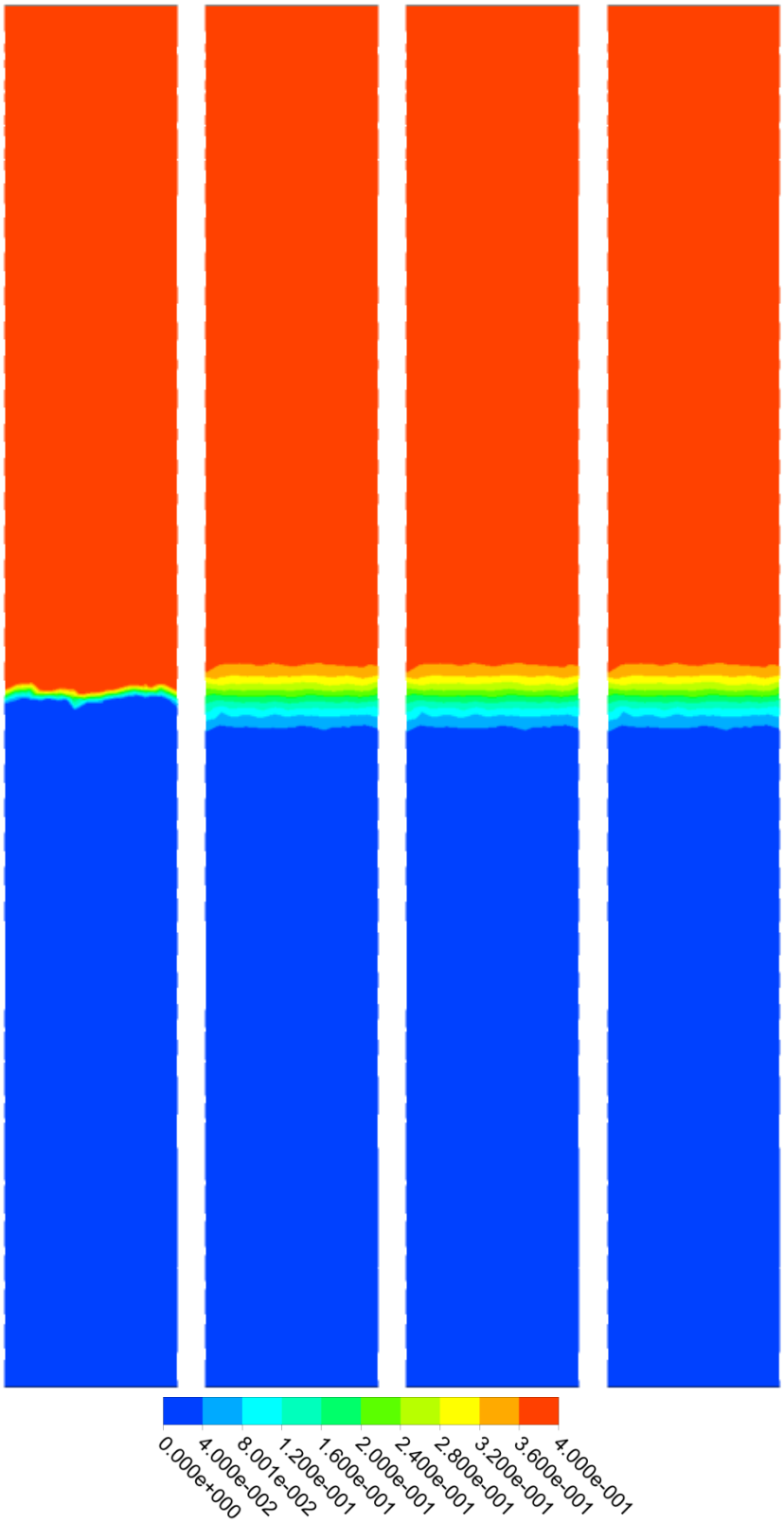


Figure 10 Helium molar fraction predictions from Simulation S5 on a tetrahedral mesh at (from left to right) t = 0 s, t = 600 s, t = 1200 s and t = 1800 s.

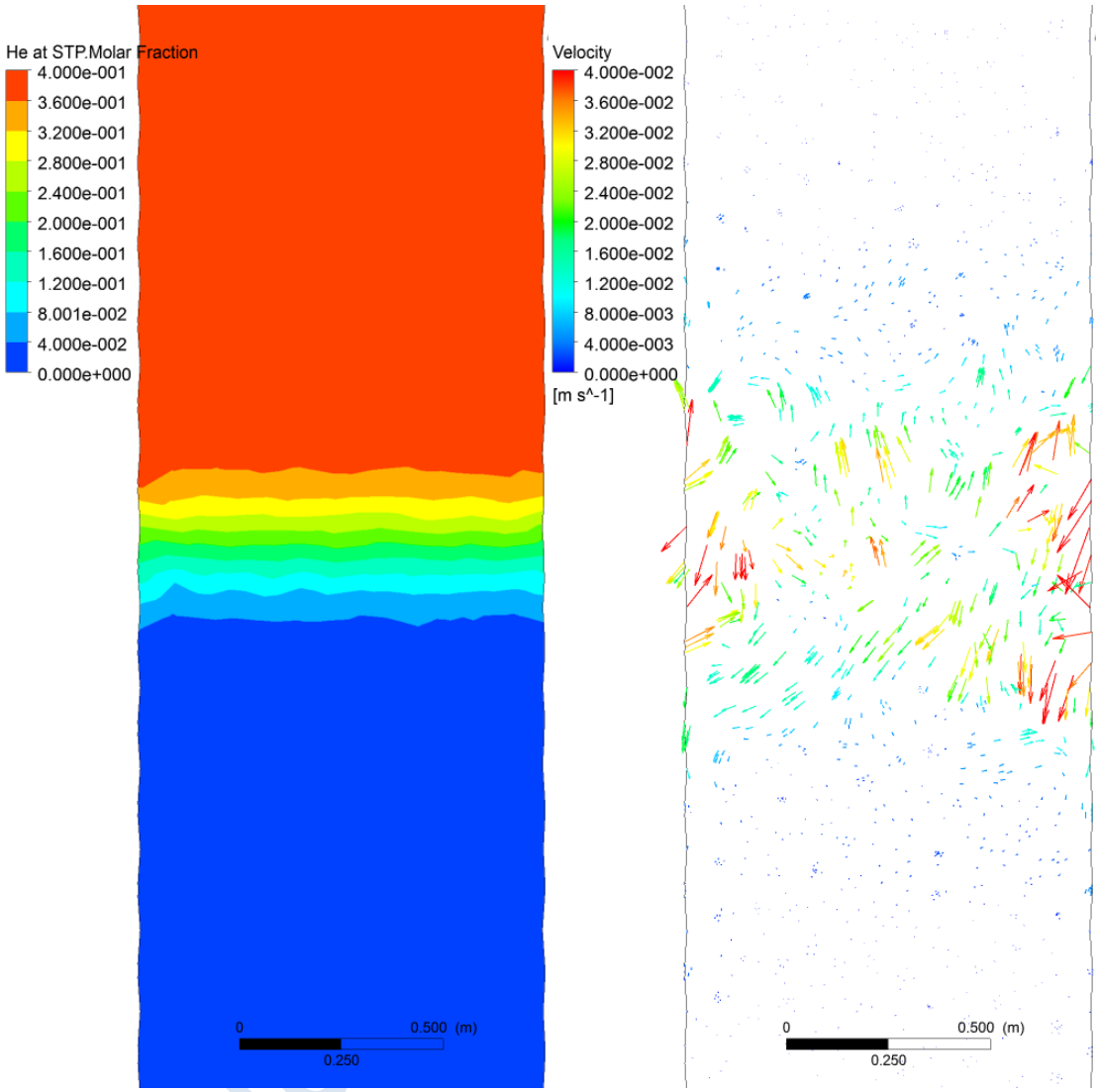


Figure 11 Helium molar fraction predictions (left) and velocity vectors (right) from Simulation S5 on a tetrahedral mesh at t = 1800 s.

2.7 Using the Verification Database

A database of Hydrogen Safety-related CFD verification procedures has been assembled and is available at:

http://www.support-cfd.eu/index.php/verification-database

In line with advice on best practice in the literature[15], database entries are grouped according to the *type* of verification undertaken. Reflecting the overview on verification already provided in this chapter, the grouping is:

Analytical Solutions: where the accuracy of numerical outputs from a code can be assessed against an analytical solution to the same equations.

Code verification: checking for consistency of outputs following simple operations such as translating or rotating the domain, mirroring the domain, mass continuity tests.

Manufactured Solutions: where source terms are added to the governing equations such that the solution to the modified equations is amenable to an analytical solution.

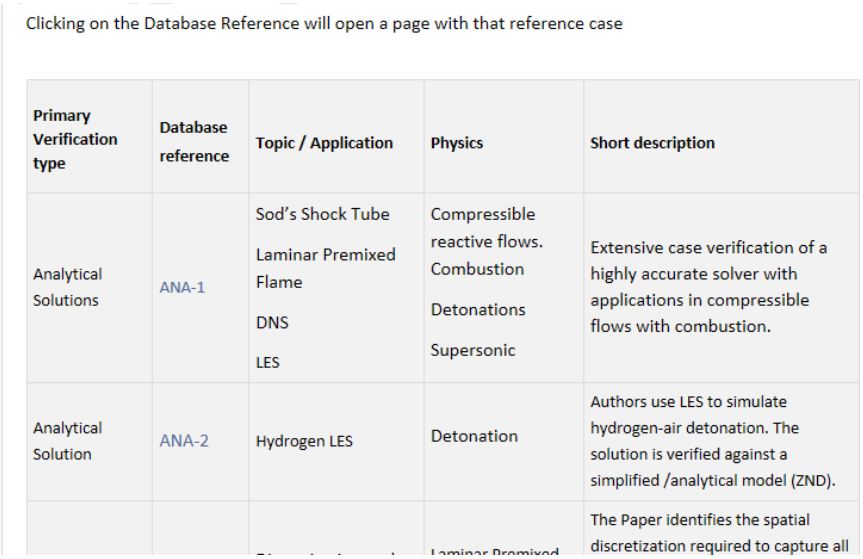
Methodology: A reference which explains verification processes or terminology.

Numerical Solutions: where the accuracy of numerical outputs from a code can be assessed against the outputs from other codes which have been well tested and are of known high quality.

Sensitivity Studies (Grid and Parameter Sensitivity): where the impact of numerical parameters (such as grid size) and case parameters (such as fluid properties, boundary conditions) are assess.

Each summary entry on the landing page follows the structure given on the right.

To aid the identification of useful references, the tables use key words for:



Clicking on the Database Reference will open a page with that reference case

Primary Verification type	Database reference	Topic / Application	Physics	Short description
Analytical Solutions	ANA-1	Sod's Shock Tube Laminar Premixed Flame DNS LES	Compressible reactive flows. Combustion Detonations Supersonic	Extensive case verification of a highly accurate solver with applications in compressible flows with combustion.
Analytical Solution	ANA-2	Hydrogen LES	Detonation	Authors use LES to simulate hydrogen-air detonation. The solution is verified against a simplified /analytical model (ZND).
				The Paper identifies the spatial discretization required to capture all

[15] Oberkampf and Trucano, "Verification and Validation benchmarks", Nuclear Engineering and Design 238 (2008) 716-743.

- The main **topic / application** area for the reference (for example, Nuclear, Fire Safety etc) this helps the user understand the relevance of the database entry to their industrial application, as well as the methodologies used by others for undertaking verification tests.
- The **physical phenomena** tested in that reference (combustion, turbulence, etc) this aids the used to understand which terms in the equations can be tested and what the most appropriate verification method is to exercise these terms in a verification test.

Each database entry follows a common structure as shown opposite:

The information provided gives sufficient information for the user to determine whether the database reference is suitable or valid for their purposes. Links are provided back to the original reference.

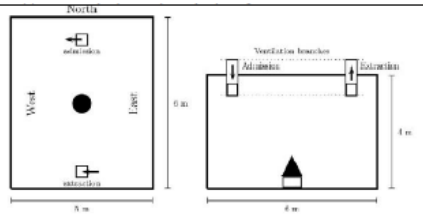
Note that in some cases, entries provide more than one type of database source. Where this occurs they are presented according to the "main" verification type given, and information on other verification data is also noted.

In the process of producing the on-line version of the database, we took the opportunity to add a small number of references, and some references were more logical in the new structure to split into a number of entries. However the dataset itself is nearly identical to that shown previously. There are 52 entries the database

This dataset is the first of its kind to be assembled for verification. It meets the objective in providing a very useful resource for practitioners to understand what verifications methods can and should be applied to the numerical code they are using, as well as identifying what those tests cases are.

SUSANA

SUpport to SAfety ANalysis of Hydrogen and Fuel Cell Technologies

Verification type	Analytical Solutions
Database reference	ANA-4
Topic / Application	Analytical Solutions Manufactured Solutions Numerical Solutions Validation
Physics	Compartment Fires Taylor Green Vortices Beltrami Flows Laminar Flow around circular obstacle
Summary	This paper contains a comprehensive set of references for analytical solutions to flowfields of relevance to fires and internal flows. MMS and Numerical solutions are also used on more complex flows.
Description	The paper outlines verification (and validation) processes on a fire field model developed by the authors. The terminology and methodology given in the reference literature are fully respected in that verification deals with mathematics and validation with physics. The verification process compares numerical results with highly accurate solutions given by analytical, manufactured or published benchmark solutions. The paper collates a very useful set of references for analytical solutions to flow cases In contrast, the validation phases of the code use a building-block approach to divide a complex system into simpler validation cases through three intermediate tiers: the unit problems, the benchmark cases and finally, the subsystem cases.
Case Title	Verification and validation of a CFD model for simulations of large-scale compartment fires
Authors	S. Suarda, C. Lapuertaa,b, F. Babika, L. Rigollet
Year	2011
Online reference	Nuclear Engineering and Design 241 (2011) 3645–3657
Case image	 Top view (left) and side view (right) of the fire.
Governing equations	
Results	

3. Validation Procedures

Validation assessment process can be defined as a comparison process between the predictions of a model which has been run to simulate a given event and the observations made in connection with the same event[16]. See chapter 2 for the definitions adopted by the SUSANA project.

The objectives of the validation procedure are:

- to define the variables that are the most important for predictions
- to define how the comparison between the model outputs and experimental observations should be done
- to highlight who will be the users and how the models results should be used

In the validation process, several steps should be done, firstly the selection of experimental data then the selection of the variables which will be compared with the experimental measures, the definition of how those variables will be compared and finally the estimation of the uncertainties.

Indeed the validation can be either qualitative by means of graphs/plots of observed versus modelled values or more quantitative by means of statistical measures between the observed and modelled values. In the SUSANA project, the validation has been chosen to be a quantitative one via the use of statistical measures performance (detailed in the paragraph 3.2)

After verifying the model is correctly implemented and defining the set of experimental data that will serve as comparison with simulation results, the following step into the validation process is the definition of the target parameters and the statistical performance measures.

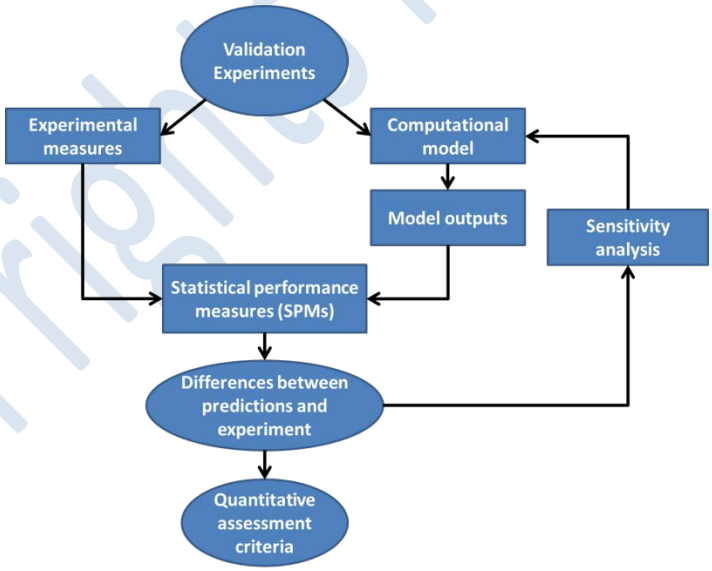


Figure 12 : Diagram of validation procedure

[16] Chapyer 19. Evaluation methodologies for dense gas dispersion models. Nijs Jan Duijm and Bertrand Carissimo

The main steps of the validation procedure are (based on IVINGS-2007)[17]:

a. Specification of the objective: this being the quantification and assessment of model performance for a selected phenomenon.
b. Identification and selection of suitable validation data sets.
c. Define the specific content and design the format of the validation database.
d. Selection of specific cases from these datasets so as to cover the range of target scenarios.
e. Definition of target variables that are measured or derived from measurements and which form the basis of comparisons with model predictions.
f. Selection of statistical performance measures (SPM) that allow quantitative comparison of predictions against measurements.
g. Review and definition of quantitative assessment criteria that define the acceptable numerical range of the SPM which result from applying this validation procedure.
h. Provide guidance on model application for the validation cases.
i. Apply the validation procedure and refine as necessary in the light of experience.

After the selection of various experimental data, the target variables can be selected and will permit to give an idea of which parameters should be followed during the CFD calculation. After running the model(s) the statistical performance measures are a set of formula that allows the comparison between the computed and measured variables. The quantitative assessment criteria can be defined as the ranges of values where the computed target variables are statistically considered to be correctly calculated.

3.1 Model Validation Database

A model validation database has been developed within the framework of the benchmark exercises and is available on the website http://www.support-cfd.eu/mvdb/. For all the experiments classified into 5 main physical categories, a set of information about the experiment is given in 10 topics. The 10 topics include variety aspects of the experiment and let the users have a detailed understanding of the experiments. The 10 topics include:

- Summary: Short description of the experiment, including the draft drawing, simple description and keywords.
- Author: Who did the experiment and who are responsible to the experiment.
- Experimental Setup: Detailed description of the experimental facility, boundary setting and location of instrumentations.
- Objective of Experiment: Which physical phenomena are investigated in this experiment.
- Application Calculation: Which kinds of numerical model can be validated by this experiment.
- Experimental Procedure: Detailed description of experimental phenomena, including the figures or movies.
- Experiment Data: Results of the experiment, including some explanations for the experiment data.

[17] IVINGS-2007-Evaluating Vapor Dispersion Models for Safety Analysis of LNG Facilities Research Project

- Performed Simulation: Some validation cases by using the experiment.
- Reference: Publications related to the experiments.
- Comments: Some suggestion from the user, the interface for the communication

The deliverable D5.1 "Model Validation Database – Part 1" gives a detailed description of the model validation database.

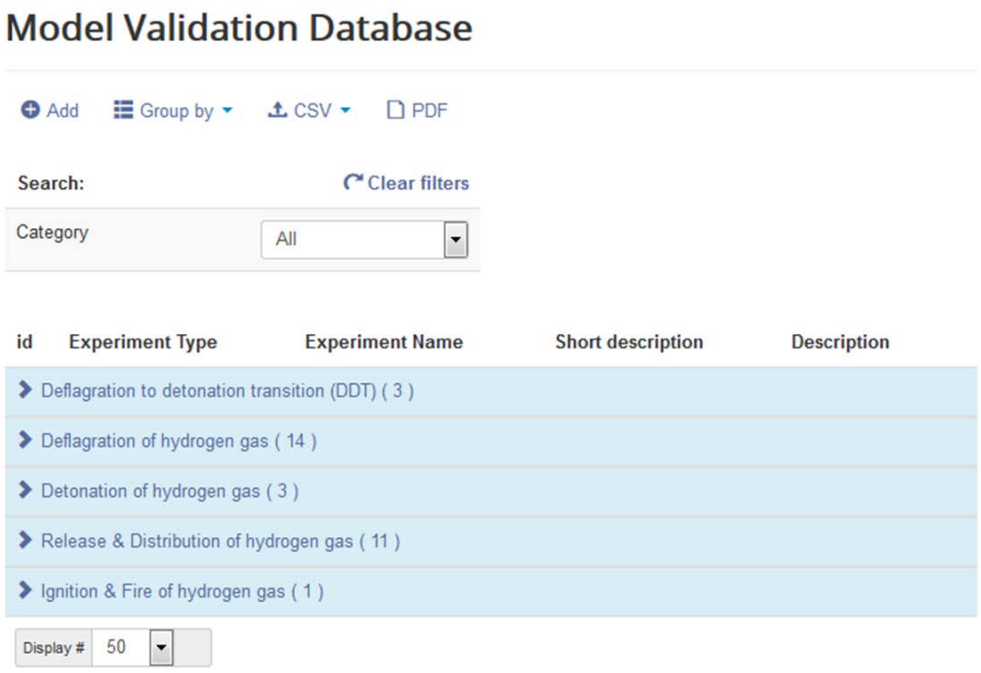


Figure 13 : Interface of Database

3.2 Target variables

The target variables are the most relevant variables for each phenomenon that will be considered for the comparison between simulations results and experimental data. Those target variables should be outputs of simulations. For each phenomenon, main and specific parameters permit to understand the physics behind the phenomenon.

Those target variables can show the evolution of the parameter in space or/and in time. All of those target variables are given in function of the different means and techniques of measures currently available and in function of the experiments/experimental measures from the validation model database.

3.2.1 Release and mixing of gaseous hydrogen, including permeation

Table 3- Target variables for release and mixing of *gaseous* hydrogen

	Direct target variable	Derived target variable	Comments
erisatio n of the leak- source	Pressure and temperature inside the hydrogen storage		This will permit to calculate the flow rate and affect flow rate and temperature of released

	vessel and in the pipe		hydrogen. If the pressure into the vessel is superior to 70b the law of perfect gases is not applicable
	Flow rate (mass / volume)		From the flow rate, the velocity can be calculated if the diameter (and density) is known
	Pressure and Temperature dynamics in the nozzle exit		Difference in temperature of released hydrogen and surrounding air in enclosure could affect mixing, e.g. for blowdown releases when temperature of gas in the nozzle exit is relevant.
Jet/Plume	Hydrogen concentration dynamics		For all variables, the values could be provided both in the jet and/or outside the jet areas. (distribution in space and time)
		Size of jet; Length, distance to the LFL and UFL	
		Mass and volume of hydrogen in flammable envelope	Derived from the concentration distribution field. Can give an idea of the total quantity of hydrogen released
	Velocity flow field		in the jet, at the nozzle (distribution in space and time)
	Turbulent fluctuation velocity		Should include the turbulence intensity u' and length scale Lt (Turbulent flows only)
	Visualisation of jet shape		Schlieren and BOS techniques of visualisation of changes in gas density are useful for validation, e.g. for transition of momentum-dominated jet to buoyance-controlled.

Dispersion	Hydrogen concentration dynamics	Concentration field	In order to describe the transitory regime, steady regime and the transition
		Gradient of concentration	
	Flow Rate	Average velocity	
		Residual turbulence	
	Pressure dynamics into the enclosure		Most relevant for releases indoors, e.g. the pressure peaking phenomenon (for combination of relatively large flow rate and small vent openings)
	Flow rate through the opening vents		

3.2.2 Release and mixing of liquid hydrogen

Table 4 - Target variables for release and mixing of *liquid* hydrogen

Direct target variable	**Derived target variable**	**Comments**
Flow rate (velocity) at source		
Temperature		
Evaporation rate		
GH_2 fraction at the source		
LH2 pool radius		
Hydrogen/oxygen/water vapour concentration	Condensation rate of water and air components/species	
	Flammable mass/volume	Derived from concentrations

3.2.3 Ignition

Table 5 - Target variable for ignition

	Direct target variable	Derived target variable	Comments
Delayed ignition	Type of igniter (size/shape)		Characterisation of the igniter
	Energy of igniter		
	Location of igniter		
	Pressure produced by the igniter		
Auto-ignition	Shape of reacting flow and combustion products escaping a pipe after ignition		
	Time of ignition after start of rupture disk opening	Rupture disk opening time	Time of a rupture disk opening is proved to be extremely important to reproduce accurately the ignition location and time *Remarks: this is available only for TPRD*
1st steps of combustion	Pressure field and dynamics		
	Temperature field and dynamics		
	Visualisation of fire shape		

3.2.4 Fires

Table 6 - Target variables for fires

	Direct target variable	Derived target variable	Comments
Jet fire	Mass flow rate		As a source term from release

	Flame length, width	Flame shape and development	Development of flame shape in time and space is important for unsteady releases and fireballs.
	Flame temperature		Distribution of temperature along the jet axis is important for validation of jet fire simulations.
	Concentration of OH-radicals		Visualisation of the reactional zone
	Heat flux	Radiation fraction of the total heat release rate	
Fire in an enclosure	Concentration of hydrogen and/or oxygen		When relevant to the considered safety problem. It can give an idea of the regime: •Well-ventilated jet fire regime •Under-ventilated jet fire regime: self-extinction regime or external flame regime
	Temperature inside the enclosure		
	Temperature of wall on a surface and in depth		For impinging jets.

3.2.5 Deflagrations

Table 7 - Target variables for deflagrations

	Direct target variable	Derived target variable	Comments
All cases of deflagrations	Pressure dynamics		Dynamics is for both positive and negative pressure phases, including maximum and minimum peak values. Should be controlled at different distances from ignition source, and multiple locations (inside/outside of flammable cloud).
	Location of flame		Punctual information in time

		Flame propagation velocity and acceleration	Pressure in a blast wave is a function of flame propagation velocity and flame acceleration.
	Cinematics of flame	Location of flame	High speed camera can give the global behaviour of flame propagation
		Flame propagation velocity and acceleration	
		Flame surface and volume	
	Surface of flame		
	Velocity of the flow ahead of the flame		
Confined deflagration	Pressure inside the enclosure	Overpressure in different locations	
		Rate of pressure rise	Could be important for selection of differential pressure sensors, etc.
	Dynamics of opening of weak walls/vents		
Coherent deflagrations	Shape of the expulsed flammable cloud		
	Velocity of the expulsed cloud		
	Pressure outside the enclosure		Pressure generated by the explosion of expulsed flammable cloud
fined deflagr	Pressure in different locations		Into the burnt gases and outside the flammable cloud

		Impulse	Should include both the positive and negative phases, indeed impulse and deflagration overpressure are important to determine damage to civil structure from a blast wave.
		Coefficient of reflection/reflected overpressure	
	Flame propagation	Shape of the flame	

3.2.6 Detonations

Table 8 - Target variables for detonations

Direct target variable	**Derived target variable**	**Comments**
Detonation overpressure	P_{CJ} and P_{ZND}	Comparison between theoretical and experimental values
	Reflected overpressure / Coefficient of reflection	Reflection pressure peaks
	Impulse/shape of signal	
	Pressure field	In different locations
Size of the detonation cells		
Detonation velocity		As derived from sequence of pressure dynamics records from different sensors Deficit of coupled flame front/shock wave propagation velocity compare to the theoretical CJ

		value may be observed due to losses in geometries with obstacles.
Velocity of the gases behind the shock wave		

3.2.7 Deflagration to detonation transition – DDT

Table 9 - Target variables for deflagration to detonation transition

Direct target variable	Derived target variable	Comments
Pressure dynamics		In various locations.
Flame propagation dynamics		
Run up distance to DDT		The distance of pre detonation

3.3 Statistical analysis methodology

3.3.1 Statistical performance parameters (measures)

Qualitative evaluation of models can be undertaken by comparison of plots of the relevant variables and this can give a general indication of the ability of a model to predict a particular scenario. This "exploratory data analysis" is recommended by Chang and Hanna (Chang and Hanna, 2005) as a first step in model evaluation, possibly including scatter plots, quantile-quantile plots, residual (box) plots and conditional scatter plots. Such analysis "by eye", while essential and informative, may become subjective or introduce variability. For a more rigorous evaluation, a procedural quantitative approach can be adopted. Statistical Performance Measures (SPMs) provide a means of comparing measured and predicted physical comparison parameters. They are non-dimensional and therefore the comparison made is independent of the units of any observed and predicted quantities. A number of different SPMs have been used by model evaluators over the years and an overview is given by Duijm et al. (Duijm et al., 1996) who suggest the following requirements for a set of SPM:

- They should give an indication of the model's ability, i.e. whether it under- or over-predicts values, such as the maximum concentration or overpressure.
- They should give an indication of the level of scatter i.e. the deviation from the average.
- Equal weight should be given to all measurements/predictions regardless of their absolute values.

A further consideration when selecting SPM is that it is beneficial to be consistent with those previously used in other model evaluations. By doing so, it is possible to gain experience with values of SPM that constitute a model that is performing well. Commonly used SPM in model evaluation are the Mean Relative Bias (MRB), Mean Relative Square Error (MRSE), Geometric Mean (MG), Geometric Variance (VG) and Factor of *n* (FACn).

MRB is based upon the difference between measured (C_o) and predicted (C_p) values, but to meet the requirement for equal weight given to all measure/predicted pairs, the values are normalised by the average of the two:

$$MRB = \left\langle 2\frac{(C_o - C_p)}{(C_p + C_o)} \right\rangle \tag{18}$$

Where the angle brackets $\langle \ldots \rangle$ denote an average over all the measured/predicted pairs. MRB gives an indication of a model's ability to predict the measured values on average, and its sign indicates whether the model is under- or over-predicting. A perfect model would result in an MRB of 0, but under- and over-predictions cancel each other out and a model may appear to perform well for the wrong reason. Therefore, MRB is paired with MRSE which sums the squares of the errors and therefore gives an indication of the scatter in the predictions:

$$MRSE = \left\langle 4\frac{(C_o - C_p)^2}{(C_p + C_o)^2} \right\rangle \tag{19}$$

MG and VG similarly follow MRB and but are based on the logarithms of the measurements and predictions (and therefore proportional to their ratio). This means that equal weight is given to all the pairs and the logarithm also acts to draw in outliers so that the SPM are not dominated by a few

extreme values, which can occur in atmospheric dispersion modelling. MG and VG are defined as follows:

$$MG = exp\left\langle ln\left(\frac{C_o}{C_p}\right)\right\rangle \quad (20)$$

$$VG = exp\left\langle ln\left(\frac{C_o}{C_p}\right)^2\right\rangle \quad (21)$$

A perfect model would result in MG and VG of 1.

A final SPM based upon the ratio of measured to predicted values is FACn, which is:

$$FACn = fraction\ of\ predictions\ where\ 1/n \leq \frac{C_P}{C_O} \leq n \quad (22)$$

FACn is easily visualised and *n* is often 2.

The additive measures, MRB, MRSE and FACn are robust in that they can accept zero values for measurements or predictions, whereas MG and VG cannot. This may cause problems in dispersion simulations in which a model may not predict any concentration at a particular sensor location. Threshold values are sometimes used to avoid this problem, but can give erroneous results and this is discussed further in the following section. The geometric measures, while they cannot accept zero values, are useful in that they can accommodate large ranges.

3.3.2 Methodology

Before the SPM can be calculated, it is important to consider how the model is to be compared with the measurements as this can influence how the data are processed and how the measured and predicted pairs, C_o and C_p are arrived at. At the most basic level, the comparisons can be as per (Chang and Hanna, 2005):

- In time only (measurements and predictions are spatially averaged).
- In space only (measurements and predictions are time averaged at each spatial location).
- In both time and space.

The decision must take into account the particular physics scenario that is being modelled and the type of output from the model, in addition to the potential complexity of the data processing steps. For example, if a model predicts only the time averaged overpressure at a particular location, then the same process can be applied to the experimental data, if time varying values were measured. On the other hand, for a complex time varying atmospheric dispersion simulation, care needs to be taken regarding how the data are processed, in order to avoid misrepresenting the underlying physics. Through inappropriate experimental data processing, it is possible to construe a dispersing plume with different dimensions to that which was originally measured. Converting raw measurement data into a suitable form for model evaluation is therefore a non-trivial task.

Data processing

In many physics scenarios, the measurements of a particular variable will be time series (of concentration or pressure). In some cases, the time series will contain zero values, but more realistically will consist of very small or even negative values which may arise from the sensor inaccuracy or drift. This often occurs around the Limit Of Detection (LOD) for many sensors. If it is only the peak or time averaged values that are of interest then consideration does not need to be given to this step. However, if the time series are of interest, then appropriate consideration needs to be given to how the values below the LOD are treated as this can have an influence on the SPM, particularly MG and VG, which cannot accept zero values.

Two common methods of dealing with values below the LOD are to remove them altogether or to replace them with a fixed value. The latter option was used by Carissimo et al. (Carissimo et al., 2001) where concentration measurements of zero were replaced by a value of 10^{-3} units. The authors acknowledged it would be preferable to base the thresholds on sensor sensitivity but such information was not always available. Helsel (Helsel, 2005) argues that both removal and substitution are overly simplistic. If the measured and predicted values below the LOD are both set equal to the LOD, or some fraction of it, datasets with many low concentrations would make a model appear to perform overly well, because the measurements and predictions would be identical in many cases.

An alternative method is to use Maximum Likelihood Estimation (MLE). This involves fitting a probability distribution to the measurements/predictions (excluding those below some low threshold value). This distribution is then used to replace values below the low threshold value with values obtained by sampling the fitted distribution, i.e. extrapolating the distribution to lower levels. An important consideration in using this approach is to ensure that the MLE distribution fits the measurements well. The method becomes more prone to error as the proportion of very low values increases, since less data is available to fit the distribution. Although the MLE method has advantages, it does not completely resolve the problem of zero or low measured values. It can still result in the generation of small C_o and C_p values, which may cause problems in computing MG and VG. In any case, it is worthwhile identifying which data points represent “genuine” data points and those which have been generated by substitution or the MLE method.

Averaging

If model comparisons are not to be made on peak values or time series then consideration needs to be given to the technique used to average the data. The effect of averaging technique is particularly important where a model predicts a steady-state value which needs to be compared with inherently time varying experimental data such as atmospheric dispersion of dense gases. For atmospheric dispersion data, the aim of time averaging is to capture a relevant snapshot of a cloud over a particular duration or “averaging window”. Setting appropriate averaging windows can be highly subjective and usually one of two approaches is used. The first is a mechanistic one of the type used by Carissimo et al. (Carissimo et al., 2001) in which the arrival and departure of a cloud is set by determining when 10% and 90% of the total dose (the concentration-time product) respectively are reached. The second approach is to visually assess the concentration-time series to determine the periods over which the data should be time averaged. This technique was used by Coldrick et al. (Coldrick et al., 2009) for processing certain time varying atmospheric dispersion datasets into steady state values. For other physics scenarios, similar techniques may be adopted.

3.4 Quantitative criteria

Being able to define what constitutes a 'good' or 'acceptable' model is not straightforward. Indeed, this decision should be based on a combination of different elements: firstly, the scientific assessment; secondly, the verification and finally, the validation.

Quantitative evaluation of the performance of a given model requires the definition of appropriate SPMs; presented in detail in the section 3.3. Previous works; (Duijm et al., 1996), (Carissimo et al., 2001), (Chang and Hanna, 2004) and (Chang and Hanna, 2005); presented a wide range of SPMs and for each, their own associated advantages and disadvantages. Duijm and Carissimo (Duijm and Carissimo, 2002) defined the main requirements of SPMs and divided the SPMs into two main categories (as set out above):

- An SPM should provide a measure of the bias in predictions, i.e. the tendency of a given model to over/under-predict its output
- An SPM should provide a measure of the spread in the predictions made, i.e. the level of scatter from the average over/under-predictions.

However and unfortunately, only limited experiences have been conducted such in-depth model evaluations and quantitative criteria for validation of model performance have only been defined for atmospheric dispersion models, based on previous benchmarking exercises. These values have been adopted for other physical scenarios, but may not be appropriate for other applications. Therefore a certain degree of uncertainty is remained.

The target variables (as detailed in the section 3.2) are the physical parameters against which the performance of the model is evaluated. They can be directly measured or derived from measurements, and can be separated into parameters based on point-wise and arc-wise data:

- Point-wise parameters involve a comparison that are paired at specific points
- Arc-wise data involves comparisons made at specific distances (radius).

The particularities of the scenario under investigation determine which to these two measures is most appropriate. For example, if continuous (or quasi-continuous) releases are considered the most commonly-used physical comparison parameter is the maximum concentration at a specific distance downstream from the release (arc-wise data). Additionally, for this case, to gain a great understanding of the performance of a given model, the maximum concentration should be combined with a comparison of the plume width, as described by (Hanna et al., 1993), (Duijm et al., 1996) and (Duijm and Carissimo, 2002). Point-wise time-averaged concentrations at specific locations are also included in SMEDIS as a physical comparison parameter for this scenario, referring to a continuous release, and as stated by (Carissimo et al., 2001), are known to provide a more stringent test of model performance than arc-wise comparisons.

Continuing the example of a continuous release scenario, appropriate selected parameters would be:

- Maximum concentration across an arc at a given radius
- Cloud width across this arc at the same radius
- Concentration at specific sensor locations

3.4.1 Results for Quantitative Criteria

Once again being able to say the predictions from this simulation are “good” or “acceptable” isn’t straightforward. Previous works on dense gas dispersion models made in the 90’s (Hanna et al, 1993) (Touma et al, 1995) or more generally on gas dispersion models (Hanna et al, 2004) gave some tracks and suggestions for the establishment of quantitative validation criteria.

SMEDIS (Carissimo et al, 2001), based on the works of (Hanna et al, 2004), suggested to use as statistical performance measures[18]:

- The FB (Fractional Bias) and MG (Geometric Mean) for the bias in the mean
- The NMSE (Normalized Mean Square Error) and VG (Geometric Variance) for the scatter about the mean

SMEDIS also attempted to establish that a “good” model should have as quantitative criteria:

- A mean bias within ±50% of the mean (i.e. -0.4<MRB<0.4 and 0.67<MG<1.5)
- A scatter of a factor of three of the mean (i.e. MRSE<2.3 and VG<3.3)
- A fraction of model observations within a factor of 2 of observations to be at least 50%

Most of these previous works used the maximum arc-wise concentration and plume width as target variables and highlighted the difficulty to apply SPM on point-wise concentration.

Lately, NCSRD considers that a “good” model would be expected to have mean bias +/- 30% of the mean, i.e. |FB|<0.3 or 0.7<MG<1.3, and random scatter about a factor of two to three, i.e. NMSE<1.5 or VG<4 (see Deliverable D5.2). This depends on the physics involved.

The results of a statistical analysis are usually presented in the form of scatter plots of MRB against MRSE or MG against VG. Those plots are a useful indication of model performance and tendency to under/over predict. As reminder each SPM has an ideal or optimum value. For FB/MRB the optimum value is 0, consequently if FB has a negative value, the model is underpredictive while if FB has a positive value, the model is overpredictive. For MG, the optimum value is 1 and if MG>1, the model is underpredictive and if MG<1, the model is overpredictive.

Another point is that FB is symmetric about the ideal value; this allows an easier comparison between value due to an equal weight to under/over prediction while MG is not symmetric and is often plotted using a logarithmic scale.

In the framework of WP5 benchmark exercises, simulations had been performed on different experiments (see Validation Database). Among them, NCSRD found the following SPMs for their simulation of the experiment GAMELAN.

Table 10 : SPMs found for GAMELAN by NCSRD

	ideal value	prediction

[18] Fractional bias can be also named Mean Relative Bias MRB and Normalized mean square error named Mean Relative Square Error MRSE

FB	0	-0.025
NMSE	0	1.52
MG	1	0.97
VG	1	1.001

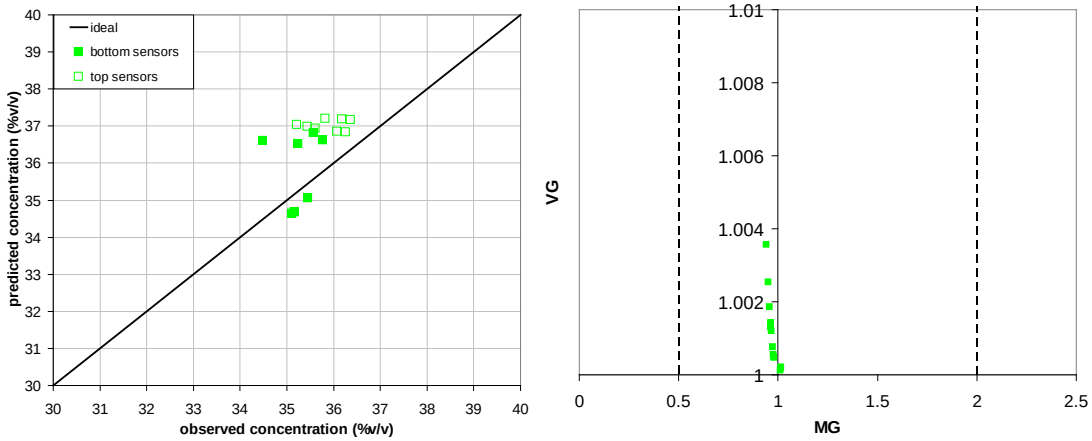


Figure 14 : The scatter plot with the observed versus the predicted concentration (right) and the MG versus VG plot (left)

Table 11 : Validation Criteria found in the framework of the benchmarking exercise on Garage Facility (WP5)

	Bias in the mean		Scatter about the mean	
	MG (SPM01)	FB (SPM02)	VG (SPM03)	NMSE (SPM04)
Mean	±25% of the mean	|FB|<0.3	VG < 2	NMSE < 0.5
Release (Peak concentration)	*±20% of the mean*	*|FB|<0.3*	*VG < 1.5*	*NMSE < 0.2*
Dispersion (Concentration at t=7000s and 20 000s)	*±30% of the mean*	*|FB|<0.3*	*VG < 2*	*NMSE < 0.5*

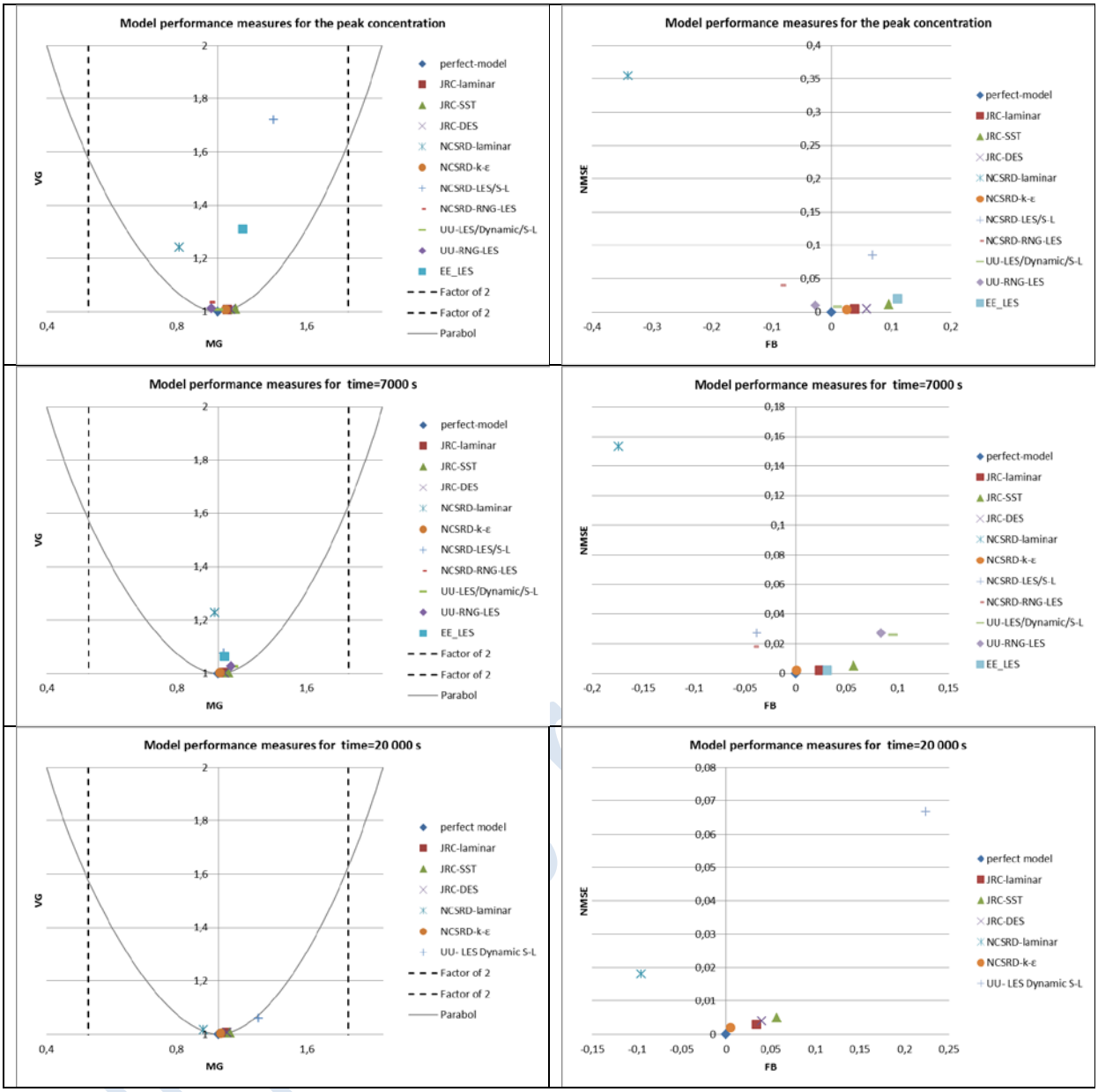


Figure 15 : Plots of MG against VG and FB against NMSE results extracted from the deliverable D5.3

As considering by NSCRD a “good” model would be expected to have mean bias ±30% of the mean, i.e. |FB|<0.3 or 0.7<MG<1.3. However, regarding the results of the benchmark exercise, a “good” model would be expected to have a random scatter about a factor of two, i.e. NMSE<0.5 or VG<2.

Unfortunately in front of the knowledge gaps in the field of fires, deflagrations and detonation and the lack of previous works on fires/deflagrations/detonations quantitative assessment criteria; what is a “good” model or a “performant” model is not well known by the partners. Regarding this fact, no proper criteria could be determined. In order to have a proper QAC, first knowledge gaps should be

overcome and secondly more benchmarking exercises should be performed with SPM calculated for specific moments (peak pressure or peak flame speed).

4. Sensitivity and uncertainty

In the verification and validation process the user needs to consider the effects of errors and the level of uncertainty when using models. Although it might be possible to minimize uncertainties by following best practice it might not be possible to eliminate them. This section reviews ways of treating uncertainty. In general, validation is about uncertainty, though possibly not always quantification of uncertainty. To validate simulations of physical systems observations and predictions of quantities are compared to determine whether the model, described by the mathematical equations, "replicates reality to an acceptable degree" (Ivings et al, 2013). Validation therefore involves assessing the difference between observed and predicted quantities (as set out in Section 3) both of which will have associated uncertainties to decide whether the model is acceptable given the difference and uncertainty. The need to consider uncertainty was recognised when the Model Evaluation Protocol (MEP) (MEG, 1994) for models used in hazard assessment was being developed. One of the items listed in the documentation describing MEPs by the Model Evaluation Group is "uncertainty estimation (of model and data)". If a model has not been verified then there can be no confidence that the solutions it produces are correct, therefore the complete process of validation can be described as Verification, Validation and Uncertainty Quantification (Roy and Oberkampf, 2010, Jatale et al, 2015).

In the following subsections, sources of uncertainty in model use are reviewed, followed by a brief description of different types of uncertainty. The approach to treating uncertainty used in MEPs is described, followed by other approaches that are used to treat uncertainty.

4.1.1 Sources of uncertainty

There are a number of different sources of uncertainty and identifying these provides a basis for understanding the uncertainty in model validation and prediction.

Model setup

Model setup uncertainty relates to propagation of uncertainty in simulations, from uncertainty about model input and boundary conditions and model parameters. In Section 3.5, two practical examples are provided on the effect of location of computational domain boundaries for release and dispersion and deflagration simulations. In Section 3.6, further examples are provided on the effects of applying different boundary conditions.

Model solution

In physical simulations the code must be verified (Section 2) to ensure that the equations are being solved correctly. This step occurs before validation, because if the solution is incorrect the predictions cannot be validated.

Code verification is typically in the responsibility of the code developer. If the code is being sold a user may not have access to the source code and code verification is regarded as a responsibility of the vendor. There is an element of software engineering in code verification, but codes for simulating physical systems will involve the use of numerical analysis which must also be verified, software engineering techniques developed for other types of code may not cover the requirements for numerical analysis.

Solution verification should also be performed for software used to perform numerical analysis. Checks must be performed to ensure that the solution approach is correct and stable, and for CFD, checks that the mesh refinement used is appropriate, either by demonstrating mesh independence or by calculating error due to the mesh. An example of solution verification is given in Section 2.6.

Experimental uncertainty

Validation compares predictions with experimental observations to check whether the model predictions of the phenomena of interest are acceptable. Therefore, in addition to the model related uncertainties, experimental uncertainty should also be considered during validation. Particularly for older data sets information on experimental uncertainty may not be available. The Fire Dynamics Simulator (FDS) validation manual (McGrattan et al, 2015) provides one possible approach to this problem where measurement uncertainties from well documented experiments (Hamins et al, 2006) are combined with engineering judgement to estimate uncertainties for experiments where that information is not available. This approach is only available where experiments performed and the instruments used are similar.

4.1.2 Types of uncertainty

Many labels are attached to uncertainties but two categories can be used to describe uncertainty:

- Aleatory uncertainty, also described as variability or irreducible uncertainty, and
- Epistemic uncertainty, also described as uncertainty or reducible uncertainty.

Identifying the type of uncertainty provides help in deciding whether and how uncertainties can be reduced. Broadly, uncertainty due to a lack of knowledge can be reduced.

Aleatory uncertainty

Aleatory uncertainty is stochastic, and a parameterised probability distribution is used to describe this type of uncertainty. The uncertainty is irreducible, as collecting further information would not remove the need to use a distribution over a range of values to describe the quantity. Since aleatory uncertainty cannot be reduced it has to be recognised in an analysis, unless the system can be changed so that the influence of the sources of aleatory uncertainty is reduced. That may not be possible. For example, aleatory uncertainty is intrinsically part of practical atmospheric dispersion.

Epistemic uncertainty

Epistemic uncertainty involves quantities where there is uncertainty about the value they take which could, in principle, be reduced by the collection of additional information.

4.1.3 Descriptions of uncertainty

There is agreement that probability distributions are an appropriate way to describe aleatory uncertainty. However, there is disagreement about whether epistemic uncertainty in quantities can also be described by probability distributions. Since both probabilistic and non-probabilistic descriptions of epistemic uncertainty are in use and will continue to be used, the disagreement is noted but not explored further.

4.1.4 Combined

There may be uncertainty about the parameters used to describe a probabilistic distribution, so there can be combined uncertainty. For atmospheric dispersion there can be significant aleatory and epistemic uncertainty, that is measurement may reduce uncertainty about the parameters describing a distribution, epistemic uncertainty, but the system is stochastic, and aleatory uncertainty will remain.

4.1.5 Approaches to the treatment of uncertainty

Treatment of uncertainty in MEPs

In MEPs, Statistical Performance Measures (SPMs) are used to quantify the performance of models for their validation. The SPMs are metrics comparing observation and prediction and are discussed in Section 3. Uncertainty in observations and predictions is recognised by specifying ranges of values for the SPMs, a 'good' model should achieve SPM values within these ranges. An MEP for examining dispersion of Liquefied Natural Gas (LNG) is reported in Ivings et al. (2007), the MEP has been applied to models used in a regulatory environment and the results reported (Hansen et al, 2010, Witlox et al, 2013). The SPMs and the acceptable ranges used in the LNG MEP were suggested by Hanna et al. (1993) and are based on evaluation of the performance of a number of dense gas dispersion models. More recently the MEP for emergency response models developed under COST ES1006 (COST, 2015) suggests acceptable ranges of SPMs for urban dispersion models based on the work of Hanna and Chang (2012). The ranges suggested for urban dispersion in Hanna and Chang (2012) were a factor of two larger than those suggested for atmospheric dispersion in rural settings in Chang and Hanna (2004). In setting the acceptance criteria the aim was that they should not allow all models to be accepted, nor should all the most widely used models be rejected. Deciding appropriate ranges to use should therefore be based on knowledge of model performance from a number of models.

In the MEP approach to validation the model is treated as a whole, though the necessary physics and the model components needed to represent them should have been considered during the scientific review in the MEP, and the validation cases should be chosen to check the ability to predict the necessary physics. Also, the ranges specified for SPMs represent the total contribution from different sources of uncertainty affecting the comparison of observation and prediction, without breaking down the contributions from different sources of uncertainty. Calculating the values of the SPMs for a single experiment only requires a model to be run at the experimental conditions. However, for a complete MEP the model might have to be run for a large number of experiments to cover the different physics required for an application.

If SPMs have been calculated using different models for relevant experiments then the choice of ranges can be based on this experience. However, if experience does not exist for an application area then selection of the ranges to use could be a problem. There is no reason to think that the ranges used in one area, atmospheric dispersion, should be applied to a different application, for example, fire and explosion. In the emergency response MEP (COST, 2015) it is noted that while the measured quantity should be the same as that calculated by the model this may not be true for atmospheric dispersion. SPM ranges suggested based on experience are making allowance for this type of discrepancy. If no validation has been performed for an application area it is difficult to make allowance for such issues and there may be little choice but to start by using ranges specified for other application areas. Performing a model evaluation as part of the development of a protocol gives an opportunity to check that the initial ranges neither accept nor reject all models, before the

protocol is published. Also, ideally, the ranges specified for the SPMs should be reviewed, as experience is gained with using an MEP.

In addition to ranges to describe acceptable model performance, confidence intervals can be calculated for the values of individual SPMs. Chang and Hanna (2005) describe the BOOT statistical model evaluation software package. This software can be used to calculate the SPMs described in Section 3 and, using bootstrap resampling, confidence intervals can be calculated for the SPMs.

Licari (2010) suggests that SPMs fulfil the purpose of allowing evaluation and comparison of models, but that they do not give a measure of the confidence in predictions. The performance metric proposed by Licari (2010) calculates the ratio of predicted to observed for each observation in a dataset and assumes that the values of the ratio are samples from a normal distribution. The probability that a specified ratio of predicted to observed is exceeded can then be calculated from the sample mean and standard deviation of the ratios for each observation. This performance metric has been developed more recently than the SPMs described in Section 3. The FAC2 SPM, the number of predictions that are within a factor of 2 of the observed values, is based on the same calculation, but only considers a single value, rather than a distribution. There appear to be no citations of the use of Licari's approach and practical experience of applying this metric, for example, the treatment of zeros in either predicted or observed values, is not available.

Other approaches to uncertainty quantification

MEPs, requiring verification and validation have been used to evaluate models for use in regulatory environments. However, interest in verification and validation of computer models, and the associated quantification of uncertainty, is much wider than the regulatory environment and the amount of work in this area is growing. SIAM (Society for Industrial and Applied Mathematics)/ASA (American Statistical Association) have held biennial uncertainty quantification workshops since 2012 and launched a Journal of Uncertainty Quantification in 2013. ASME (The American Society of Mechanical Engineers) has standards for verification and validation in computational solid mechanics (ASME, 2006, 2012) and computational fluid dynamics and heat transfer (ASME, 2010). They have held an annual verification and validation symposium since 2012, and launched a Journal of Verification, Validation and Uncertainty Quantification in 2016. An effect of this interest is that both standards and methods are changing and developing, a revision of ASME V&V10 should be issued in 2016.

The reason for performing V&V remains to determine whether a model has acceptable performance for a purpose. Those purposes may be different and the systems that V&V is applied to may be very different to those considered in MEPs.

The approach to performing validation remains the comparison of observation and prediction, but in the examples given below the acceptability for a purpose is based on the estimation of model form uncertainty. That is, the uncertainty that remains when other sources of uncertainty have been identified and quantified, due to description of the physical system used in the model and the assumptions made to reach that description. Compared to the use of ranges on SPMs in MEPs this requires the uncertainty to be broken down into different sources of uncertainty and the definition of treatments for different types of uncertainty. The uncertainties considered in V&V20 ASME (2009) are from solution verification, experimental error and input uncertainty; these are combined to estimate the model form uncertainty. The solution verification estimates the uncertainty due to the numerical solution approach, for CFD this would usually be described as the error due to the mesh and discretisation used. The experimental error is the uncertainty in the quantity to be predicted and the input uncertainty is the uncertainty in input conditions and properties.

An estimate of model form uncertainty could be used to decide whether further effort is required to reduce this uncertainty to an acceptable level, V&V10 ASME (2006). In ASME V&V20 a further restriction on the definition of validation is used, that a model can only be considered to be validated for the conditions where experimental observations are available. The standard states that away from those points engineering judgement must be used to consider the effects of uncertainty. It is likely that once a model form uncertainty has been calculated it will be used to state intervals on the prediction of quantities, though care should be taken with interpolation, and, especially, extrapolation beyond the region for which experimental validation data is available.

Other considerations are that V&V10 (ASME, 2006) suggests a system approach, starting with the verification and validation of low-level components of a system and moving on to sub-systems containing more than one component. It is likely that at the level of the complete system experimental data will not be available.

The V&V10 standard (ASME, 2006) does not provide a methodology for performing verification and validation. The aim of the standard was to provide a language to describe, and a conceptual framework to understand, verification and validation. The intention was that this would help provide a foundation for the development of verification and validation methodologies. V&V10.1 (ASME, 2012) was produced to provide a simple example, illustrating some of the key concepts and procedures presented in V&V10 (ASME, 2006). The treatment of uncertainty within the standard was retained, as a key element of verification and validation, but the example uses generated, rather than actual experimental data.

In contrast the V&V20 standard (ASME, 2009) proposes a methodology for verification and validation where all uncertainties are treated the same. The approach used is based on the Guide to the Expression of Uncertainty in measurement (International Organization for Standardization, 1995). Verification is required before validation, and in V&V20 two elements are considered; Code verification to check that the code is doing what was intended and solution verification. The solution verification is used to estimate the uncertainty in the numerical solution, in CFD simulations this is treated for the mesh and discretisation. This term is included in the assessment of model form uncertainty. Two alternative methods of calculating the effect of input uncertainty are suggested, a local method and a Monte Carlo approach for global uncertainty. Since validation is always against experimental data the uncertainty in the experimental measurements must be considered. These sources of uncertainty are then combined to give the model form uncertainty.

The approach described in the FDS validation manual (McGrattan et al, 2015) is another approach related to the Guide to the Expression of Uncertainty in Measurement (International Organization for Standardization, 1995). In this approach comparison is made between fire experiments and simulations, without considering the component sub-models used within the model. The solution verification term is included in the model form uncertainty, though the influence of the mesh is examined using different mesh resolutions as part of the validation. The approach used to describe the model uncertainty is described in McGrattan and Toman (2011), in addition to the use of an approach where the model errors are not broken down into components from sub-models the errors are assumed to be normally distributed. This results in an analytical solution for the model form uncertainty composed of the mean over- or under-prediction, the bias, and the uncertainty about the mean.

Use of the information from an FDS validation study is described in McGrattan et al. (2106). Information on the experimental data used in validation studies can indicate the range for which the validation applies. While the uncertainty analysis can be used to predict the likelihood a given threshold is exceeded, incorporating the model uncertainty.

The FDS validation and uncertainty approach is in regular use, as cases are added to the FDS validation suite and documented in the FDS validation manual (McGrattan et al, 2015). Additionally all the validation cases are run before minor releases of FDS to check that there are no unexpected discrepancies between code releases. An issue that should be remembered with all these approaches is the computing resource required. At the end of 2012 it took between one and two weeks to perform the 800 calculations in the FDS validation suite on a 256-core Linux cluster[19]. While available computing power has increased cases continue to be added to the FDS validation suite, running all the validation cases will continue to require a significant commitment of computing resource.

4.1.6 Conclusions

The use of SPM ranges in MEPs allows the evaluation of model uncertainty by validation comparing observations and predictions. Based on the evaluation, uncertainty bounds can be stated for use when applying a model.

Alternative methods are being developed, these consider contribution to model uncertainty by source (Section 3.3.1) and type (Section 3.3.2). A disadvantage of these methods is that they depend on the availability of more detailed information on uncertainty and in most cases would require more computing to be performed for the uncertainty analysis. An advantage, compared to the use of SPM ranges, is that if it is decided that model performance is unacceptable there is a basis for performing sensitivity analysis to identify important components in the uncertainty and to help decide how uncertainty could be reduced.

Uncertainty in predictions can also be affected by the user and information on best practice is necessary to try and reduce this source of uncertainty.

4.2 Worked examples

In the following sections, examples of model form uncertainty are provided. The approach taken has been to identify uncertain parameters and vary those to assess the effect on model results.

4.2.1 Effect of location of computational domain boundaries

The size of the computational domain should be carefully chosen. Domain boundaries should be located far enough from the area of interest in order to minimize the impact of the boundary conditions on the results. In the case of hydrogen dispersion in a vented enclosure, the computational domain should be expanded in order to include not only the enclosure, but also the area surrounded the enclosure. Vents are areas of great importance with complex flow around them, therefore it is necessary to ensure that the boundary conditions have no impact on them.

In ignition and fire modelling it is important to include sufficient expanse of ambient atmosphere into the domain design to prevent the undesirable impact of the outer boundary conditions on the numerical solution. Modelling of the fire in the enclosure typically requires the addition of an external domain outside of the openings in order to ensure proper boundary conditions. It is recommended to move the “far field” boundary to a distance of up to two characteristic sizes from the fire enclosure. While removal of outer boundaries to a large distance from the main simulation area of interest may significantly increase computational costs, which would appear to be spent on

[19] https://groups.google.com/forum/#!topic/fds-smv/jmIyOy2wzFA (accessed 10-02-2016)

areas where no phenomena of interest take place, the experience of numerical simulations of both ignited and unignited releases performed at Ulster University emphasizes the advisability to move the ambient boundary as far as practically possible from the release origin/vent location.

In deflagration modelling, the extent of the domain has the potential to greatly affect the results of computations. If the domain is too small the propagation of the pressure wave will not be correctly captured. Generally, the domain should be much larger than the expected flammable volume.

The effect of changing computational domain size was shown in the benchmark problem SBEP-V20 (Papanikolaou et al. 2010) where an increase of the size of the computational domain produced a significant improvement in the agreement between simulation results and the experimental measurements. Therefore it is always essential to investigate the effect of the size of the computational domain on the simulation results, performing the same simulation with an increasingly bigger domain until the effect on the relevant variables becomes negligible. Such sensitivity tests on the extent of the computational domain should be undertaken unless there is supporting information from the literature. Two representative examples about domain extension and sensitivity studies are presented next.

4.2.2 Release and dispersion example

The effect of the computational domain boundaries was examined in helium release and dispersion case inside a garage. The geometry of the problem is shown in Figure 16. The dimensions of the facility are 5.76 m (length) x 2.96 m (width) x 2.42 m (height). A small circular vent of 200 mm diameter exists in the west wall. Concentrations were measured at 57 positions within the garage (small spheres in Figure 16). The sensor named Vol1 is closest to the vent. Helium mass flow rate is equal to 0.054 g/s from a circled orifice with diameter equal to 29.7 mm. Release duration is equal to 3740 s. The concetrations after the release were also measured (diffusion phase) until 20000 s. More details about the experiment can be found in (Gupta et al. 2009).

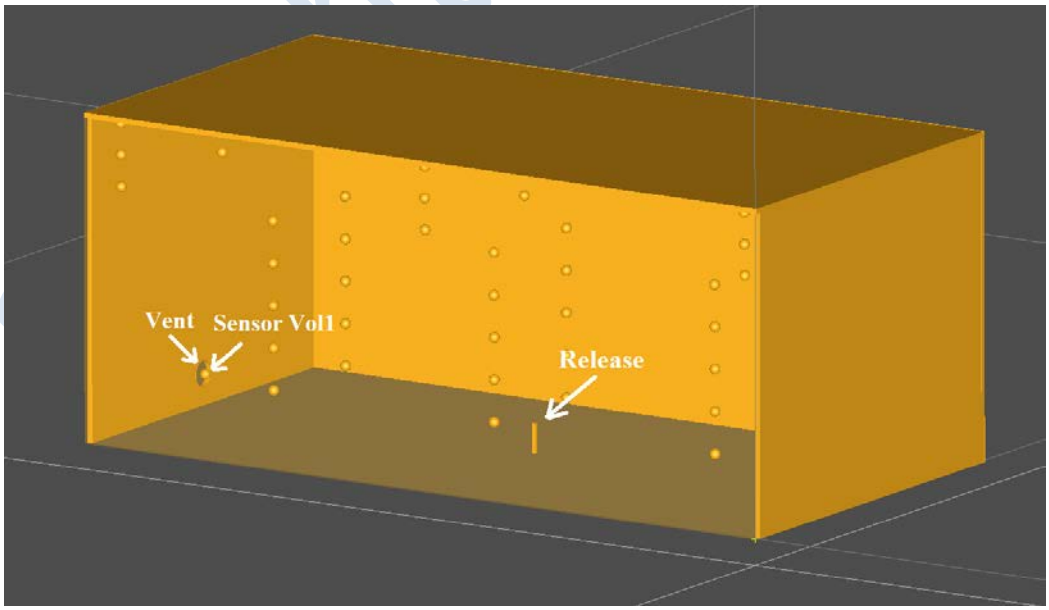
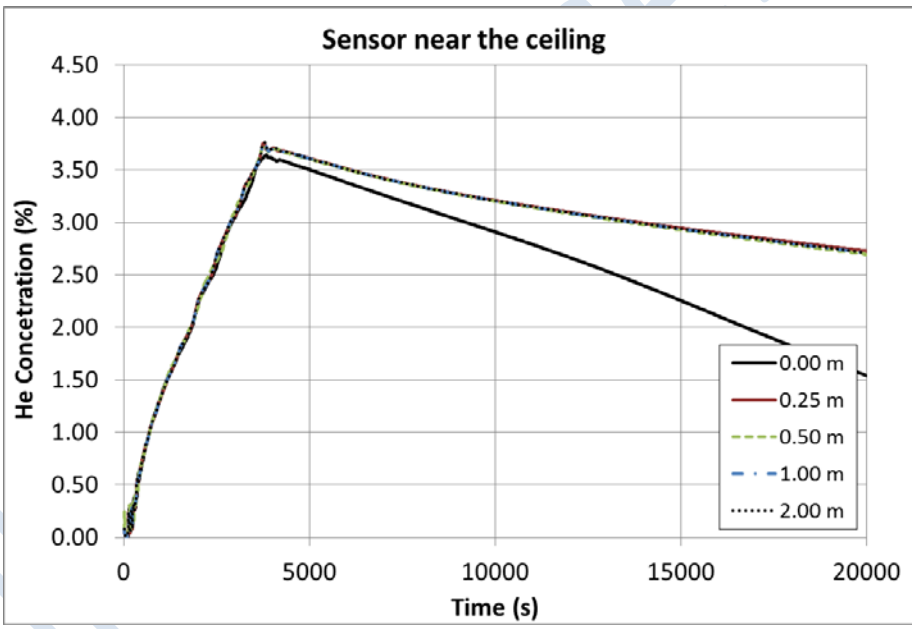


Figure 16: Geometry of the problem

A domain size sensitivity study was carried out. Four different domain expansions were applied: 0.25 m, 0.5 m, 1 m and 2 m. The domain was extended only upwind of the wall with the vent. Since the vent is placed approximately in the center of the wall and in the lower part of the wall no expansion was applied in the y-and z-directions. The case without any domain expansion was also examined. The zero gradient boundary condition was applied in all variables at the east domain (x-direction).

In Figure 17 the computational results are presented for two sensors, one at the ceiling and one next to vent (sensor Vol1). We observe that in both sensors the results with 1.00 m and 2.00 m expansion are identical. At the sensor near the ceiling, the results are similar even with the 0.25 m expansion. Significant differences are observed only for the no expansion case, at the diffusion phase. On the other hand at the sensor near the ceiling, differences among the results are observed even between 0.50 m and 1.00 m expansion. This is explained by the fact that this sensor is the closest sensor to the domain boundary.

As a result, we conclude that the location of computational domain boundaries need to be chosen with caution. A sensitivity study should be carried out in order to assure that the solution is unaffected by the boundaries location. In the examined case, an expansion of 1.00 m is needed in order to achieve independent results.



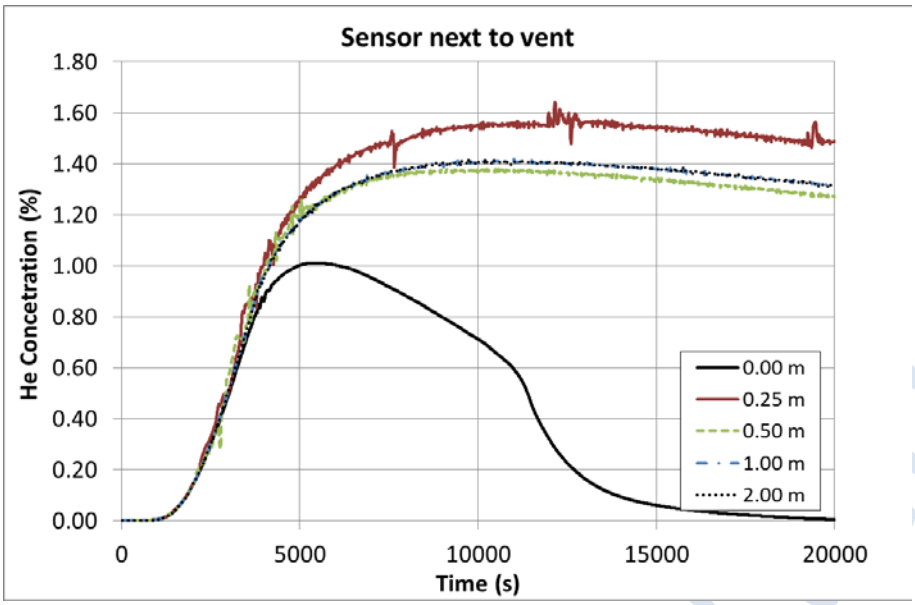


Figure 17: Computational results at a sensor near the ceiling (top) and at the sensor Vol1 next to the vent (bottom) for various domain expansions.

4.2.3 Deflagration example

The effect of the computational domain boundaries was examined in hydrogen deflagration simulation. A hydrogen-air mixture of 29.7% by volume occupies an unconfined hemispherical volume of 20 m diameter. Explosion pressure was measured at 2.0, 3.5, 5.0, 6.5, 8.0, 18.0, 25.0, 35.0, 60.0 and 80.0 m from the ignition point which it was located at the center of the hemisphere. More details about the experiment may be found in (Molkov et al. 2006).

Various domain-sizes were studied in order to examine the impact on the results. The domain-sizes that were tested are presented in Table 12. At all exit planes (lateral, front, back and top) the non-reflecting type boundary conditions for the normal velocities is chosen, while for the parallel to the exit planes' velocity components, zero gradient boundary conditions are applied.

In Figure 18 the pressure at 5, 8, 35 and 80 m from the center of the hemisphere, for three different domain sizes are presented. We observe that the domain size has a significant impact on the results at the closest to the boundary sensor (80 m). At the other sensors, the extended domains affect the results only at the tail of the pressure-time curve. When the Domain 1 is used (200 x 200 x 100 m), the pressure fails to return to its initial value. Domains 2 and 3 (extended domains), however, reproduce this physical behaviour. Small differences between Domain 2 and 3 are observed only at the tail of the pressure-time curve at the last position (80 m). At that sensor, even the Domain 2 fails to restore the initial value of the pressure and the more extended Domain 3 is required.

Table 12. Dimensions of the numerical domain

	Length (m)	Width (m)	Height (m)
Domain 1	200	200	100
Domain 2	300	300	150
Domain 3	400	400	200

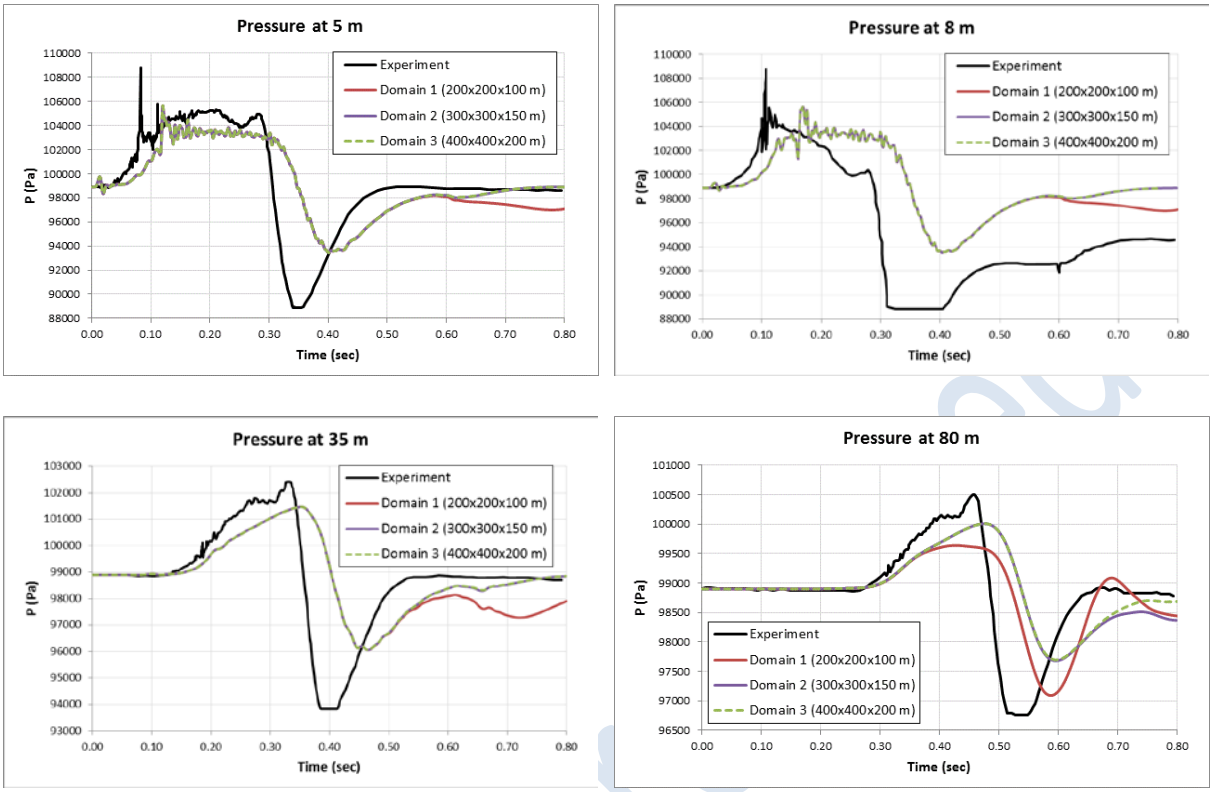


Figure 18: Pressure at 5, 8, 35 and 80 m from the center of the hemisphere, for three different domain sizes.

4.3 Effect of boundary conditions

The choice of the boundary conditions is significant for the accuracy of the computational results. There are several options available for boundary conditions and the user must decide the most appropriate boundary conditions for their application based on the Guide to best practices (SUSANA, 2014). In inflow boundaries where the Dirichlet boundary condition (given value) is mainly applied, there are some uncertainties concerning the values of the variables. These uncertainties can affect the results. Some of these uncertainties that are met in hydrogen release problems are;

- The **wind** (in open environment releases): In the presence of wind its velocity and its turbulence characteristics (e.g. k and ε values) should be imposed as the inlet boundary conditions. These values can be obtained from a 1-D simulation that produces the vertical profile or using the power law profile. In general, estimating the wind profile encounters several uncertainties and difficulties. Wind speed and direction are transient and high oscillations may occur with time. This transient behaviour is not easily modelled and usually there is not enough available experimental information to assist its modelling. (Giannissi et al. 2014) modelled the transient wind direction using the available experimental data and it is shown that transient wind direction affects significantly the predicted concentration levels at the sensors that were placed in line with the release, even though the average wind direction was in line with the release. Another factor that

affects the wind profile (speed, temperature and turbulence) is the atmospheric stability conditions (stable, neutral, unstable), which are not always experimentally available and may have an impact on the results.

- The hydrogen inlet boundary in **compressed releases**: In compressed hydrogen release an under-expanded jet will be formed close to the release point. It will rapidly accelerate and expand to atmospheric pressure through a series of shocks. The numerical modelling of the region close to the release is very demanding in terms of the high grid resolution that is required. Therefore, several modelling approaches have been developed introducing the notional nozzle, in order to minimize the computational demands. Each notional nozzle approach would estimate different inlet values (velocity, temperature, etc.) and consequently it could affect the prediction; therefore, the choice of the appropriate approach for each case is crucial. For low storage pressures (Birch et al. 1987) approach can be used. The main assumption of the approach is that isentropic expansion occurs at the nozzle. The size of the notional diameter and the value of the velocity that are estimated with the approach are set on the hydrogen inlet boundary. (Birch et al. 1987) model is built on the ideal gas equation of state. For gas storage pressures above 10- 20 MPa, the non-ideality of the mixture could be accounted for (Schefer et al. 2007) by using the Abel-Noble equation of state. An alternative to the (Schefer et al. 2007) method developed by (Molkov et al. 2009) which is based on mass and energy conservation equations rather than mass and momentum equation can also be used. The effect of each modelling approach on the results based on several experiments is presented in (Papanikolaou & Baraldi 2011), (Papanikolaou & Baraldi 2012).

  Moreover, simulation of hydrogen releases from high pressure storage tanks often involves modelling of blowdown problem, with pressure and consequently flow rate in the tank decreasing during the release. This presents a problem for the simulation utilizing notional nozzle approach, since the diameter of notional nozzle is itself dependent on the parameters in the tank. Modelling of blowdown release, therefore, would require implementation of a movable grid to account for the change of notional nozzle diameter with time, which will significantly complicate problem setup and increase computational resource requirements. An alternative volumetric source approach (Molkov et al. 2009), which allows blowdown simulations to be performed on a stationary grid can be used. This approach is based on the introduction of volumetric release in a small portion of the calculation domain around the inflow, where distributed volumetric sources are applied to momentum, energy, species and other equations to mimic parameters of the modelled inflow.

- The hydrogen inlet boundary in **LH2 (liquid hydrogen) releases**: In LH2 release one can treat the source as a gas phase boundary condition (evaporating pool) or as a two phase boundary condition (two phase jet). In a recent study regarding liquefied natural gas release (Giannissi et al. 2013) concluded that the two phase source provides better results compared to the evaporating pool. Moreover fewer assumptions, such as the pool size, are required. In the two phase jet both liquid phase and vapour phase of hydrogen enter the computational domain. The estimation of the flashed vapour mass fraction is very significant, because it affects the vapour dispersion to a great extent. In general, high vapour mass fractions lead also to higher velocities at the source. The flashed vapour mass fraction can be provided by either by assuming isenthalpic expansion (Venetsanos & Bartzis 2007), (Giannissi et al. 2014) or isentropic expansion (Statharas et al. 2000). The inlet velocity is calculated with the help of the mixture density, the orifice diameter and the measured spill rate. Alternatively, a sensitivity study (Ichard et al. 2012) regarding the flashed vapour fraction can be performed.

- The **discharge coefficient** (c_D) of the nozzle should also be considered, in order to estimate the source boundary conditions. The value of the discharge coefficient depends on the nozzle (the ideal nozzle has a value equal to 1). The actual nozzles have a discharge coefficient below unity. A value ranged between 0.8-1 can be imposed. In general, values smaller than unity can be tested, in order to examine the effect of the discharge coefficient on the results.
- **Turbulence intensity** at hydrogen inlet boundary: Its value is usually not kwon exactly so a sensitivity study could be performed to assess its effect on the results. The value of turbulent intensity at the source can be ranged between 5-15%. Higher turbulence intensity at source would lead to more diffusive results near the release point.
- **Ground temperature** in LH2 releases or in cryogenic releases (low temperature): In such releases the heat flux from the ground is a very important factor that influences considerably the hydrogen dispersion, especially if the release point is close to the ground. Therefore, on the bottom (ground) boundary a transient given value of temperature by solving a 1-D temperature equation inside the ground should be imposed, because the solid substrate gets colder with time. Otherwise (if a constant given value is imposed) high heat transfer rates will be predicted resulting in more buoyant cloud. The constant temperature boundary condition can be applied in releases above water, because it can be safely considered that water temperature remains constant due to its high heat capacity and because natural convection occurs.

5. V&V procedures in other protocols: LNG, SMEDIS

Techniques for model evaluation have been in existence since the early days of computer simulation and numerous model evaluation protocols have been produced. This Section provides a brief overview of the approaches adopted for verification and validation in three of these protocols, relevant to the SUSANA project.

In the 1990's, a Model Evaluation Group (MEG) was set up to address issues relating to model quality and also to identify areas for research into major industrial hazards. The model evaluation group initially produced a very generic model evaluation protocol (MEG, 1994a) and then formed several working groups to generate more specialised versions in the following areas:

- Dense gas dispersion
- Pool fires
- Gas explosions

Each working group was composed of people with more in-depth knowledge specific to their area of application and were therefore able to consider the requirements for an MEP. In addition to the generic model evaluation protocol, the model evaluation group produced a set of "guidelines for model developers" (MEG, 1994b). Of the three working groups formed by the MEG, only two resulted in adapted versions of the MEP. These were the Heavy Gas Dispersion Expert Group (HGD) and the gas explosion group, or Model Evaluation Group Gas Explosions (MEGGE).

The generic model evaluation protocol is a very brief document and verification is covered briefly in that "assessors should ensure that code is producing output in accordance with the model specification." The MEG protocol also suggests that verification is a task for the model developers, and should be recorded in the documentation.

The first activity in validation is a statement of its aims and which model parameters are to be tested. Validation then consists of selecting appropriate data and parameters and making an assessment of the uncertainty of both the model and the data. How the model is to be compared with the data appears to be covered by "selection of validation parameters", leaving the choice to the evaluator to decide which technique to use, and whether to adopt a statistical method for example. The final aspects of validation are forming conclusions and making recommendations, and these activities may result in a need to revisit certain aspects as deficiencies may be found in particular datasets.

The SMEDIS (Scientific Model Evaluation of Dense gas DISpersion models) project was a continuation of the MEG and HGD work and was also part sponsored by the CEC. As previous evaluation studies had dealt only with releases over flat unobstructed terrain, real release scenarios from process plants would involve more complex problems such as aerosol sources, obstacles and complex terrain. A need was therefore identified to address these scenarios (Daish et al., 2000). The SMEDIS project aimed to produce a model evaluation protocol to address these "complex effects." Rather than a tool for ranking models in terms of performance, the SMEDIS project intended to encourage continual model development and leave in place a protocol and database for use by future model developers. Although the SMEDIS protocol was based on the MEG and HGD protocols, it was designed to be much more specific to the three complex effects scenarios. This was because the HGDEG protocol was considered to be not explicit enough in its description of the evaluation procedure. Another area where SMEDIS differs from the MEG protocols is that a significant aspect of it is concerned with development and refinement of the protocol, or versions of it, for specific uses.

While the protocol is based upon the structure of the MEG protocol, there are additional activities which are specific to evaluation of the protocol, as much as evaluation of the models.

SMEDIS treats verification “passively” and evidence is therefore sought during the scientific assessment. The reason for this is the labour intense nature of verification and the practicality of carrying it out in full for each model.

Validation is the only part of the SMEDIS protocol that is treated actively. It involves running the model against the test cases listed in the SMEDIS database, or the experiments identified in the pre-evaluation stage and computing the statistical performance measures. Since the protocol is concerned with complex effects, it is recognised that not all models are able to take these effects into account. Therefore, it allows the user to only select only a subset of the data to run the model against.

The LNG dispersion model evaluation protocol is set out in Ivings et al. (2007) and summarised in Ivings et al. (2013). It follows much of the structure set out in SMEDIS, but was adapted to specifically account for the physics seen in the dispersion of LNG vapours.

The approach to verification follows that set out in SMEDIS, where it is treated passively, by reviewing evidence collected during the scientific assessment. Verification is recorded in the MER, but not included in the qualitative assessment criteria. The reason given for this is that the absence of information or evidence of verification would not be a sufficient reason to reject a model. Also the judgment that needs to be made on whether a model has been verified is subjective as well as being reliant on claims made by the model developer/proponent which are impractical to substantiate.

The validation procedure in the LNG dispersion model evaluation protocol again adopts the approach set out in SMEDIS. In this approach, careful consideration is given to identifying the key physics and variables involved in LNG dispersion and selecting appropriate test cases to cover the range of target scenarios. An alternative approach to validation would be to amass a large quantity of test data and run the model against as many scenarios as possible. However, because validation is extremely time consuming such an approach would be unfeasible and would also carry the risk of not testing the model correctly. In other words, the emphasis is on matching the domain of validation with the domain of application of the model.

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