Novel **E**ducation and **Tr**aining **Tools** based on digital applications related to hydrogen and fuel cell technologies

Deliverable D3.2:

e-Engineering toolbox, 1st version

D3.2: e-Engineering Toolbox 1st Version

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If deliverable does not get finished as scheduled in description of activity, please add a short explanatory statement. (To be done by responsible person of deliverable)

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30.04.2018	1.6	Final compilation before submission by V.Shentsov (UU)

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1   Introduction

The content of e-Engineering was prepared before the first project meeting and delivered in milestone MS3.1 (M4). It consists of 23 tools in e-Engineering toolbox and 10 tools in e-Science toolbox summing total of 33 tools to be developed. The table of contents which was outlined in milestone MS3.1 is going to be used as a substructure for this deliverable. The content of the deliverable is formed from the tool's descriptions and realisation of them into the platform that are due in M14 as they deployed up to now based on the template for the tool's description developed and presented as an annex in MS3.1.

In the next Sections, a description of the tools that were to be delivered by M14 is provided. Most of them have been already programmed and implemented in the platform as well. The description of the rest tools will be presented in D3.3.

2   e-Laboratory website

The e-Laboratory webpage is shown in Figure 1. This page contains a current structure of the available tools which are deployed, tested and validated and will be updated in the final deliverable D3.3. The interface of the e-Laboratory is being developed as the project progresses.
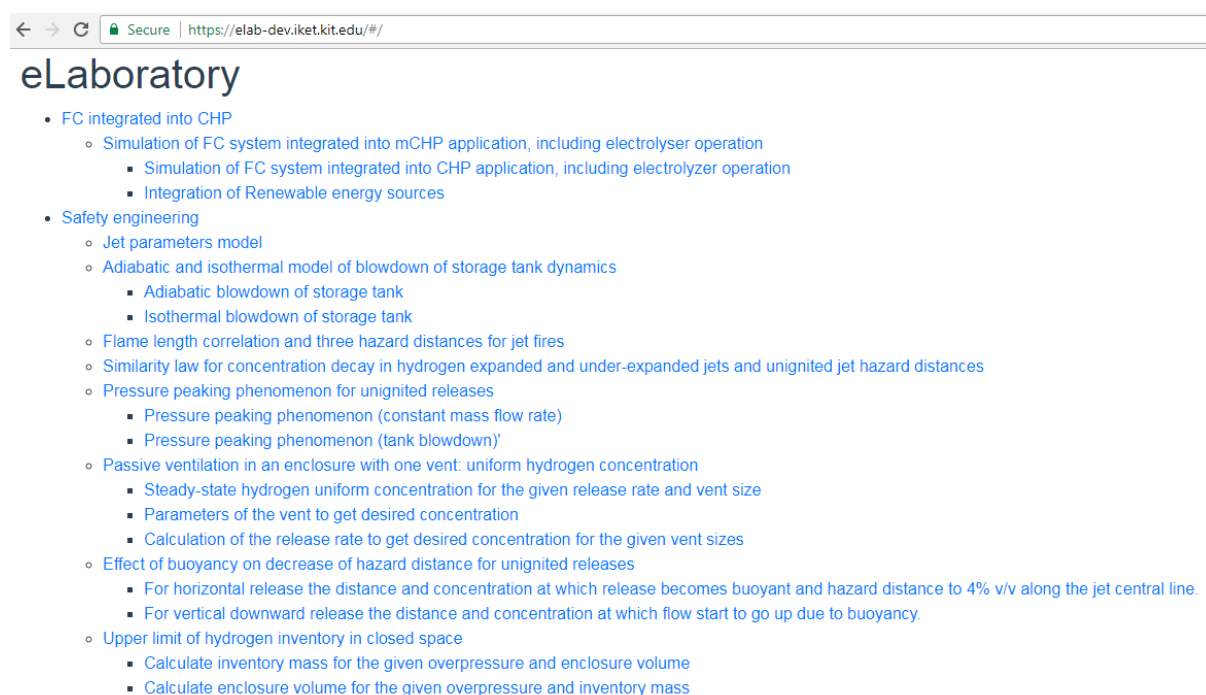
Figure 1 Screen shot of e-Engineering toolbox homepage.

3   e-Engineering

3.1   Renewable energy system (RES) tools

The tool description due date for the RES tool was initially M12. The RES tool delivery date was swapped with the date of the storage tool of the e-science toolbox. This action was necessary due to

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some issues encountering in obtaining the software that is used for the development of the RES tool, i.e. the HOMER software developed by NREL of US DOE. The software used to be available for free. However, the policy changed recently and a fee is charged. Some delays in the purchase of the software were the main reasons for the need for tool swapping. All issues have now been resolved and the RES tool is expected to be delivered by the end of M18. The storage tool of the e-science toolbox was ready earlier than planned and thus NCSRD recommended implementing that tool instead of the RES tool in the platform. The new delivery dates of the tools are shown in the updated table in Section Structure and planning of e-Laboratory delivery.

3.1.1   Design and optimisation of hybrid RES - hydrogen autonomous power systems for isolated communities and sites (NCSRD)

Due in D3.3

3.2   Fuel cells (FC) tools

Due in D3.3

3.2.1   Simulation of SOFC based on natural gas as fuel (DTU)

Due in D3.3

3.2.2   Energy balances and hydrogen costs for various electrolysis techniques (DTU)

Due in D3.3

3.2.3   Cell and stack models for both fuel cells and electrolysis (DTU)

Due in D3.3

3.2.4   Thermo-mechanical models to predict lifetime of high temperature FCs and electrolysers (DTU)

Due in D3.3

3.3   Storage /Separation tools

3.3.1   Storage material properties estimation and performance assessment based on a "materials-by-design" multi-scale approach (NCSRD)

The storage tools were renamed to storage/separation tools, in order to better reflect their functionalities. Three tools are included:

1. *Hydrogen Storage in Carbon-based Materials*
2. *Hydrate equilibrium pressure of H2 mixtures*
3. *Hydrate-based separation of the binary mixture H2 + CO2*

The first tool is a storage tool, the second tool is a tool that can be used for both gas storage and gas-mixture separation industrial applications and the third tool is a separation tool. All three tools target to both academic and industrial users.

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3.3.1.1   Hydrogen Storage in Carbon-based Materials

The objective of the *Hydrogen Storage in Carbon-based Materials* tool is to provide a tutorial (H2CNT simulation tutorial), in order to guide the user through the steps required to set up an atomistic simulation of hydrogen sorption in a carbon-based nanoporous material using the Grand Canonical Monte Carlo (GCMC) method.

Monte Carlo (MC) simulations entail properly constructed algorithms to sample the configuration space of physical systems by means of the probability density function describing the system's energy states in a particular ensemble. The choice of the statistical ensemble depends on the imposed macroscopic conditions. Of particular interest, for studying phase equilibria within porous media, is the Grand Canonical MC (constant chemical potential μ, volume V and temperature T).

The proposed methodology is implemented on the case of hydrogen sorption in carbon nanotubes. The manual is designed as a primer; no prior familiarization with pertinent software tools is needed. Freeware and open source software are used. This tutorial can serve as a starting point to proceed with different and/or more complex systems.

The basic software requirements are a molecular builder for the digitization of the host matrix and a molecular simulator package performing GCMC simulations.

The Carbon Nanostructure Builder incorporated in Visual Molecular Dynamics (VMD)[1] will be used for the generation of carbon nanotube structures. In VMD software the general case is that the atomic positions and, hence, distances and bond lengths, are specified in Ångström. Bond angles and dihedral angles are measured in degrees.

Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)[2] will be used to perform the GCMC simulations. LAMMPS is a classical molecular dynamics simulation code with the GCMC option available through an optional package that enables Monte Carlo attributes. Input data and parameters necessary for running a GCMC simulation are specified in the input script; therein, there is the option to choose among eight different styles for the units to be used in the simulation via a command that is launched at the beginning of the script. This command determines the units of the quantities that are specified in both the input and output files.

Performing sorption simulation experiments presupposes the reconstruction of a digitized model for the host. The molecular builder software allows users to create atomistic digitized carbon nanostructures, e.g. carbon nanotubes.

Subsequent to host digitization is the force field choice for the proper description of the physicochemical interactions of the system. A force field encompasses the functional form and optimized parameter sets used to compute the potential energy of a system of particles (Kowalczyk et al., 2007).

Finally, the MC method is implemented in the Grand Canonical statistical ensemble. In the GCMC method there are three types of attempted moves for the efficient sampling of the configuration space of the system: (i) displacement: a particle is randomly selected and displaced (translation

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[1] VMD software, http://www.ks.uiuc.edu/Research/vmd/

[2] LAMMPS software, http://lammps.sandia.gov/index.html

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and/or rotation) by a random vector; (ii) creation: a particle is created at a random position in the simulation box; and (iii) destruction: a particle is randomly selected and destroyed. The attempt of a creation or a deletion is performed randomly with equal probabilities. Displacement is handled using the Metropolis method. The detailed description of the GCMC method is given in the tutorial.

3.3.1.2   Tools realisation

Through the platform the user will be able to download the tutorial and all the necessary input files, while a link for redirection to the official websites of the VMD and LAMMPS softwares will be also provided. The tool has not been implemented in the platform yet. However, the recommended structure is the following.

- Storage/Separation tools
  - Hydrogen Storage in Carbon-based Materials
    - Click here to download the tutorial and the input files
    - Click here to download the LAMMPS code
    - Click here to download VMD code
  - Hydrate equilibrium pressure of H2_mixtures
  - Hydrate-based separation of the binary mixture H2 + CO2

3.3.1.3   Hydrate equilibrium pressure of H2 mixtures

The objective of the *Hydrate equilibrium pressure of H2 mixtures* is to provide a user friendly web-based tool to calculate the three-phase (i.e., Hydrate – Liquid water – Vapour; H–L$_w$–V) equilibrium pressure (Sloan and Koh, 2007) of a binary gas mixture (A + B), where in our notation gas component A is always H$_2$, while component B could be either CO_2 or CH_4. The three-phase equilibrium pressure is an important thermodynamic property for all processes that use hydrate formation for gas storage or gas-mixture separation industrial applications.

The calculations are performed using the methodology introduced by Lipenkov & Istomin (Lipenkov and Istomin, 2001), (Thomas et al., 2009). The methodology combines the use of the hydrate equilibrium pressures of the pure gases. The hydrate equilibrium pressure, P_i, of pure gases is given by a simple expression (Holder et al., 1988),

$$P_i = 1000 * exp\left(C_i + \frac{D_i}{T}\right)$$

where C_i and D_i are component-specific parameters and the factor 1000 is used in order to have the pressure expressed in units of Pa. The parameters for each gas are calculated by fitting the aforementioned equation to three-phase equilibrium experimental data for each gas hydrate system (Holder et al., 1988).

The three-phase equilibrium pressure of the mixture is provided by the following expression:

$$P_{AB} = \frac{P_A \cdot P_B}{(P_A + P_B) - (Y_A P_A + Y_B P_B)}$$

3.3.1.4   Tools realization

The tool has not been implemented in the platform yet. However, the recommended structure is the following.

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Please select the binary gas mixture (A + B) to consider:

1. H_2 (A) + CO_2 (B)

2. H_2 (A) + CH_4 (B)

The user would be able to select between two binary mixtures, H2/CO2 and H2/CH4. Upon selection of the gas mixture to consider, the following two option will be available:

Please select the type of calculation to consider:

(a) Perform calculation at a specific temperature, T, in the range [273 – 298 K] and gas composition, Y_A, in the range (0 – 1).

(b) Perform calculations at a specific gas composition (Y_A) in the temperature range 273 – 298 K.

In the first option, the user should give as input data a specific temperature and the gas composition and the output data, i.e. the equilibrium pressure of pure components and of the mixture, will be displayed in a table format. In the second option, the user should define only the gas composition and the output data will be displayed in table and plot format over a temperature range with increments specified by the user. The user would be able to export both the table and the plot for further editing.

3.3.1.5   Hydrate-based separation of the binary mixture H2+CO2

The current tool calculates the separation efficiency of the binary gas mixture (A + B) where, in our notation, gas component A is always H_2, while component B is CO_2. The separation process is based on hydrate formation. The mixture H2/CO2 is of great significance due to its encounter in the newer Integrated Gasification Combined Cycle (IGCC) technology.

IGCC is a technology that turns coal and other carbon based fuels into pressurized gas—synthesis gas (syngas), which is a fuel gas mixture consisting of hydrogen, carbon dioxide and carbon monoxide. The syngas can then be converted into a mixture of CO_2 and H_2. Separation of CO_2 from this mixture would result in pure H_2 that can be used in fuel cells. A cleaner power generation cycle is then achieved with low non-carbon greenhouse gas emissions.

There are several methodologies to separate the H2/CO2 mixture. An attractive relatively new technology is the use of hydrate formation to separate the gas mixture. Consider the following schematic (Figure 2):

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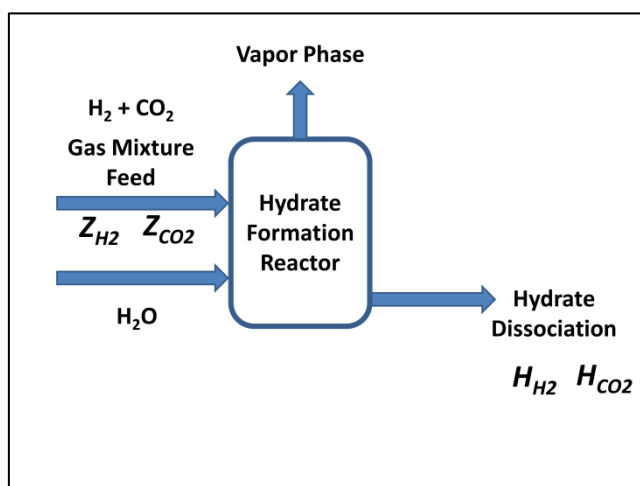
Figure 2 - Schematic depiction of H2/CO2 separation using hydrate technology.

Subsequently, consider a gas mixture that contains H_2 and CO_2 and has a composition (expressed in mole fraction): Z_{H2} and Z_{CO2} for H_2 and CO_2 respectively. If the gas mixture is introduced in a vessel with water, at appropriate temperature, T, and pressure, P, hydrate can be formed (i.e., "ice-like", solid, inclusion material). The solid phase can selectively incorporate part of the gas phase. Upon dissociation of the hydrate material (i.e., by reducing the pressure or increasing the temperature), the enclathrated gas phase can be released. However, the final composition (i.e., H_{H2} and H_{CO2} for H_2 and CO_2 respectively) of the released gas phase is different than the initial gas feed composition. Therefore, some degree of gas mixture separation can be achieved (Sloan & Koh, 2007), (Holder et al., 1988) following such a methodology. The particular approach has been used for industrial gas separation, with a particular example being the system $H_2 + CO_2$. The above process requires multiple steps for greater levels of separation.

This tool presents some important parameters that are related to the separation process of the $H_2 + CO_2$ mixture using hydrate technology. The tool's calculations are carried out with the help of a database, which contains the three-phase equilibrium pressure and the hydrogen composition in the hydrate phase based on the composition in the feed mixture and on the temperature. This database is produced using the van der Waals – Platteeuw theory and will be thoroughly validated against available experimental data.

3.3.1.6   Tools realisation

It has not implemented in the platform yet. The main idea is to allow the user to define the temperature and the mole fraction of hydrogen in the gas feed mixture and the tool will provide as output data: the pressure, the CO2 composition in the gas feed mixture, the composition of the hydrate phase, the split fractions and the separation efficiencies. The data will be displayed in table format, which the user will be able to export it for further editing.

3.4   FC integrated into CHP tools

3.4.1   Simulation of FC system integrated into CHP application, including electrolyser operation (UNIPG)

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3.4.1.1   Introduction

This model allows the calculation of payback time of a Fuel Cell CHP unit once installed in an existing building. The model is based on monthly energy production and consumption, while energy prices are considered constant during the overall period. The tool is divided in two different sections. Section one is the study of system payback when no additional energy sources are included. In this first part the user should know the average heat and electrical monthly consumption of the building as input for the calculations. Section two, that is a continuation of the first study, evaluates the integration into the building of a renewable energy system (RES), such as PV panels or micro wind turbine, and a long-term storage realized with an electrolyzer and hydrogen tank. If the user activates this latter option, additional inputs on the availability of the RES, are required.

Nomenclature

Parameter	Symbol	Unit
Monthly energy consumption	Ec_n	kWhe
Monthly gas consumption	Gc_n	Scm
Boiler efficiency	η_b	
Retail price	*Erp*	€/kWhe
Electricity cost	*Ec*	€/kWhe
Gas cost	Gc	€/SCM
CHP unit electrical size	P_{CHP}	kW
Electrical efficiency of CHP unit	η_e	
Thermal efficiency of CHP unit	η_t	
CHP unit cost	U_c	€/kW
Monthly cogeneration utilization factor	UF_n	

Additional parameters are introduced and commented during calculations.

Energy is measured in kWh with additional subscript: *e*, in case of electrical energy; *t*, in case of thermal energy; *g*, in case of chemical energy in a gas such as hydrogen or natural gas.

3.4.1.2   CHP base model description

Note: Model description should appear upon pressing the appropriate button on the home screen of the tool.

This model calculates the payback of a fuel cell system for cogeneration of heat and power (CHP) when introduced in an existing building to optimize energy efficiencies and reduce energy price. CHP integration is based using, as main range of time, month. This means that the energy balance and the valorization of the energy in terms of consumption or supply is evaluated at the end of every month. Thermal or electric buffer can be used to match the production and the consumption for smaller range of time such as days, hours, minutes and seconds. The aim of the tool is to evaluate system payback and not to optimize system design.

Required inputs:

- Building inputs: monthly electricity and heat consumption, efficiency of the existing boiler.
- CHP inputs: unit size, thermal and electrical efficiency, unit cost.

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- Market inputs: electricity cost, retail price and gas cost.
- Integration strategy: utilization factor of the unit during the year.

General assumptions:

- The CHP unit operates in steady state with only ON/OFF operation;
- Energy values of gas and electricity are not time dependent;

Integration strategies:

- All balances in terms of energy are realized with month as range of time;
- Extra heat produced by CHP is not valorized into the building but can be released to atmosphere with no additional cost;
- Extra production of electricity is sold to the grid at input defined retail value;

Calculations:

CHP instant gas consumption (G_{CHP} - kWh) is calculated as follows:

CHP gas consumption $$G_{CHP} = \frac{P_{CHP}}{\eta_e}$$ (1.1)

CHP monthly electrical production (E_{eCHPn} – kWh) is calculated as the electricity produced by the system multiplied to the operation hours of the month:

Power from CHP $E_{eCHPn} = (P_{CHP}) \cdot (24 \cdot D_n \cdot UF_n)$ D_n = days in month n   (1.2)

Month	Gen	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Dn	31	27	31	30	31	30	31	31	30	31	30	31

CHP monthly thermal production (E_{tCHPn} – kWhe) is calculated as the heat produced by the system multiplied to the operation hours of the month:

Heat from the CHP $$E_{tCHPn} = (\frac{P_{CHP}}{\eta_e} \cdot \eta_t) \cdot (24 \cdot D_n \cdot UF_n)$$ (1.3)

CHP monthly gas consumption (G_{CHPn} – kWhg) is calculated as the system gas consumption multiplied to the operating hours:

Gas consumption $$G_{CHPn} = G_{CHP} \cdot (24 \cdot D_n \cdot UF_n)$$ (1.4)

Electricity balance (DE – kWhe) is calculated as the difference between the electricity produced by the CHP unit and electricity consumption of the building. This is also the energy that is supplied from the market:

Energy from the market $$DE_n = E_{eCHPn} - Ec_n$$ (1.5)

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Thermal balance (DT – kWht) is calculated as the difference between the heat produced by the CHP unit and heat requirement of the building. Such amount as to be supplied from the additional boiler. Building heat requirement is calculated starting from gas consumption multiplying to the boiler efficiency multiplied to natural gas low heating value, 9.59 kWh/Sm^3:

Heat from the boiler $DT_n = \text{Gc}_n \cdot 9.59 \cdot \eta_b - E_{tCHPn}$ (1.6)

Annual OPEX$_{CHP}$ costs (€/year) is calculated as difference between costs, electricity and gas, and income, electricity. Over production of heat is not considered as a possible income for the economic evaluations. The equation calculates electricity and gas value as cost or income depending on the relative balance.

$$OPEX_{CHP} = \sum_{1}^{12} (G_{CHPn} \cdot G_C) - (DE_n \cdot E_C{}^*{}_n) + \left(\frac{DT_n}{\eta_b} \cdot T_C{}^*{}_n\right)$$

$$E_C{}^*{}_n = \begin{bmatrix} Erp, DE_n > 0 \\ Ec, DE_n \leq 0 \end{bmatrix}$$ (1.7)

$$T_C{}^*{}_n = \begin{bmatrix} G_c, DT_n > 0 \\ 0, DT_n \leq 0 \end{bmatrix}$$

Annual OPEX$_{SOA}$ costs (€/year) is the operational cost without the CHP unit and is calculated as the sum of monthly electricity and gas costs of the building.

$$OPEX_{SOA} = \sum_{1}^{12} (Gc_n \cdot G_C \cdot 9.59) + (E_n \cdot E_{C_n})$$ (1.8)

CAPEX$_{CHP}$ cost (€), is calculate as system size multiplied to unit cost:

$$CAPEX_{CHP} = P_{CHP} \cdot U_c$$ (1.9)

The PAYBACK$_{CHP}$ (years) is the ration between CAPEX and the economies, calculated as difference between OPEX$_{SOA}$ and OPEX$_{CHP}$:

$$PAYBACK_{CHP} = \frac{CAPEX_{CHP}}{OPEX_{SOA} - OPEX_{CHP}}$$ (1.10)

3.4.1.3   Input values

Values to calculate payback of CHP unit.

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Monthly energy consumption*	Ec$_n$		kWhe	> 0	-
Monthly gas consumption*	Gc$_n$		SMC	> 0	-
Boiler efficiency	η_b			0-1,2	0.9
Retail price	Erp		€/kWhe	> 0	0.14
Electricity cost	Ec		€/kWhe	> 0	0.29
Gas cost	Gc		€/SCM	> 0	0.075

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Size of CHP unit	P_{CHP}		kW	> 0	
Electrical efficiency of CHP unit	η_e			0-1	0.6
Thermal efficiency of CHP unit	η_t			0-1	0.22
CHP unit cost	U_c		€/kW	> 0	4000
Monthly CHP utilization factor*	UF_n			0-1	

* The input is a vector of 12 values, one for each month of the year

3.4.1.3.1 Calculation procedure

1.1	Gas consumption G_{CHP}	G_{CHP}	$$G_{CHP} = \frac{P_{CHP}}{\eta_e}$$	kWhg
1.2	Monthly electrical production E_{eCHPn}	E_{eCHPn}	$E_{eCHPn} = (P_{CHP}) \cdot (24 \cdot D_n \cdot UF_n)$ D_n = days in month n	kWhe
1.3	Monthly thermal production E_{tCHPn}	E_{tCHPn}	$$E_{tCHPn} = (\frac{P_{CHP}}{\eta_e} \cdot \eta_t) \cdot (24 \cdot D_n \cdot UF_n)$$	kWht
1.4	CHP monthly gas consumption G_{CHPn}	G_{CHPn}	$G_{CHPn} = G_{CHP} \cdot (24 \cdot D_n \cdot UF_n)$	kWhg
1.5	Electricity balance DE	DE_n	$DE_n = E_{eCHPn} - Ec_n$	kWhe
1.6	Thermal balance DT	DT_n	$DT_n = Gc_n \cdot 9.59 \cdot \eta_b - E_{tCHPn}$	kWht
1.7	Annual OPEX$_{CHP}$ costs	$OPEX_{CHP}$	$$OPEX_{CHP} = \sum_{1}^{12}(G_{CHPn} \cdot G_C)$$ $$- (DE_n \cdot E_{C}{}^{*}{}_{n})$$ $$+ \left(\frac{DT_n}{\eta_b} \cdot T_{C}{}^{*}{}_{n}\right)$$ $$E_{C}{}^{*}{}_{n} = \begin{bmatrix} Erp, DE_n > 0 \\ Ec, DE_n \leq 0 \end{bmatrix}$$ $$T_{C}{}^{*}{}_{n} = \begin{bmatrix} G_c, DT_n > 0 \\ 0, DT_n \leq 0 \end{bmatrix}$$	€/year
1.8	OPEX of state of art	$OPEX_{SOA}$	$$OPEX_{SOA} = \sum_{1}^{12}(Gc_n \cdot G_C \cdot 9.59)$$ $$+ (E_n \cdot E_{C_n})$$	€/year

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| 1.9 | CAPEX of CHP layout | $CAPEX_{CHP}$ | $CAPEX_{CHP} = P_{CHP} \cdot U_c$ | € |
| 1.10 | PAYBACK of the CHP | $PAYBACK_{CHP}$ | $PAYBACK_{CHP} = \dfrac{CAPEX_{CHP}}{OPEX_{SOA} - OPEX_{CHP}}$ | year |

3.4.1.3.2 Output values

Main output of the calculation tool is the payback time.

Parameter name	Symbol	Output value	Unit
$PAYBACK_{CHP}$	$PAYBACK_{CHP}$	5,79	year

In addition, a dynamic bar graph will show month results based on user requirements. Based on a selection menu is possible to show inputs, such as Ec_n or Gc_n, and calculated parameters, such as E_{eCHPn}, E_{tCHPn}, DE_n or DT_n.

On request, the tool shows additional parameter such and $OPEX_{CHP}$ and $CAPEX_{CHP}$.
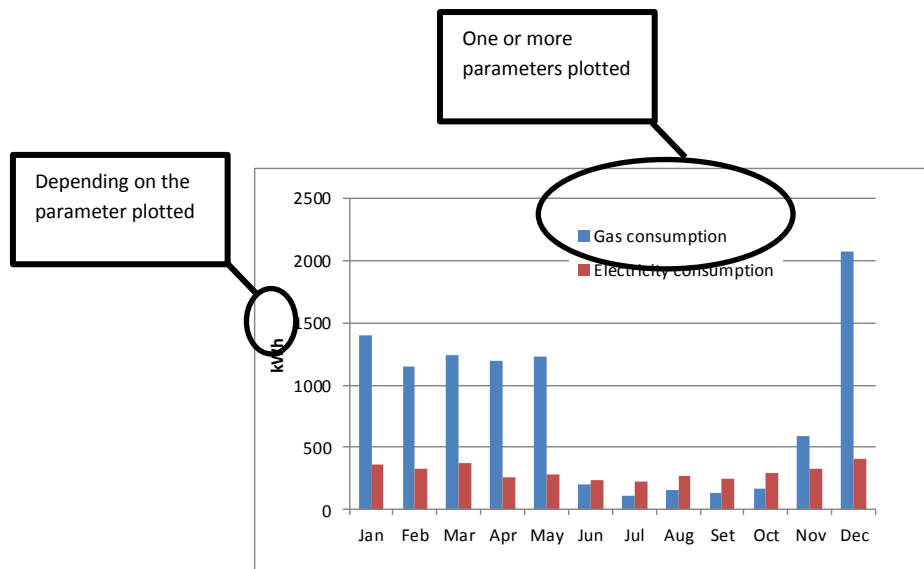
Example of results panel which should appear after calculation.

3.4.1.4   Tool realisation

The snapshot of tool realisation is presented in Figure 3.

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Figure 3 - Simulation of FC system integrated into CHP application, including electrolyser operation tool snapshot.

3.4.2   Integration of Renewable energy sources

After the first section, the tool allows the user to continue the study considering the integration of a renewable energy source (RES). A specific button should be available for such option. In the case a RES is introduced into the system additional inputs are required.

3.4.2.1   Input values

Values to calculate payback in case RES unit is introduced.

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
RES utilization factor *	P_{uf}		-	> 0	-
Power of RES unit	P_{RES}		kW	> 0	
RES unit cost	RES_C		€/kW	> 0	
Electrolyser unit cost	E_C		€/kW	> 0	
Hydrogen storage unit cost	S_C		€/kWh	> 0	
Fuel cell unit cost	FC_c		€/kWh	> 0	
Electrolyser efficiency	η_{el}		-	0-1	
Fuel cell efficiency	η_{fc}			0-1	

* The input is a vector of 12 values, one for each month of the year

3.4.2.2   RES-CHP model description

Note: Model description should appear upon pressing the appropriate button on the home screen of the tool.

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This section of the model evaluates the introduction of a renewable energy source in the building and a storage system realized with an electrolyser and a hydrogen storage tank.

Required inputs:

- RES inputs: monthly RES utilization factor, RES power size and RES unit cost;
- Storage inputs: electrolyser and fuel cell efficiency and unit cost, hydrogen storage unit cost.

General assumptions:

- The RES production and electricity consumption is balanced every month. Additional buffer for electricity balance is considered as part of the RES cost;

Integration strategies:

- Electrolyzer and fuel cell are considered in steady state operation. Electrolyzer utilization factor is the same of RES while fuel cell operates in the remaining time of the period;

Electricity produced by RES every month, (RES_n- kWhe), is calculated as follows:

Renewable energy produced $\qquad\qquad RES_n = RES_{uf} \cdot P_{RES} \cdot 24 \cdot D_n$ $\qquad\qquad$ (2.1)

Monthly balance, (DE_{RESN} -kWhe), is the difference between RES production and electricity consumption of the building:

Energy balance $\qquad\qquad\qquad DE_{RESn} = RES_n - Ec_n$ $\qquad\qquad\qquad$ (2.2)

Whenever Energy balance is negative, there is an extra renewable energy ($RESdn$ – kWhe) that can be stored and is calculated as follows:

Extra RES for storage $\qquad\qquad RESd_n = \begin{bmatrix} -DE_{resn}, DE_{resn} \leq 0 \\ 0, \qquad DE_{resn} > 0 \end{bmatrix}$ $\qquad\qquad$ (2.3)

The size of electrolyzer, (P_{el} - kW) is calculates from $RESdn$, and is the maximum the maximum amount of electricity stored when RES balance is negative:

Electrolyzer
power $\qquad\qquad P_{el} = max_{n=1..12} \left(\dfrac{RESd_n}{D_n \cdot 24 \cdot RES_{uf}} \right)$ $\qquad\qquad$ (2.4)

Hydrogen produced (H_{2p} - kWhg) is calculated from the electrolyzer size and the operative time of the system or, equivalent, dividing the $RESdn$ per the electrolyzer efficiency:

Hydrogen produced $\qquad\qquad\qquad H_{2pn} = \dfrac{RESd_n}{\eta_{el}}$ $\qquad\qquad\qquad$ (2.5)

Hydrogen necessary ($H2rn$ – KWhg) to supply all the electrical energy necessary to the user, can be calculated with following equation:

Hydrogen request $\qquad\qquad H_{2rn} = \begin{bmatrix} 0, DE_{resn} \leq 0 \\ \dfrac{DE_{RESn}}{\eta_{fc}}, \qquad DE_{resn} > 0 \end{bmatrix}$ $\qquad\qquad$ (2.6)

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Comparing the hydrogen available and the request is possible to calculate the storage volume and the hydrogen that can be really converted in the fuel cell. The hydrogen available is the sum of the produced plus the amount available in the previous month. The storage is calculated starting from June (n=6) as first month of produced hydrogen starting from an empty hydrogen storage. Hydrogen in the storage (H_{2sn} - kWhg) is calculated as follows:

Hydrogen in the storage
$$H_{2sn} = \begin{bmatrix} H_{2pn} + H_{2sn-1} - H_{2rn}, & H_{2pn} + H_{2sn-1} > H_{2rn} \\ 0, & H_{2pn} + H_{2sn-1} \leq H_{2rn} \end{bmatrix} \quad n = 6..12, 1..5 \qquad (2.7)$$

Hydrogen used in the fuel cell (H_{2fc} – kWhg) can be easily calculated as follows:

Hydrogen used in the fuel cell
$$H_{2fc} = H_{2sn-1} - H_{2sn} \qquad (2.8)$$

The power of the fuel cell (P_{fc} – kW) can be calculated based on the hydrogen used:

Fuel cell power
$$P_{fc} = max_{n=1..12} \left(\frac{H_{2fc}}{D_n \cdot 24 \cdot (1 - RES_{uf})} \cdot \eta_{fc} \right) \qquad (2.9)$$

The electricity produced from the fuel cell (E_{FCn} – kWhe) is calculated as follows:

Fuel cell electrical energy
$$E_{fcn} = H_{2fc} \cdot \eta_{fc} \qquad (2.10)$$

Total amount of electricity produced from renewable energy (RES_{tn} – kWhe) is the following:

Total RES electrical supply
$$RES_{tn} = E_{fcn} + RES_n - RESd_n \qquad (2.11)$$

The difference between the total energy consumption (E_{cn}) and the total RES supply (RES_{tn}) is the new monthly energy consumption that can be used as input for the cogeneration design as described in phase 1.

New energy consumption
$$Ec_n^* = E_{cn} - RES_{tn} \qquad (2.12)$$

The CAPEX of the RES and storage system, ($CAPEX_{RES}$ - €) is calculated as follows:

$$CAPEX_{RES} = P_{RES} \cdot RES_c + P_{el} \cdot E_c + P_{fc} \cdot FC_c + H_{2s} \cdot S_c \qquad (2.13)$$

Total CAPEX cost (CAPEX - €), is $CAPEX_{CHP}$, obtained from phase 1 calculation based on the new energy request, and $CAPEX_{RES}$:

$$CAPEX = CAPEX_{CHP} + CAPEX_{RES} \qquad (2.14)$$

The payback (PAYBACK - years) is the ration between CAPEX and the economies, calculated as difference between $OPEX_{SOA}$ and $OPEX_{CHP,}$ considering that RES unit has no OPEX costs:

$$PAYBACK = \frac{CAPEX}{OPEX_{SOA} - OPEX_{CHP}} \qquad (2.15)$$

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

3.4.2.2.1 Calculation procedure

Input parameters from user

Calculate Eq. 12-16 for n=1..12

Calculate Eq. 2-6 for n=1..12 using $E_{cn} = E_{cn}^*$

Calcualte Eq. 7-8

Calculate Eq. 17-19
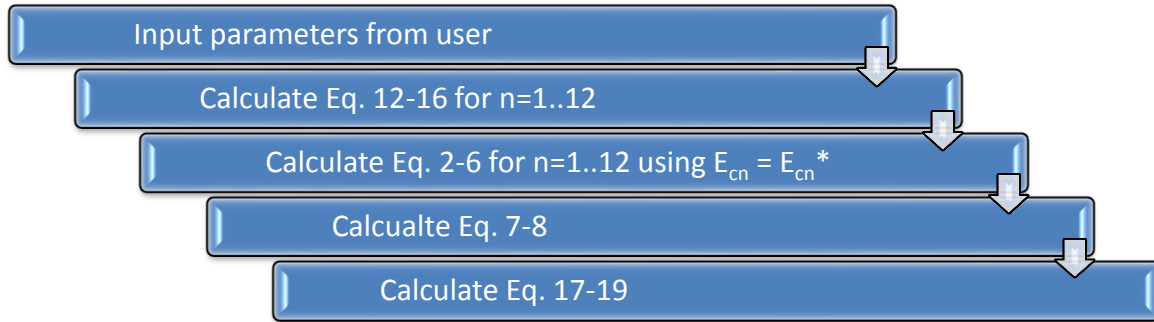
2.1	Renewable energy produced	RES$_n$	$$RES_n = RES_{uf} \cdot P_{RES} \cdot 24 \cdot D_n$$	kWhe
2.2	Energy balance	DE$_{RESN}$	$$DE_{RESn} = RES_n - Ec_n$$	kWhe
2.3	Extra RES for storage	RESd$_n$	$$RESd_n = \begin{bmatrix} -DE_{resn}, DE_{resn} \leq 0 \\ 0, \qquad DE_{resn} > 0 \end{bmatrix}$$	kWhe
2.4	Electrolyzer power	P$_{el}$	$$P_{el} = max_{n=1..12}\left(\frac{RESd_n}{D_n \cdot 24 \cdot RES_{uf}} \right)$$	kW
2.5	Hydrogen produced	H$_{2pn}$	$$H_{2pn} = \frac{RESd_n}{\eta_{el}}$$	kWhg
2.6	Hydrogen request	H$_{2rn}$	$$H_{2rn} = \begin{bmatrix} 0, DE_{resn} \leq 0 \\ \frac{DE_{RESn}}{\eta_{fc}}, \qquad DE_{resn} > 0 \end{bmatrix}$$	kWhg
2.7	*Hydrogen in the storage*	H$_{2sn}$	$$H_{2sn} = \begin{bmatrix} H_{2pn} + H_{2sn-1} - H_{2rn}, \qquad H_{2pn} + H_{2sn-1} > H_{2rn} \\ 0, \qquad H_{2pn} + H_{2sn-1} \leq H_{2rn} \\ n = 6..12, 1..5 \end{bmatrix}$$	kWhg
2.8	*Hydrogen used in the fuel cell*	H$_{2fc}$	$$H_{2fc} = H_{2sn-1} - H_{2sn}$$	kWhg
2.9	*Fuel cell power*	P_{fc}	$$P_{fc} = max_{n=1..12}\left(\frac{H_{2fc}}{D_n \cdot 24 \cdot (1 - RES_{uf})} \cdot \eta_{fc} \right)$$	kW
2.10	*Fuel cell electrical energy*	E_{fcn}	$$E_{fcn} = H_{2fc} \cdot \eta_{fc}$$	kWe
2.11	*Total RES electrical supply*	RES_{tn}	$$RES_{tn} = E_{fcn} + RES_n - RESd_n$$	kWe
2.7	New electricity consumption	Ec_n^*	$$Ec_n^* = E_{cn} - RES_{tn}$$	kWhe

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		E_{cn}*			
			Consider eq. 1.1 – 1.10		
2.8	CAPEX of RES	$CAPEX_{RES}$	$CAPEX_{RES} = P_{RES} \cdot RES_c + P_{el} \cdot E_c + P_{fc} \cdot FC_c + H_{2s} \cdot S_c$	€
2.9	Total CAPEX	CAPEX	$CAPEX = CAPEX_{CHP} + CAPEX_{RES}$	€
2.10	Total PAYBACK	PAYBACK	$PAYBACK = \dfrac{CAPEX}{OPEX_{SOA} - OPEX_{CHP}}$	year

3.4.2.2.2 Output values

Main output of the calculation tool is the payback time.

Parameter name	Symbol	Output value	Unit
PAYBACK	PAYBACK	4,13	year

In addition, a dynamic bar graph will show month results based on user requirements (see previous paragraph). Based on a selection menu is possible to show inputs, such as Ec_n or Gc_n, and calculated parameters, such as RES_n, D_{RESn}, $H_{2n}E_{eCHPn}$, E_{tCHPn}, DE_n or DT_n.

On request, the tool shows additional parameter such and P_{el}, H_{2s}, $OPEX_{CHP}$ and $CAPEX_{RES}$, $CAPEX_{CHP}$.

3.4.3   References

Desideri, U., Cinti, G., Discepoli, G., Sisani, E., Penchini D*., "SOFC Micro-CHP integration in residential buildings",* (2012) Proceedings of the 25th International Conference on Efficiency, Cost, Optimization and Simulation of Energy Conversion Systems and Processes, ECOS 2012, 7, pp. 261-272.

R. Atochero Velasco, A. Lubrano Lavadera , S. Scarfogliero, G. Cinti, G. Bidini, V. Cigolotti, M. Minutillo, "*Electrical energy storage systems based on resoc technology: a novel approach for the grid integration of renewable energy sources*", European Fuel Cell Technology & Applications Piero Lunghi Conference, Naples, December 16-18, 2015, ISBN 978-88-8286-324-1.

3.5   Safety engineering tools

3.5.1   Jet parameters model (UU)

3.5.1.1   Introduction

Note: Model description should appear upon pressing the appropriate button on the home screen of the tool.

This model describes the parameters in either an expanded or an under-expanded jet.

Shown in Figure 1 is a simple schematic of an 'expanded' (red lines) and an 'under-expanded' (black lines) jet.

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]
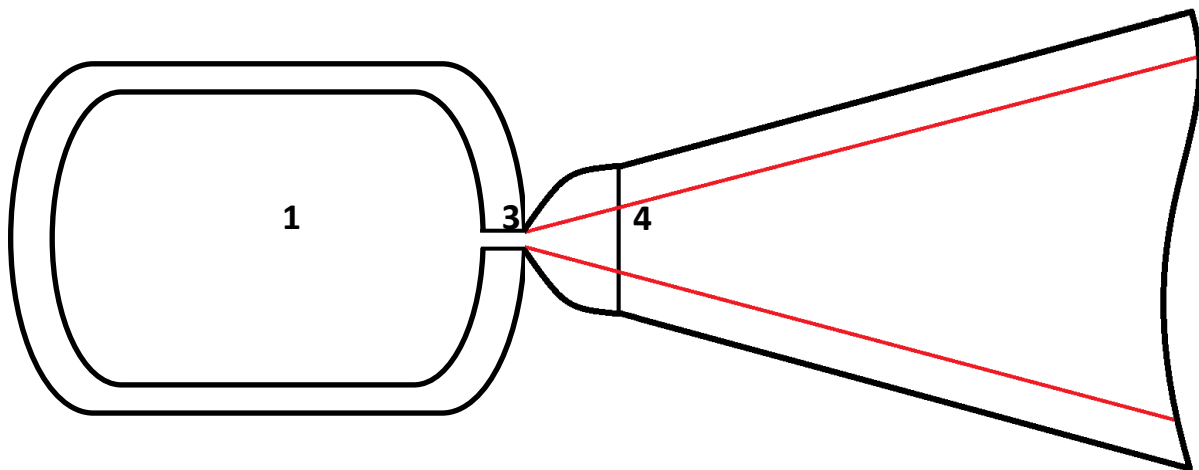
Figure 4 – Simple schematic of 'expanded' (red lines) and 'under-expanded' (black lines) jet.

1 = Reservoir

3 = Nozzle (orifice)

4 = Pressure and velocity is equal to ambient and local speed of sound respectively (condition 4 exists only for under-expanded jet)

The critical pressure ratio across the leak, p^*, determines whether the flow is subsonic or sonic / supersonic.

$$p^* = \frac{p_1}{p_{atm}} = \left(\frac{(\gamma + 1)}{2}\right)^{\gamma/(\gamma-1)}$$

Therefore the critical pressure ratio for the transition to sonic flow for hydrogen is $\approx$ 1.9. If p^* < 1.9, the flow is subsonic and expanded, as long as p^* > 1.9, the exit velocity remains locally sonic and the jet is underexpanded. The exit pressure rises above ambient with the result that expansion, down to ambient pressure, p_{atm}, takes place outside of the real nozzle at location downstream of the Mach disc, called the "notional" nozzle or effective diameter.

Therefore different equation sets are solved depending on whether the flow is expanded or under-expanded. The equation set relating to an under-expanded jet is detailed in (V. Molkov & Bragin, 2009) and (Molkov, 2012) and is based on the Abel-Noble equation of state for hydrogen; conservation equations for mass and energy; assumption that at state (4) (so called "effective nozzle diameter") pressure is equal to ambient and velocity is equal to the local sound speed.

The expanded jet equation set utilises the isentropic pressure and density relationships.

3.5.1.2   Nomenclature

Parameter	Symbol	Unit
Universal gas constant	R	J/(kmol K)
Molecular mass	M	kg/kmol
Hydrogen specific gas constant	R_{H2}	J/ (kg K)

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Hydrogen co-volume constant	$b=0.007691$	m^3/kg
Pressure in reservoir	p_1	Pa
Adiabatic index	$\gamma=1.405$	-
H$_2$ density in reservoir	ρ_1	kg/m^3
Temperature in reservoir	T_1	K
Orifice diameter	d_3	m
Ambient pressure	p_4	Pa
Mass flow rate	$\dot{m}$	kg/s

3.5.1.3 Input values

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Hydrogen pressure in reservoir	p_1	20500000	Pa	190000-100000000	20500000
Hydrogen temperature in reservoir	T_1	288	K	230-330	288
Orifice diameter	d_3	0.0095	m	0.0001-0.1	0.0095
Ambient pressure	p_4	101325	Pa	33700-107900	101325

3.5.1.4 Calculation procedure

	Initial conditions		
1	Hydrogen pressure in reservoir	p_1 - user input	Pa
2	Hydrogen temperature in reservoir	T_1 - user input	K
3	Orifice diameter	d_3 - user input	m
4	Ambient pressure	p_4 - user input	Pa
	Calculation		
5	Universal gas constant	$R=8314.47$	J/K/kmol
6	H2 molar mass	$M_{H2}=2.016$	kg/kmol
7	Hydrogen specific gas constant	$R_{H2}=R/M_{H2}$	J/ (kg K)
8	H2 co-volume constant	$b= 0.007691$	m^3/kg
9	Adiabatic index	$\gamma=1.405$	-
10	H$_2$ density in reservoir	$$\rho_1 = \frac{p_1}{\left(p_1 b + R_{H2} T_1\right)}$$	kg/m^3

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

Algorithm of solution:

If statement 1:

IF	$1.0 < \dfrac{p_1}{p_4} < 1.9$	
Ambient pressure	$p_3 = p_4$	[kg/m^3]
Mach number at the orifice, M_3 :	$M_3 = \sqrt{\dfrac{2\left[\left(\frac{p_1}{p_4}\right)^{\frac{(\gamma-1)}{\gamma}}-1\right]}{(\gamma-1)}}$	[ND]
Temperature at the orifice	$T_3: \quad T_3 = T_1 \cdot \left(\dfrac{p_4}{p_1}\right)^{(\gamma-1)/\gamma}$	[K]
Speed of sound at orifice	$C_3: \quad C_3 = \sqrt{\dfrac{\gamma \cdot R \cdot T_3}{M_{H_2}}}$	[m/s]
Velocity at the orifice (actual)	$V_3: \quad V_3 = M_3 \times C_3$	[m/s]
Mass flow rate, $\dot{m}$:	$\dot{m} = \rho_3 \times V_3 \times \dfrac{\pi \cdot d_3^2}{4}$	[kg/s]

ELSE

If statement 2:

IF $\qquad\qquad\qquad\qquad\qquad\qquad \dfrac{p_1}{p_4} \leq 1.0$ **Stop calculation**

NB: Calculation cannot proceed: Box containing p$_1$ should turn red. Note beside p$_1$ box should appear: "Value of p$_1$ (reservoir) must be greater than p$_4$ (ambient)"

ELSE

Procedure for ρ_3:

$\Delta = 0.1$ $\qquad\qquad\qquad\qquad\qquad\qquad$ /* Δ Index (Required within 'If' loop) */

$i_\Delta = 0$

$\rho_3 = 0.6\rho_1$ $\qquad\qquad\qquad\qquad\qquad$ /* first guess for r3*/

$$LHS = \left(\frac{\rho_1}{1-b\rho_1}\right)^{\gamma}$$ /* Left hand side of equation */

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

$$RHS = \left(\frac{\rho_3}{1-b\rho_3}\right)^{\gamma}\left[1+\left(\frac{\gamma-1}{2(1-b\rho_3)^2}\right)\right]^{\frac{\gamma}{\gamma-1}}$$ /* Right hand side of equation */

Loop:

WHILE $(\rho_3<\rho_1)$ and (LHS-RHS)/LHS≥0.00001   **DO**

/* This loop should continue until condition $\left|\frac{(LHS-RHS)}{LHS}\right| < 0.00001$ is met*/

If (RHS < LHS)   { i∆=0; $\rho_3=\rho_3+\Delta$ } **else**

If (RHS > LHS and i∆=0)   { ∆=∆/2; i∆=1; $\rho_3=\rho_3-\Delta$ } **else**

If (RHS > LHS and i∆=1)   {$\rho_3=\rho_3-\Delta$}

/* Purpose of this loop is to iterate ρ_3 calculation until LHS = RHS (to specified accuracy)*/

Temperature at the orifice, T_3:	$T_3 = T_1/\left(1+(\gamma-1)/2(1-b\rho_3)^2\right)$	[K]
Pressure in orifice, p_3:	$p_3 = \dfrac{\rho_3 R_{H2} T_3}{1-b\rho_3}$	[Pa]
Velocity in orifice, V_3:	$V_3^2 = \gamma R_{H2} T_3/(1-b\rho_3)^2$	[m/s]
Temperature in effective nozzle, T_4:	$T_4 = \dfrac{2T_3}{(\gamma+1)}+\dfrac{(\gamma-1)}{(\gamma+1)}\dfrac{p_3}{\rho_3(1-b\rho_3)R_{H2}}$	[K]
Velocity in effective nozzle, V_4:	$V_4^2 = \gamma R_{H2} T_4$	[m/s]
Density in effective nozzle, ρ_4:	$\rho_4 = \dfrac{p_4}{(p_4 b + R_{H2} T_4)}$	[kg/m³]
Effective nozzle diameter, d_4:	$d_4 = d_3(\rho_3 V_3/\rho_4 V_4)^{1/2}$	[m]
Mass flow rate, $\dot{m}$:	$\dot{m} = \rho_4 V_4 \cdot \pi d_4^2/4$	[kg/s]

3.5.1.5   Output values

Parameter name	Symbol	Output value	Unit
Density in the reservoir,	ρ_1	15.237	kg/m3
Density at the orifice,	ρ_3	9.489	kg/m3
Pressure in orifice,	p_3	9839437.89	Pa
Velocity in orifice,	V_3	1254	m/s
Temperature at the orifice,	T_3	233	K
Diameter of effective nozzle exit,	d_4	0.0942544	m

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Density in effective nozzle exit,	ρ_4	0.1024997	kg/m3
Velocity in effective nozzle exit,	V_4	1179	m/s
Temperature in effective nozzle exit,	T_4	239.5	K
Mass flow rate,	$\dot{m}$	0.84302	kg/s

3.5.1.6   Tool realisation

The snapshot of tool realisation is presented in Figure 5. The user can select the required units for Temperature, Length, Volume and Pressure before or after calculation by selecting appropriate units in the dropdown list above the input fields. The conversion units described in section 4. Upon pressing the Show description button user can read the model details and see all appropriate links to the publications that were used to develop the tool. After user specified all initial values in the input field and pressing calculate, all output values will be provided as shown in Figure 5. All results can be exported to coma separated file *.CSV and saved by pressing the "Export to CSV" button.

Figure 5 - Snapshot of Jet parameters model realisation.

3.5.2   Adiabatic and isothermal model of blowdown of storage tank dynamics (UU)

3.5.2.1   Introduction

This model consists of two options to allow for the calculation of high-pressure hydrogen tank blowdown with adiabatic and isothermal conditions.

1. Adiabatic blowdown of storage tank
2. Isothermal blowdown of storage tank

3.5.2.2   Choice of the model

When the tool is selected, the screen with the choice should appear prompting to select the option.

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

> **Please choose the option you want to calculate:**
>
> ○ 1. Adiabatic blowdown of storage tank
>
> ○ 2. Isothermal blowdown of storage tank

Note: Example of the model choice is the Option (radio) Button. When checked the screen with appropriate input parameters should appear below, together with button to initiate calculation (choice of RUN, CALCULATE, START etc. to be uniform across the e-Laboratory).

3.5.2.3   Option 1: Adiabatic blowdown of storage tank (Model description)

3.5.2.3.1 Introduction

Note: Model description should appear upon pressing the appropriate button on the home screen of the tool.

This model allows user to calculate the adiabatic blowdown of storage hydrogen tank.
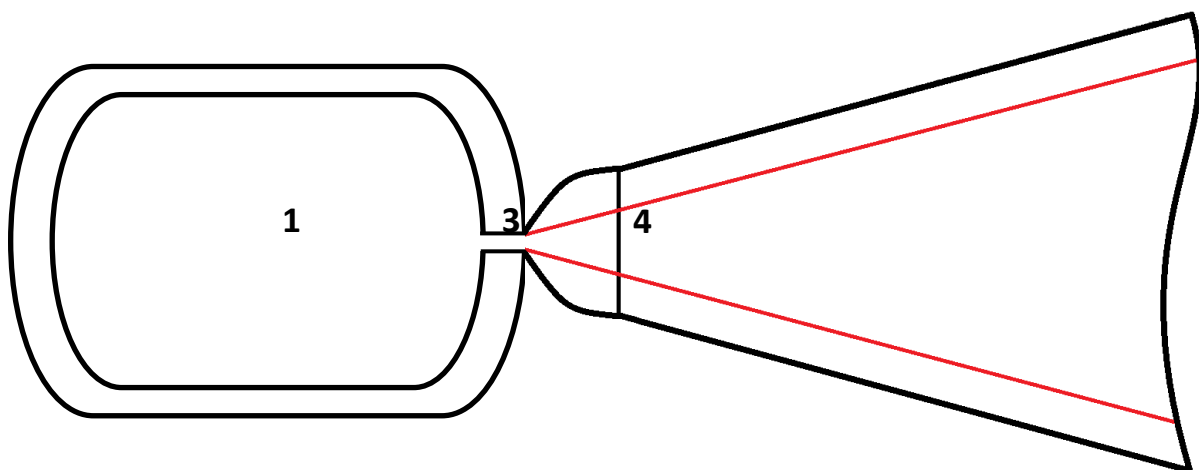
Figure 6 – Simple schematic of 'expanded' (red lines) and 'under-expanded' (black lines) jet

1 = Reservoir

3 = Nozzle (orifice)

4 = Pressure and velocity is equal to ambient and local speed of sound respectively (condition 4 exists only for under-expanded jet)

The adiabatic blowdown model is based on the assumption of a quick release from a high-pressure reservoir and negligible heat transfer effects to the released hydrogen temperature.

It is built on the model for expanded and under-expanded jet parameters (Molkov, 2012), which describes parameters in an expanded and under-expanded jet through the characteristic stages of its development – in reservoir (1), orifice (3), and effective nozzle diameter (4).

The under-expanded jet parameters model is derived from the Abel-Noble equation of state for hydrogen and the conservation equations for mass and energy. The outflowing mass flow rate,

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

determined according to the under-expanded jet parameters mode, is integrated until the ratio of the pressure in the vessel, p_1, to the ambient pressure, p_4, reaches the critical value corresponding to the chocked flow conditions in the orifice:

$$p_1/p_4 = \left[(\gamma+1)/2\right]^{\gamma/(\gamma-1)}$$, which for hydrogen (γ =1.405) is equal to: $p_1/p_4 < 1.9$. (Schefer, Houf, Marchi, Chernicoff, & Englom, 2006)

Where:

- p_1 = Pressure in reservoir
- p_4 = Atmospheric pressure
- γ = Ratio of specific heats (1.405)

At this time, when $p_1/p_4 < 1.9$, the jet is considered to be expanded, and the outflowing mass flow rate is then calculated using isentropic pressure and density relationships.

NB1:   The realised algorithm attempts to determine blowdown time starting from an initial guess provided by the user as an input parameter.

NB2:   Initial number of time steps for integration is chosen as n = 1000 to avoid a prolonged calculation. Though n = 1000 is usually sufficient to provide precise integration, users are advised to use a larger number of time steps (e.g. n = 2000) to check if the pressure dynamics in the vessel remains essentially the same (after blowdown time is determined using the initial time step number n = 1000). It is recommended to increase time step number until the pressure dynamics are time step insensitive, i.e. time step convergence has been reached.

3.5.2.3.2 Nomenclature

Parameter	Symbol	Unit
Universal gas constant	R	J/(kmol K)
Molecular mass	M	kg/kmol
Hydrogen specific gas constant	R_{H2}	J/ (kg K)
Hydrogen co-volume constant	$b=0.007691$	m^3/kg
Pressure in reservoir	p_1^0	Pa
Adiabatic index	$\gamma=1.405$	-
Critical pressure	p_{crit}	Pa
Initial H_2 density in reservoir	ρ_1^0	kg/m^3
Initial temperature in reservoir	T_1	K
Initial H2 mass in reservoir	m	kg
Initial time	t	s
Initial mass flow rate	$\dot{m}$	kg/s
Iteration counter	i	-
Time step size	Δt	s

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

3.5.2.3.3 Input values

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Initial hydrogen pressure in reservoir	p_1^0	20500000	Pa	190000-100000000	20500000
Initial hydrogen temperature in reservoir	T_1	288	K	230-330	288
Tank volume	V_1	0.196	m	0.01-10	0.196
Orifice diameter	d_3	0.0095	m	0.0001-0.1	0.0095
Ambient pressure	p_4	101325	Pa	33700-107900	101325
Initial guess for integration time	t_{f0}	1000	S	10-5000	1000
Number of time steps for integrations	n	1000	-	500-5000	1000

3.5.2.3.4 Calculation procedure

	Initial conditions		
1	Initial hydrogen pressure in reservoir	p_1^0 - user input	Pa
2	Initial hydrogen temperature in reservoir	T_1 - user input	K
3	Tank volume	V_1 - user input	m^3
4	Orifice diameter	d_3 - user input	m
5	Ambient pressure	p_4 - user input	Pa
6	Initial guess for integration time	t_{f0} - user input	S
7	Number of time steps for integrations	n - user input	-
	Calculation		
8	Universal gas constant	$R=8314.47$	J/K/kmol
9	H2 molar mass	$M_{H2}=2.016$	kg/kmol
10	Hydrogen specific gas constant	$R_{H2}=R/M_{H2}$	J/ (kg K)
11	H2 co-volume constant	$b= 0.007691$	m^3/kg
12	Adiabatic index	$\gamma=1.405$	-
13	Critical pressure	$p_{crit} = p_4 \cdot \left[(\gamma+1)/2 \right]^{\gamma/(\gamma-1)}$	Pa
14	Initial H$_2$ density in reservoir	$\rho_1^0 = \dfrac{p_1^0}{\left(p_1 b + R_{H2} T_1\right)}$	kg/m^3
15	Initial H2 mass in reservoir	$m = V\rho_1$	kg
16	Initial time	$t=0$	s
17	Initial mass flow rate	$\dot{m} = 0$	kg/s
18	Iteration counter	$i=0$	-

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

19	Time step size	$\Delta t = t_{f0}/n$	s

Algorithm of solution:

Mark 1

Create new data file
INTEGRATION NEXT STEP

New H₂ mass in the reservoir, m : $\quad m = m - \dot{m} \cdot \Delta t$ [kg]

Density in the reservoir, ρ_1: $\quad \rho_1 = m/V$ [kg/m³]

Pressure in reservoir, p_1: $\quad p_1 = p_1^0 \left[\dfrac{\rho_1}{\rho_1^0} \dfrac{\left(1 - b\rho_1^0\right)}{\left(1 - b\rho_1\right)} \right]^{\gamma}$ [Pa]

Temperature in reservoir, T_1: $\quad T_1 = \dfrac{p_1}{\rho_1 R_{H2}} \left(1 - b\rho_1\right)$ [K]

If statement 1:

    IF $\qquad\qquad 1.0 < \dfrac{p_1}{p_4} < 1.9$

    Ambient pressure $\qquad p_4 = p_3$ [kg/m³]

    Mach number at the orifice, M_3 : $\quad M_3 = \sqrt{\dfrac{2\left[\left(\frac{p_1}{p_4}\right)^{\frac{(\gamma-1)}{\gamma}} - 1\right]}{(\gamma-1)}}$ [ND]

    Temperature at the orifice T_3 : $\quad T_3 = T_1 \cdot \left(\dfrac{p_4}{p_1}\right)^{(\gamma-1)/\gamma}$ [K]

    Speed of sound at orifice C_3 : $\quad C_3 = \sqrt{\dfrac{\gamma \cdot R \cdot T_3}{M_{H_2}}}$ [m/s]

    Velocity at the orifice (actual) V_3 : $\quad V_3 = M_3 \times C_3$ [m/s]

    Mass flow rate, $\dot{m}$: $\quad \dot{m} = \rho_3 \times V_3 \times \dfrac{\pi \cdot d_3^2}{4}$ [kg/s]

    /* Concerning output (excel file) - When this loop is active please print in each respective column:ρ_4 = N/A, T_4 = N/A and d_4 = N/A */

ELSE
If statement 2:
IF $\qquad\qquad \dfrac{p_1}{p_4} \leq 1.0$ **Stop calculation**

NB: Calculation cannot proceed: Box containing p_1 should turn red. Note beside p_1 box should appear: "Value of p_1 (reservoir) must be greater than p_4 (ambient)"
ELSE
Procedure for ρ_3:

    Δ=0.1 $\qquad\qquad\qquad$ /* Δ Index (Required within 'If' loop) */
    i_Δ=0
    ρ_3=0.6ρ_1 $\qquad\qquad\qquad$ /* first guess for r3*/

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

$$LHS = \left(\frac{\rho_1}{1-b\rho_1}\right)^\gamma$$ /* Left hand side of equation */

$$RHS = \left(\frac{\rho_3}{1-b\rho_3}\right)^\gamma \left[1+\left(\frac{\gamma-1}{2(1-b\rho_3)^2}\right)\right]^{\frac{\gamma}{\gamma-1}}$$ /* Right hand side of equation */

Loop:

WHILE $(\rho_3 < \rho_1)$ and (LHS-RHS)/LHS≥0.00001 **DO**

/* This loop should continue until condition $\left|\frac{(LHS-RHS)}{LHS}\right| < 0.00001$ is met*/

If (RHS < LHS) { i∆=0; $\rho_3 = \rho_3 + \Delta$ } **else**

If (RHS > LHS and i∆=0) { ∆=∆/2; i∆=1; $\rho_3 = \rho_3 - \Delta$ } **else**

If (RHS > LHS and i∆=1) {$\rho_3 = \rho_3 - \Delta$}

/* Purpose of this loop is to iterate ρ_3 calculation until LHS = RHS (to specified accuracy)*/

Temperature at the orifice, T_3: $T_3 = T_1 / \left(1 + (\gamma-1)/2(1-b\rho_3)^2\right)$ [K]

Pressure in orifice, p_3: $p_3 = \dfrac{\rho_3 R_{H2} T_3}{1-b\rho_3}$ [Pa]

Velocity in orifice, V_3: $V_3^2 = \gamma R_{H2} T_3 /(1-b\rho_3)^2$ [m/s]

Temperature in effective nozzle, T_4: $T_4 = \dfrac{2T_3}{(\gamma+1)} + \dfrac{(\gamma-1)}{(\gamma+1)} \dfrac{p_3}{\rho_3(1-b\rho_3)R_{H2}}$ [K]

Velocity in effective nozzle, V_4: $V_4^2 = \gamma R_{H2} T_4$ [m/s]

Density in effective nozzle, ρ_4: $\rho_4 = \dfrac{p_4}{(p_4 b + R_{H2} T_4)}$ [kg/m³]

Effective nozzle diameter, d_4: $d_4 = d_3 (\rho_3 V_3 / \rho_4 V_4)^{1/2}$ [m]

Mass flow rate, $\dot{m}$: $\dot{m} = \rho_4 V_4 \cdot \pi d_4^2 / 4$ [kg/s]

Output to file:

1) Time, t [s]
2) Iteration count, i [-]
3) H_2 mass in the reservoir, m [kg]
4) Pressure in the reservoir, p_1 [Pa/atm/bar/psi] (whichever has been chosen by user)
5) Density in the reservoir, ρ_1 [kg/m³]
6) Temperature in the reservoir, T_1 [K]
7) Pressure in orifice, p_3 [Pa/atm/bar/psi] (whichever has been chosen by user)
8) Density in orifice, ρ_3 [kg/m³]
9) Temperature in orifice, T_3 [K]
10) Density in effective nozzle, ρ_4 [kg/m³]
11) Temperature in effective nozzle, T_4 [K]
12) Effective nozzle diameter, d_4 [m]
13) M Velocity in effective nozzle, V_4 [m/s]
14) Mass flow rate, $\dot{m}$ [kg/s]

/* Please include these column headings in produced 'Excel' output file.*/

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

Updates:

Time, t:	$t = t + \Delta t$	[s]
Iteration counter, i:	$i = i + 1$	[-]
Pressure in reservoir, p_1^0:	$p_1^0 = p_1$	[Pa]
Density in reservoir, ρ_1^0:	$\rho_1^0 = \rho_1$	[kg/m³]

Go to **Mark 1**

Go to **Integration next step**

if {-0.2p₄<(p_1-p_{crit})<=0 AND t-t$_{f0}$>-0.1n} ① YES

NO

if (p_1-p_{crit})< -0.2p₄ ②

NO

NO if (t>t_{f0}) ③ YES

t_{f0}=t, $\Delta t = t_{f0}/n$

t_{f0} = 2t$_{f0}$, $\Delta t = t_{f0}/n$

STOP
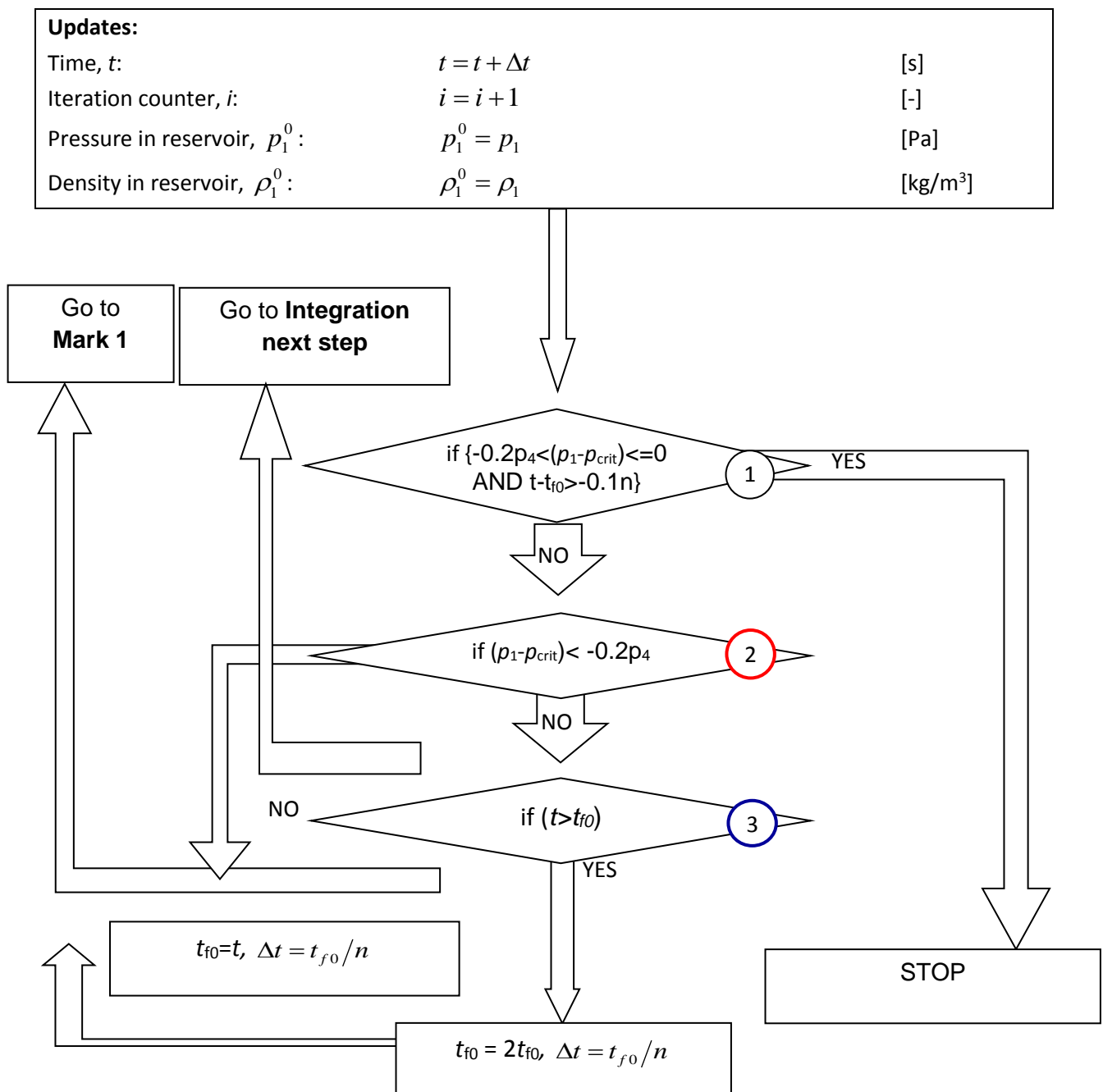
NB3: Upon calculation finished, the graph for the pressure ***p_1*** (Y-axis) against time ***t*** (X-axis) blowdown should be plotted. The pressure axis should have axis title with respect to the pressure units chosen at the beginning e.g. Pressure (bar/Pa/kPa etc.).

NB4: The link to or SAVE button should be available for save excel file with results after calculation.

3.5.2.3.5 Output values

- The results should be represented by option to save excel file and the plotted graph. The graph should have title 'Pressure':
  - X – axis = Time (s)
  - Y – axis = Pressure (bar / Pa / atm / psi), depending on the initial choice of the user

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

3.5.2.4   Option 2: Isothermal blowdown of storage tank

3.5.2.4.1 Introduction

This model allows user to calculate the isothermal blowdown of storage hydrogen tank.
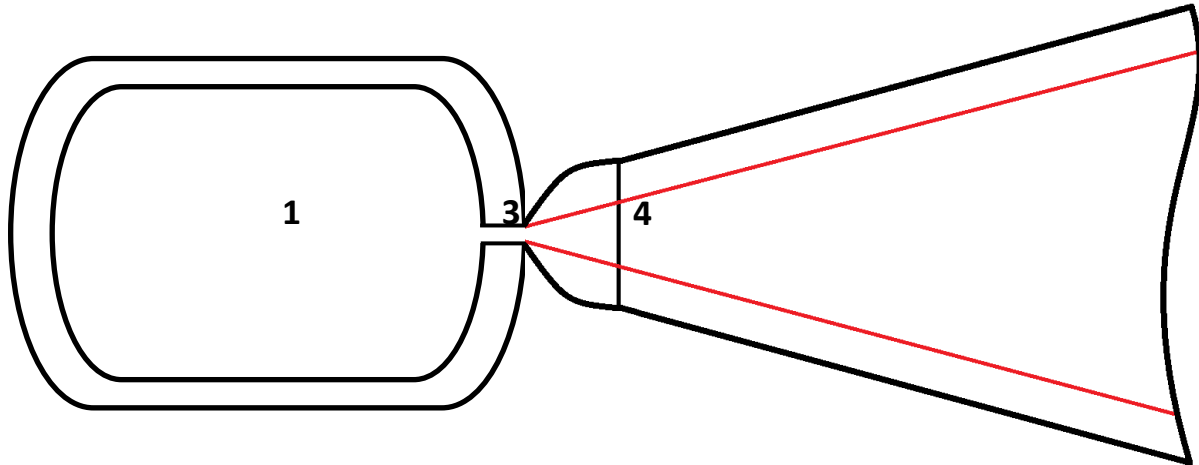
Figure 7 - Simple schematic of 'expanded' (red lines) and 'under-expanded' (black lines) jet.

The isothermal blowdown of a storage tank is based on the assumption of a relatively long release from a high-pressure reservoir, so that heat transfer significantly changes the temperature of the outflowing hydrogen.

The phenomena was observed experimentally and described in (Schefer, Houf, Williams, Bourne, & Colton, 2007) [1], where hydrogen temperature inside the reservoir initially dropped down to approximately T = -45°C, and then recovered to T ≈ -35°C during an 8 minute release from 414 bar storage, with total pipeline length of 11 m.

The procedure is built on the model for expanded and under-expanded jet parameters (Molkov, 2012) [2], which describes parameters in an expanded and under-expanded jet through the characteristic stages of its development – in reservoir (1), orifice (3), and effective nozzle diameter (4).

The under-expanded jet parameters model is derived from the Abel-Noble equation of state for hydrogen and conservation equations for mass and energy. The outflowing mass flow rate, determined according to the under-expanded jet parameters model, is integrated until the ratio of the pressure in the vessel, p_1, to the ambient pressure, p_4, reaches the critical value corresponding to the chocked flow conditions in the orifice:

$p_1/p_4 = \left[(\gamma+1)/2\right]^{\gamma/(\gamma-1)}$, which for hydrogen ($\gamma$ =1.405) is equal to: $p_1/p_4 < 1.9$. (Schefer et al., 2006 [3])

Where:

- p_1 = Pressure in reservoir
- p_4 = Atmospheric pressure

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- γ = Ratio of specific heats (1.405)

At this time, when $p_1/p_4 < 1.9$, the jet is considered to be expanded, and the outflowing mass flow rate is then calculated using isentropic pressure and density relationships.

NB1:   The user is prompted to specify a low temperature limit for hydrogen in the reservoir, T_{1lim}. The model algorithm will calculate reservoir temperature T_1 according to the adiabatic model until this low temperature limit is reached, after which the reservoir will be treated as isothermal with temperature equal to T_{1lim}. Specification of a low temperature limit equal to the initial temperature, i.e. $T_{1lim}=T_1$, will correspond to an infinitely fast heat transfer between the ambient environment and the reservoir.

NB2:   The realised algorithm attempts to determine blowdown time starting from an initial guess provided by the user as an input parameter.

NB3:   Initial number of time steps for integration is chosen as n=1000 to avoid a prolonged calculation. Though n=1000 is usually sufficient to provide precise integration, users are advised to use a larger number of time steps (e.g. n=2000) to check if the pressure dynamics in the vessel remains essentially the same (after blowdown time is determined using the initial time step number n=1000). It is recommended to increase time step number until the pressure dynamics are time step insensitive, i.e. time step convergence has been reached.

3.5.2.4.2 Input values

As per Adiabatic blowdown model (Section 3.5.2.3) one additional low temperature limit term required for user input **T_{1lim}**:

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Low limit hydrogen temperature in reservoir	T_{1lim}	288	K	200-330	288

(No change required from existing model)

3.5.2.4.3 Calculation procedure

As per Adiabatic blowdown model (Section 3.5.2.3), one addition of a minimum temperature limit applied to T_1. In this model the minimum allowable value of T_1 (temperature in the reservoir) is the value of T_{1lim}, as set by the user.

"If statement" should be added in iteration loop for calculation of temperature in reservoir after calculation of p_1:

if (T_1 != T_{1lim}) { $$T_1 = \frac{p_1}{\rho_1 R_{H2}}\left(1 - b\rho_1\right)$$ }

                    if ($T_1 < T_{1lim}$) { $T_1 = T_{1lim}$;   }

3.5.2.4.4 Output values

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

- The results should be represented by option to save excel file and the plotted graph. The graph should have title 'Pressure':
    - X – axis = Time (s)
    - Y – axis = Pressure (bar / Pa / atm / psi), depending on the initial choice of the user

3.5.2.5   Tool realisation

The snapshot of tool realisation is presented in Figure 8. Same features as for the Jet parameters tool but also user can plot the pressure curve.
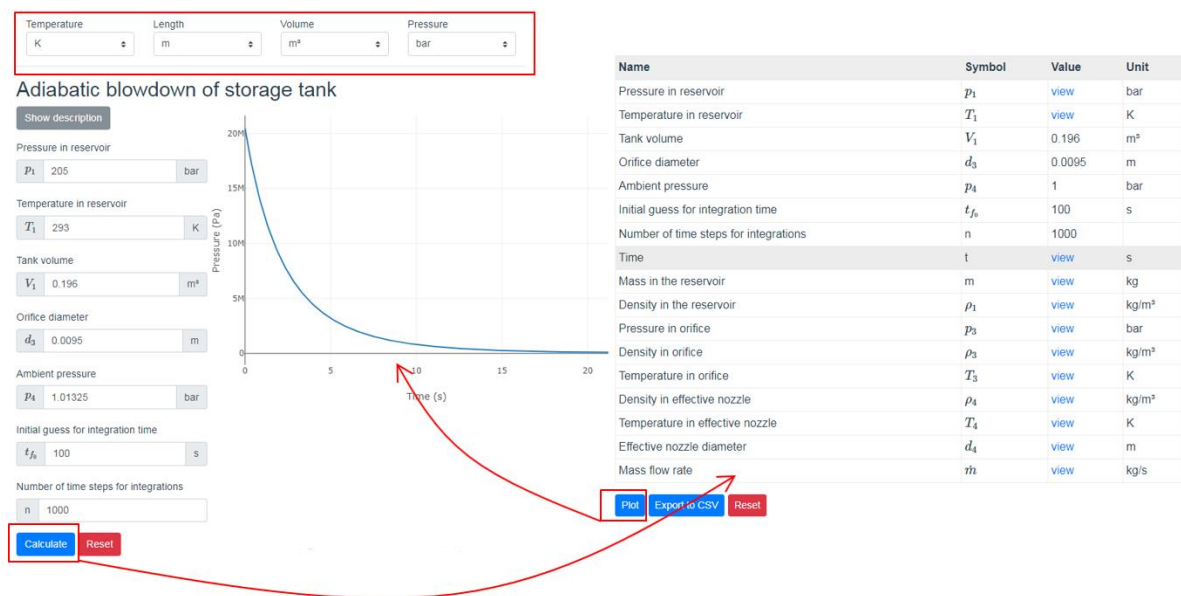
Figure 8 - Snapshot of Adiabatic blowdown model realisation.

3.5.3   Flame length correlation and three hazard distances for jet fires (UU)

3.5.3.1   Introduction

Note: Model description should appear upon pressing the appropriate button on the home screen of the tool.

This mode allows to calculate two features associated with hydrogen jet fires:

- Flame length
- Separation distances (depending on chosen hazard criteria)

Each of these features is briefly introduced below:

3.5.3.2   Flame length

The model utilizes a dimensionless flame length correlation (described by (Vladimir Molkov and Saffers, 2013)) for laminar and turbulent flames, buoyancy- and momentum-controlled fires,

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

expanded (subsonic and sonic) and under-expanded (sonic and supersonic) jet fires, thereby covering the entire spectrum of hydrogen reacting leaks.

The only dependence of the dimensionless flame length, L_F/D, is on parameters at the nozzle exit and on the density of the surrounding air. These parameters are: density, ρ_N and velocity, U_N at the nozzle exit. Density and velocity can be normalized as ρ_N/ρ_S and U_N/C_N respectively. Using the assumption that the kinetic energy flux in the nozzle exit is a conserved scalar of the process, a relationship between the density and the velocity in the dimensional group is introduced as $(\rho_N/\rho_S) \cdot (U_N/C_N)^3$.

This dimensionless hydrogen flame length correlation is shown in Figure 9. The parameters needed to predict the flame length are those at the *actual* nozzle exit only meaning that consideration of flow parameters at the *notional* nozzle exit are not required.
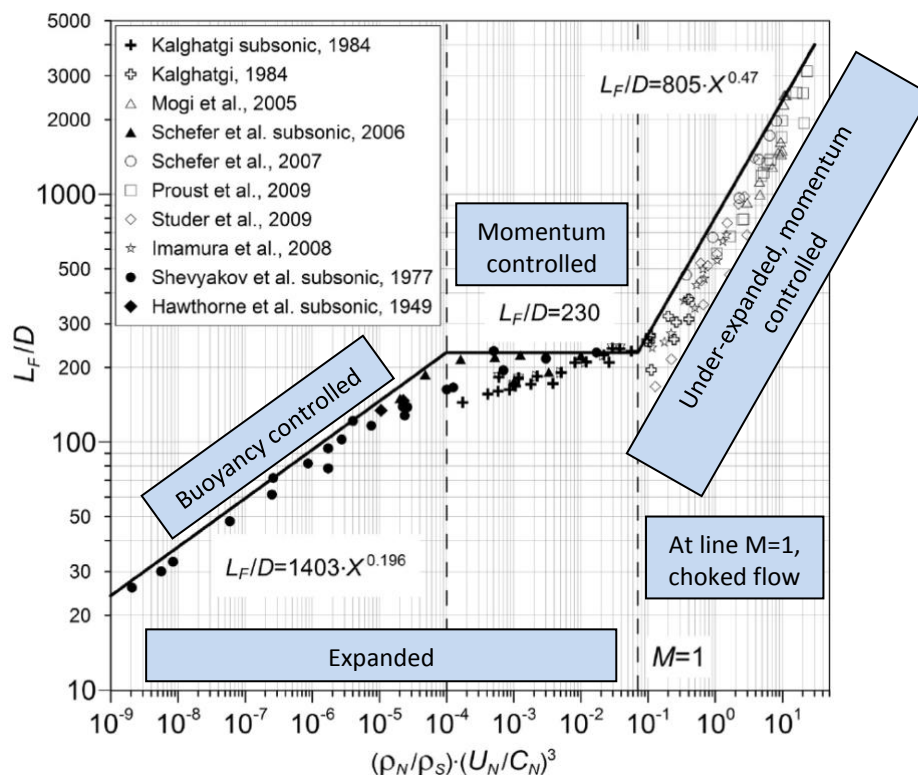
Figure 9 – Dimensionless (conservative) correlation for hydrogen jet flames (in formulas shown in figure "X" denotes the similarity group $(\boldsymbol{\rho_N/\rho_S}) \cdot (\boldsymbol{U_N/C_N})^3$) (Vladimir Molkov and Saffers, 2013).

The shape of Figure 1 has three distinct parts, each with a physical meaning based on knowledge of jet flame behaviour. The dimensionless flame length, L_F/D, increases for laminar and transitional flames (buoyancy-controlled), then it is practically constant for transitional and fully developed turbulent expanded flames (momentum-dominated) and finally it increases again for under-expanded jets (momentum-dominated). To describe this final part of the curve, the use of the "hydrogen jet parameters model" (please include hyperlink to this model) is required. It should be noted that the equations shown on Figure 1, and used during calculations, provide a conservative estimate of the flame length.

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

The hydrogen flow parameters presented in Figure 9 are either taken directly from experiments (dimensionless flame length, L_F/D) or calculated using under-expanded jet theory (density, flow rate, and speed of sound in the nozzle exit) following (V. Molkov, Makarov, & Bragin, 2009). Details of the experimental data utilised is described in (V. Molkov & Saffers, 2011).

Using this correlation it can be concluded:

- For subsonic flows (where M < 1) the dimensionless flame length depends on the nozzle Mach number only, as the density ratio ρ_N/ρ_S is practically constant for expanded jets.
- For choked flows (where M = 1) the dimensionless flame length depends only on the hydrogen density in the nozzle exit, ρ_N. Density increases with an increase in storage pressure, and decrease in temperature.

The dimensionless correlation is validated within the following limits:

- In the range of hydrogen storage pressures from nearly atmospheric up to 900 bar,
- At temperatures down to 80 K, and
- In the range of nozzle diameters from 0.4 to 51.7 mm.

3.5.3.3   Expanded and Under-expanded jet

Shown in Figure 10 is a simple schematic of an 'expanded' (red lines) and an 'under-expanded' (black lines) jet.
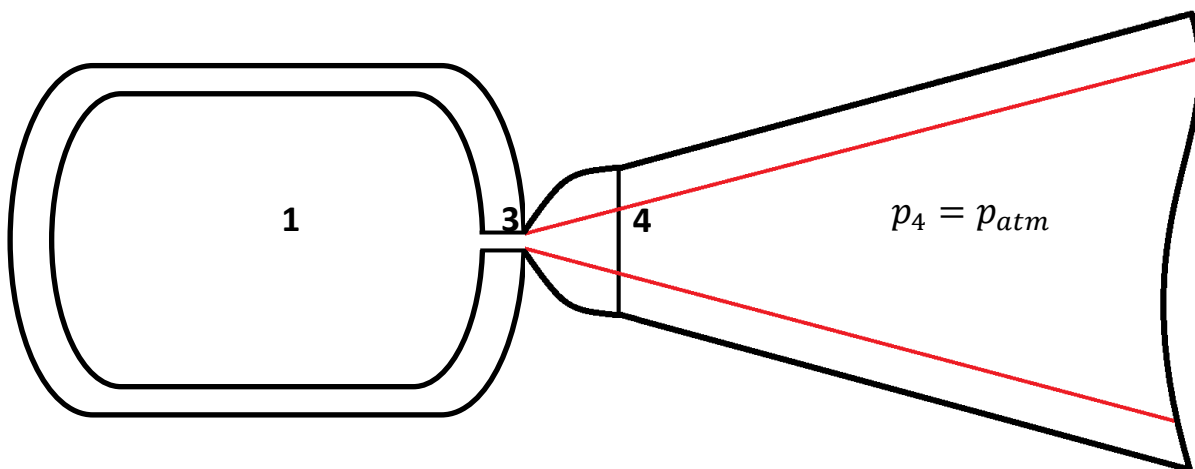
Figure 10 – Simple schematic of 'expanded' and 'under-expanded' jet.

1 = Reservoir

3 = Nozzle (orifice)

4 = Pressure and velocity is equal to ambient and local speed of sound respectively (condition 4 exists only for under-expanded case)

The critical pressure ratio across the leak, p^*, determines whether the flow is subsonic or sonic / supersonic.

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

$$p^* = \frac{p_1}{p_{atm}} = \left(\frac{(\gamma + 1)}{2}\right)^{\gamma/(\gamma-1)}$$

Therefore the critical pressure ratio for the transition to sonic flow for hydrogen is $\approx$ 1.9. If p^* < 1.9, the flow is subsonic and expanded, as long as p^* > 1.9, the exit velocity remains locally sonic and the jet is underexpanded. The exit pressure rises above ambient with the result that expansion, down to ambient pressure, p_{atm}, takes place outside of the real nozzle at a location downstream of the Mach disc, called the effective nozzle diameter.

Therefore, different equation sets must be solved depending on whether the flow is expanded or under-expanded, the equation set relating to an under-expanded jet is detailed in (Molkov, 2012).

The expanded jet equation set, based on isentropic pressure and density relationships, is summarised in Table 1:

Table 1 – System of equations for expanded jets.

System of equations for expanded jets:
$\rho_1 = p_1/[(p_1 \cdot b) + (R_{H_2}) \cdot T_1]$
$\rho_N = \rho_1 \cdot (p_{atm}/p_1)^{1/\gamma}$
$M_N = \sqrt{2[(p_1/p_{atm})^{(\gamma-1)/\gamma} - 1]/(\gamma - 1)}$
$T_N = T_1 \cdot (p_{atm}/p_1)^{(\gamma-1)/\gamma}$
$C_N = \sqrt{(\gamma \cdot R \cdot T_N)/M_{H_2}}$
$U_N = M_N \times C_N$
$\rho_{atm} = (p_{atm} \cdot M_{air})/(R \cdot T_{atm})$

3.5.3.4   Separation distances from an ignited hydrogen leak

Following release, jets can be divided into three types: fully momentum-dominated, transitional and fully buoyancy-dominated. A simple schematic of these jet types for an initially horizontal jet are shown in Figure 11:
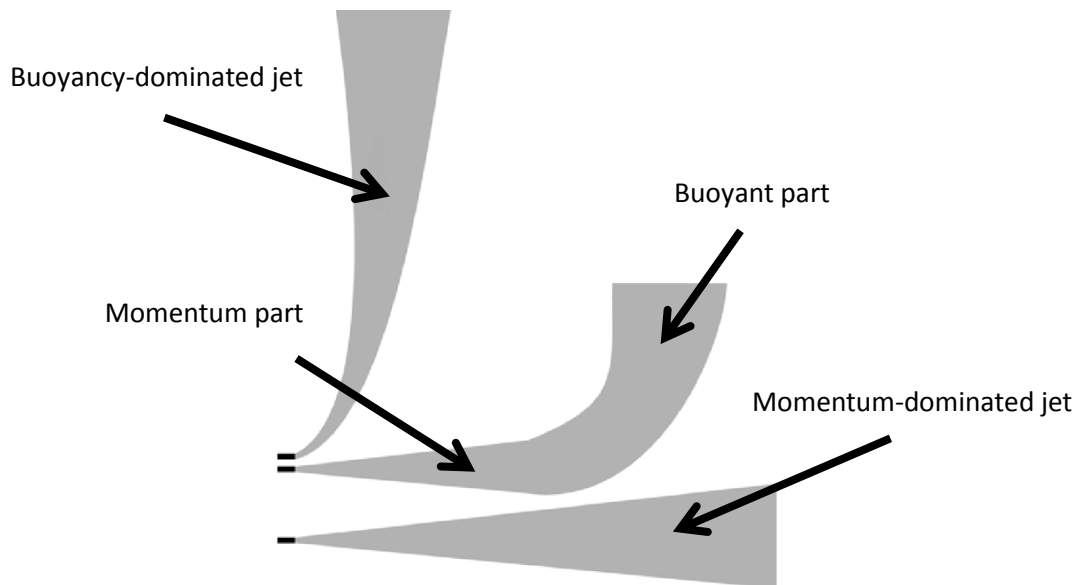
Figure 11 – Momentum-dominated, transitional, and fully buoyancy-dominated jet.

Fully momentum-dominated jets are not affected by buoyancy whereas fully buoyancy-dominated jets are quickly diverted from the horizontal to vertical flow direction. Transitional jets are initially momentum-dominated close to the nozzle and then further downstream, as velocity drops and jet diameter increases, they become buoyancy-dominated. When considering hydrogen safety engineering it is important to know when this transition takes place, as it has direct consequences for the required separation distance to maintain safety.

Using the flame length calculations performed, the required separation distance when considering **momentum dominated** straight flames for each of the criteria listed below can be calculated:

So called "harm criteria" for people can be expressed in terms of injury or death, (LaChance, 2010).

These criteria can be written as follows:

- No harm limit, 70 °C: $x = 3.5 \times L_F$
- Pain limit for 5 min exposure, 115 °C: $x = 3.0 \times L_F$
- Third degree burns (20 s), 309 °C: $x = 2.0 \times L_F$

It should be noted that the authors have selected the "harm criteria" from LaChance as a basis for the calculation of separation distance for demonstration purposes only. A universally accepted standard for this calculation has not yet been agreed at National, European or International level.

3.5.3.5   Nomenclature

Parameter	Symbol	Unit
H2 co-volume constant (0.00769)	b	m3/kg
Speed of sound	C	m/s
Orifice diameter	D	m
Flame length	L_F	m
Mach number (M=U/C)	M	Non-dimensional
H2 molecular mass (2.016)	M_{H_2}	kg/kmol

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Air molecular mass (28.97)	M_{air}	kg/kmol
Pressure	p	Pa
Critical pressure ratio (1.89595)	p^*	ND
Hydrogen specific gas constant (4124.241)	R_{H_2}	J/(kg K)
Temperature	T	K
Velocity	U	m/s
Axial distance from the nozzle	x	m
Adiabatic index (for hydrogen = 1.405)	γ	ND
Density	ρ	kg/m3
Flame length	L_F	m
Subscripts:		
Location = reservoir	1	
Location = nozzle (orifice)	N (3)	
Location = Surrounding air (atmosphere)	S (atm)	

3.5.3.6　Input values

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Hydrogen pressure in reservoir	p_1	20000000	Pa	101325 – 90,000,000	20000000
Hydrogen temperature in reservoir	T_1	293	K	> 80	293
Orifice diameter	D_3	0.003	m	0.0004 – 0.0517	0.003
Ambient temperature	T_{atm}	101325	K	233 - 313	101325

3.5.3.7　Calculation procedure

Model constants		
Parameter	**Value / Calculation**	**Unit**
H₂ co-volume constant	b=0.00769	m³/kg
Universal gas constant	R=8314.47	J/(kmol K)
H₂ molecular mass	M_{H_2}=2.016	kg/kmol
Air molecular mass	M_{air}=28.97	kg/kmol
Hydrogen specific gas constant	R_{H_2}=4124.24107	J/(kg K)
Ambient pressure	p_{atm}=101325	Pa
Adiabatic index	γ=1.405	-
Critical pressure ratio	p^*=1.89595	-

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

3.5.3.8   Flame length

3.5.3.8.1 Algorithm of solution

Check critical pressure ratio

If $\dfrac{p_1}{p_{atm}} > p^*$

No

Expanded jet

Go to Section 3.5.3.8.2

Yes

Under-expanded jet

Go to Section 3.5.3.8.3
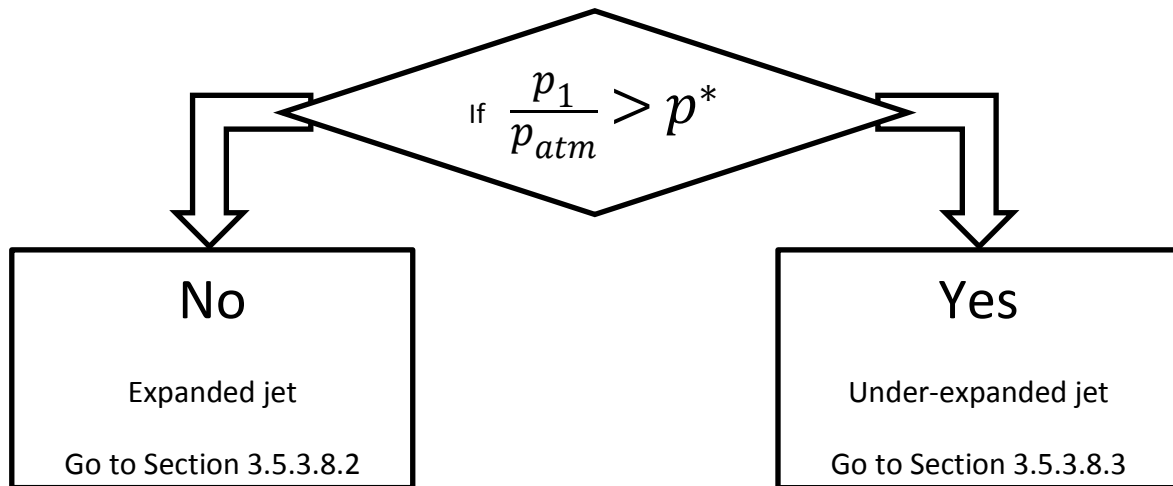
3.5.3.8.2 Expanded jet

	Initial conditions		
1	Hydrogen pressure in reservoir	p_1 - user input	Pa
2	Hydrogen temperature in reservoir	T_1 - user input	K
3	Orifice diameter	D_3 - user input	m
4	Ambient temperature	T_{atm} - user input	K
	Calculation		
5	Density in the reservoir	$\rho_1 = \dfrac{p_1}{[(p_1 \cdot b) + (R_{H_2} \cdot T_1)]}$	kg/m³l
6	Density at the nozzle	$\rho_N = \rho_1 \cdot \left(\dfrac{p_{atm}}{p_1}\right)^{1/\gamma}$	kg/m³
7	Mach number at the nozzle	$M_N = \sqrt{\dfrac{2\left[\left(\dfrac{p_1}{p_{atm}}\right)^{\frac{\gamma-1}{\gamma}} - 1\right]}{(\gamma - 1)}}$	-
8	Temperature at the nozzle	$T_N = T_1 \cdot \left(\dfrac{p_{atm}}{p_1}\right)^{(\gamma-1)/\gamma}$	K
9	Nozzle speed of sound	$C_N = \sqrt{\dfrac{\gamma \cdot R \cdot T_N}{M_{H_2}}}$	m/s
10	Velocity at the nozzle	$U_N = M_N \times C_N$	m/s
11	Ambient density	$\rho_{atm} = \dfrac{p_{atm} \cdot M_{air}}{R \cdot T_{atm}}$	kg/m³

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12	Dimensionless group	$Dimensionless\ group = \left(\frac{\rho_N}{\rho_{atm}}\right) \cdot \left[\left(\frac{U_N}{C_N}\right)^3\right]$	-
13	Flame length	Use "if" statement below	m

If $\left(\frac{\rho_N}{\rho_{atm}}\right) \cdot \left[\left(\frac{U_N}{C_N}\right)^3\right] < 0.0001$ ⟹ $L_F = D_3 \times 1403 \cdot \left[\left(\frac{\rho_N}{\rho_{atm}}\right) \cdot \left(\frac{U_N}{C_N}\right)^3\right]^{0.196}$

Or if

$0.0001 < \left(\frac{\rho_N}{\rho_{atm}}\right) \cdot \left[\left(\frac{U_N}{C_N}\right)^3\right] < 0.07$ ⟹ $L_F = D_3 \times 230$
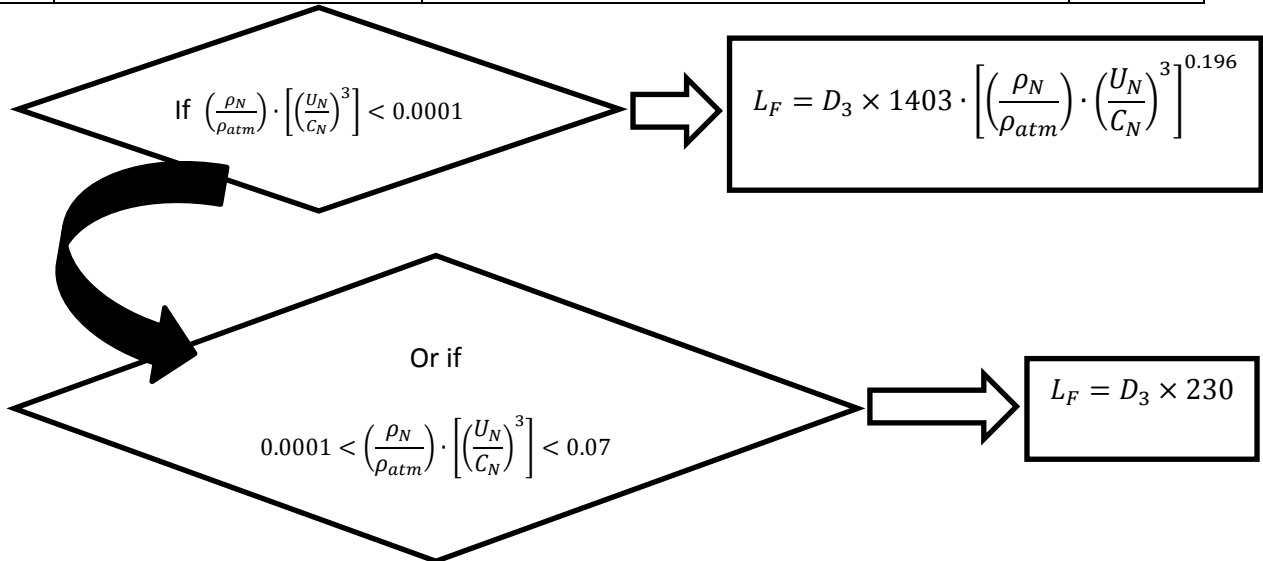
3.5.3.8.3 Under-expanded jet

Using required terms, as provided in input values and model constants, and using the same calculation procedure as carried out in the "Hydrogen jet parameters tool" calculate:

- Density at the nozzle, ρ_N:
  - Where, $\rho_N = \rho_3$ ('Density at the orifice' from "Hydrogen jet parameters tool")
- Velocity at the nozzle, U_N:
  - Where, $U_N = V_3$ ('Velocity in orifice' from "Hydrogen jet parameters tool")
- Temperature at the nozzle, T_N:
  - Where, $T_N = T_3$ ('Temperature at the orifice' from "Hydrogen jet parameters tool")

	Initial conditions		
1	Hydrogen pressure in reservoir	p_1 - user input	Pa
2	Hydrogen temperature in reservoir	T_1 - user input	K
3	Orifice diameter	D_3 - user input	m
4	Ambient temperature	T_{atm} - user input	K
	Calculation		
5	Nozzle speed of sound	$C_N = \dfrac{1}{[1 - (b \cdot \rho_N)]} \times \sqrt{\gamma \cdot R_{H_2} \cdot T_N}$	m/s
6	Ambient density	$\rho_{atm} = \dfrac{p_{atm} \cdot M_{air}}{R \cdot T_{atm}}$	kg/m^3
7	Flame length	$L_F = D_3 \times \left\{805 \cdot \left[\left(\frac{\rho_N}{\rho_{atm}}\right) \cdot \left(\frac{U_N}{C_N}\right)^3\right]^{0.47}\right\}$	m

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

3.5.3.9   Separation distances for hydrogen jet fires

"No harm" (70ºC) separation distance

$$X_{70^o C} = 3.5 \times L_F$$

Where:

- $X_{70^o C}$ – "No harm" (70ºC) separation distance, m
- L_F – Flame length, m
  - For expanded jet from Section 3.5.3.8.2
  - For under-expanded jet from Section 3.5.3.8.3

"Pain limit" (5 mins, 115ºC) separation distance

$$X_{115^o C} = 3.0 \times L_F$$

Where:

- $X_{115^o C}$ – "Pain limit" (5 mins, 115ºC) separation distance, m
- L_F – Flame length, m
  - For expanded jet from Section 3.5.3.8.2
  - For under-expanded jet from Section 3.5.3.8.3

"Third degree burns" (20 s, 309ºC) separation distance

$$X_{309^o C} = 2.0 \times L_F$$

Where:

- $X_{309 C}$ – "Third degree burns" (20 s, 309ºC) separation distance, m
- L_F – Flame length, m
  - For expanded jet from Section 3.5.3.8.2
  - For under-expanded jet from Section 3.5.3.8.3

3.5.3.10 Output values

Parameter name	Symbol	Output value	Unit
Flame length			
Flame length	L_F	6.26204	m
Required separation distances			
"No harm" (70 ºC) separation distance	$X_{70^o C}$	21.91716	m
"Pain limit" (5 mins, 115 ºC) separation distance	$X_{115^o C}$	18.78613	m
"Third degree burns" (20 sec, 309 ºC) separation distance	$X_{309^o C}$	12.52409	m

3.5.3.11 Tool realisation

The snapshot of tool realisation is presented in Figure 12.

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]
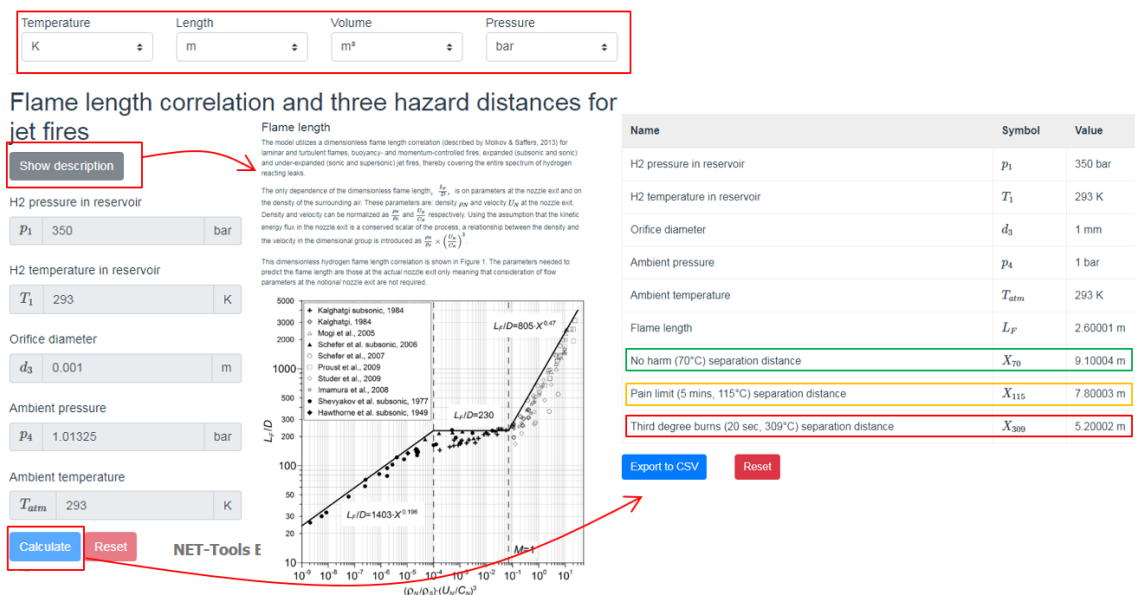
Figure 12 - Snapshot of Flame length correlation tool realisation.

3.5.4   Axial distance to H2 concentrations - similarity law for concentration decay in hydrogen expanded and under-expanded jets and unignited jet hazard distances (UU)

This model allows for prediction of axial concentration decay of a leaking gas for sub-sonic, sonic, and super-sonic jets. The similarity law is shown to be valid in a wide range of conditions from expanded to highly under-expanded jets. The model is used for calculation of hazard distances formed by the size of the flammable envelope

3.5.4.1   Introduction

Note: Model description should appear upon pressing the appropriate button on the home screen of the tool.

Analysis of experimental data has demonstrated that the longest, and therefore most hazardous, flames can be expected to be formed from under-expanded jets. With this in mind, the similarity law (S. L. Brennan, Makarov, & Molkov, 2009) for axial concentration decay in round unignited, expanded, momentum-dominated jets, as suggested by (Chen & Rodi, 1980), has now been expanded and validated for under-expanded hydrogen jets (Molkov, 2012).

The equation implemented to calculate the axial distance from the nozzle, to a prescribed concentration of hydrogen can be written as:

$$x = \frac{5.4 \times D}{C_{ax}} \cdot \sqrt{\frac{\rho_N}{\rho_S}}$$

where:

- x = Axial distance from the nozzle, m
- D = Nozzle diameter, m
- C_{ax} = Mass fraction of hydrogen at axial distance x, ND

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

- ρ_N = Density at nozzle exit, kg/m^3
- ρ_S = Air density, kg/m^3

When considering under-expanded jets knowledge of density in the nozzle, ρ_N, (as a function of storage pressure and losses in the leak pathway) is required. This density is calculated using the 'hydrogen jet parameters' engineering tool which is also available on e-Laboratory (which was developed following (V. Molkov et al., 2009)). For expanded jets, calculations are based on isentropic pressure and density relationships (this equation set is described in more detail in the description of the 'flame length and separation distance for jet fires' engineering tool, see Section **3.5.3**).

Shown below in Figure 13 is a correlation between the location of the hydrogen flame jet tip and the location of three different hydrogen concentrations (8%, 11% and 16%) in an unignited jet emanating from the same leak source. Points in Figure 13 represent the experimental flame length, L_F/D. The diagonal lines shown correspond to the dimensionless distance, x/D, i.e. to the location of three different axial hydrogen concentrations. From Figure 13, for momentum-controlled round jet fires, the flame tip is located where the axial concentration of hydrogen in an unignited jet from the same leak source is in the range from 8% to 16% by volume. More precisely, the best fit line of 70 experimental points for the flame length of momentum-dominated hydrogen jet fires is close to the line for 11%, by volume of hydrogen in air, in unignited jet releases.

This engineering tool calculates the axial distance from the nozzle corresponding to the location of various pre-selected hydrogen concentrations, namely 4%, 8%, 11%, 16% and 29.5% by volume, **in unignited jets**. This model also allows the 'user' to choose their own concentration for analysis, within the hydrogen flammability limits of 4% to 75% by volume.
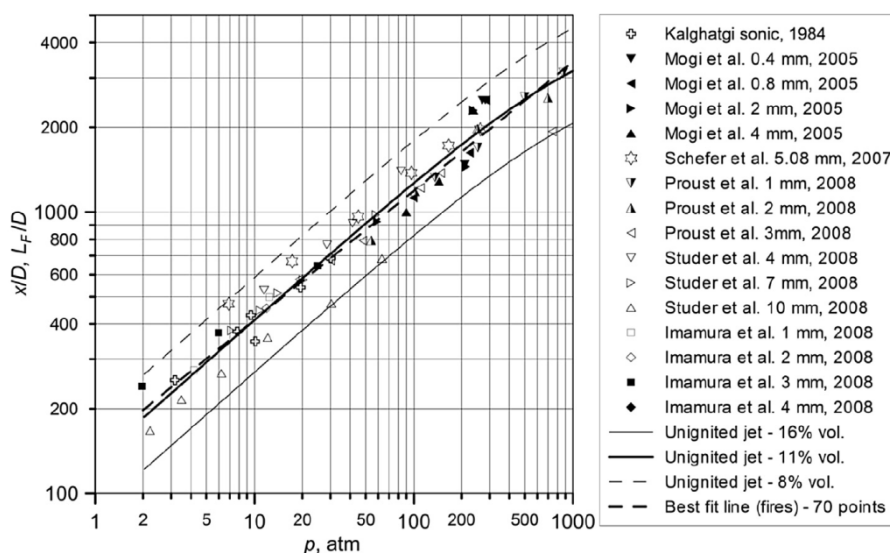
Figure 13 – Correlation between the dimensionless flame length, L_F/D, and distance to a particular concentration in a non-reacting jet, x/D for different storage pressures (Vladimir Molkov and Saffers, 2013)

3.5.4.2 Model constants

Table 2 – Model constants

Parameter	Symbol	Value / Calculation	Unit

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

H₂ co-volume constant	b	0.00769	m³/kg
Universal gas constant	R	8314.47	J/(kmol K)
H₂ molecular mass	M_{H_2}	2.016	kg/kmol
Air molecular mass	M_{air}	28.97	kg/kmol
Hydrogen specific gas constant	R_{H_2}	4124.24107	J/(kg K)
Ambient pressure	p_{atm}	101325	Pa
Adiabatic index	γ	1.405	ND
Critical pressure ratio	p^*	1.89595	ND
Mass fraction of H₂ by vol. in air, 4%	$C_{ax,4\%}$	0.002881	ND
Mass fraction of H₂ by vol. in air, 8%	$C_{ax,8\%}$	0.005994	ND
Mass fraction of H₂ by vol. in air, 11%	$C_{ax,11\%}$	0.008498	ND
Mass fraction of H₂ by vol. in air, 16%	$C_{ax,16\%}$	0.013037	ND
Mass fraction of H₂ by vol. in air, 29.5%	$C_{ax,29.5\%}$	0.0282	ND

Notes:

- This list details the constants contained within the model, required for calculation purposes.
- The user does not need to see or have access to these parameters:
- ND = Non-dimensional

3.5.4.3   Input values

Table 3 – Input values

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Hydrogen pressure in reservoir	p_1	3.5e+7	Pa	$101325 - 90,000,000$	3.5e+7
Ambient pressure	p_{atm}	101325	Pa		101325
Hydrogen temperature in reservoir	T_1	293	K	> 80 K	293
Orifice diameter	D_3	0.005	m	$0.0004 - 0.0517$ m $(0.4 - 51.7 \text{ mm})$	0.005
Ambient temperature	T_{atm}	293	K	233 - 313 K	293
User specified H₂ percentage, to calculate axial distance from nozzle	$X_{\%, H_2}$	20	%	4% - 75%	20

Notes to programmer:

- The value entered by the user must be converted into a decimal number:
  - If $X_{\%, H_2}$ (between $4 - 75$) is entered by user:
    - For calculations: $X_{\%, H_2}[decimal] = X_{\%, H_2}[4 - 75] \times 0.01$
- The range limits described above for each parameter should also appear on screen.
  - If a value outside this range is entered by the user, the entry box which contains the incorrect entry should be highlighted and a request written onto the screen that an alternative value must be entered.

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

    o   The calculation must not proceed unless a value within the allowable range for each parameter is entered.

3.5.4.4   Calculation procedure: Axial distance calculation

Check critical pressure ratio

If $\dfrac{p_1}{p_{atm}} > p^*$

No

Expanded jet

Calculate ρ_N as per:

1. Density in the reservoir

$$\rho_1 = \frac{p_1}{[(p_1 \cdot b) + (R_{H_2} \cdot T_1)]}$$

2. Density at the nozzle (expanded)

$$\rho_N = \rho_1 \cdot \left(\frac{p_{atm}}{p_1}\right)^{1/\gamma}$$

Yes

Under-expanded jet

Using required terms, as provided in Table 2 and Table 3, and using the same calculation procedure as carried out in the "hydrogen jet parameters model" calculate:

Density at the nozzle, ρ_N, where, $\rho_N = \rho_3$ ('Density at the orifice' from "hydrogen jet parameters model")

	Calculation		
1	Ambient density	$\rho_{atm} = \dfrac{p_{atm} \cdot M_{air}}{R \cdot T_{atm}}$	kg/m^3
2	Axial distance from the nozzle to 4% by vol. of H$_2$	$X_{4\%,H_2} = \dfrac{5.4 \times D_3}{C_{ax,4\%}} \cdot \sqrt{\dfrac{\rho_N}{\rho_{atm}}}$	m
3	Axial distance from the nozzle to 8% by vol. of H$_2$	$X_{8\%,H_2} = \dfrac{5.4 \times D_3}{C_{ax,8\%}} \cdot \sqrt{\dfrac{\rho_N}{\rho_{atm}}}$	m
4	Axial distance from the nozzle to 11% by vol. of H$_2$	$X_{11\%,H_2} = \dfrac{5.4 \times D_3}{C_{ax,11\%}} \cdot \sqrt{\dfrac{\rho_N}{\rho_{atm}}}$	m
5	Axial distance from the nozzle to 16% by vol. of H$_2$	$X_{16\%,H_2} = \dfrac{5.4 \times D_3}{C_{ax,16\%}} \cdot \sqrt{\dfrac{\rho_N}{\rho_{atm}}}$	m
6	Axial distance from the nozzle to 29.5% by vol. of H$_2$	$X_{29.5\%,H_2} = \dfrac{5.4 \times D_3}{C_{ax,29.5\%}} \cdot \sqrt{\dfrac{\rho_N}{\rho_{atm}}}$	m
7	Calculation of user specified mass fraction of H$_2$ by vol. in air	$C_{ax,?\%} = \dfrac{1}{1 + \left[\left(\frac{1}{X_{\%,H_2}} - 1\right) \times \left(\frac{M_{air}}{M_{H_2}}\right)\right]}$	N/D

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

| 8 | Axial distance from the nozzle to user specified % by vol. of H₂ | $$X_{?\%,H_2} = \frac{5.4 \times D_3}{C_{ax,?\%}} \cdot \sqrt{\frac{\rho_N}{\rho_{atm}}}$$ | m |

3.5.4.5   Output values

Table 4 – Model outputs

Parameter	Value	Unit
Axial distance from the nozzle, by vol. H₂		
Axial distance from nozzle to 4% by vol. H₂ (HAZARD DISTANCE)	$X_{4\%,\,H_2}$ (32.56)	m
Axial distance from nozzle to 8% by vol. H₂	$X_{8\%,\,H_2}$ (15.65)	m
Axial distance from nozzle to 11% by vol. H₂	$X_{11\%,\,H_2}$ (11.04)	m
Axial distance from nozzle to 16% by vol. H₂	$X_{16\%,\,H_2}$ (7.196)	m
Axial distance from nozzle to 29.5% by vol. H₂	$X_{29.5\%,\,H_2}$ (3.327)	m
Axial distance from nozzle to (user specified) ?% by vol. H₂	$\mathbf{X}_{?\%,\,H_2}$	**m**

Notes: Regarding Model Output (the specific % by vol. of H₂ chosen by the user) would it be possible for this percentage value to appear in this output table? So say if 20% was entered into Table 3 the output table created would look like (for row 6):

| Axial distance from nozzle to (user specified) **20%** by vol. H₂, $X_{\mathbf{20}\%,H_2}$ | Ans. (5.505) | m |

3.5.4.6   Tool realisation

The snapshot of tool realisation is presented in Figure 14.

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

Figure 14 - Snapshot of Similarity law tool realisation.

3.5.5   Pressure peaking phenomenon (PPP) for unignited and ignited releases (UU)

This model allows to calculate ignited and unignited PPP with constant mass flow rate and with tank blowdown.

3.5.5.1   Choice of the model

When the tool is selected the screen with the choice should appear prompting to select the option.

Note: Example of the model choice is the Option(radio) Button. When checked the screen with appropriate input parameters should appear below, together with button to initiate calculation (choice of RUN, CALCULATE, START etc. to be uniform across the e-Laboratory).

3.5.5.2   Option 1: Pressure peaking phenomenon (constant mass flow rate)

3.5.5.2.1 Introduction

Note: Model description should appear upon pressing the appropriate button on the home screen of the tool.

Current composite tanks for high pressure hydrogen storage have been shown to rupture in 3.5 - 6.5 min in fire conditions. As a result a large PRD venting area is currently used to release hydrogen from the tank before its catastrophic failure. However the ***unignited*** release of hydrogen from such PRDs, unlike heavier hydrocarbon gaseous fuels, is capable of resulting in unacceptably high overpressures within for example garage environments, causing major damage and the possible collapse of the structure.

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

In fact due to high flammability and low ignition energy of hydrogen most of releases are ignited. The pressure effects of hydrogen indoor jet fires were studied and it was concluded that the pressure peaking is also applicable and even more pronounced for ignited releases. Methodology for reacting release PPP estimation described in [paper to be published therefore, default coefficient is 1. To be changed.].

The phenomenological pressure peaking model allows for the simulation of the pressure dynamics in the enclosure, as a result of constant mass inflow rate of hydrogen into the enclosure through an orifice with specified diameter and venting of the enclosure to atmosphere through a vent of known area.

The pressure peaking model is based on:

- The assumption of initial pressure and temperature in the enclosure equal to those of atmosphere.
- The assumption of a perfectly stirred reactor (uniform mixture of gases in the enclosure).
- Orifice flow relation derived from Bernoulli's equation.

The model also assumes that there is uniform outflow velocity profile from the vent. However, at extremely low hydrogen mass flow rates the conditions for concurrent inflow-outflow in the vent plane may be established. *Under such conditions this particular model cannot be applied*. Therefore the minimum mass flow rate ($\dot{m}_{H2\_min}$) which will lead to 100% hydrogen concentration in the enclosure is calculated. The entered value of mass flow rate ($\dot{m}_{H2}$) is then compared to this minimum value ($\dot{m}_{H2\_min}$).

The calculation process will only proceed if $\dot{m}_{H2} > \dot{m}_{H2\_min}$.

NB1: For the assessment of the lower limit of mass flow rate that leads to 100% of hydrogen concentration in an enclosure the characteristic discharge coefficient is set to $C_{D\_100\%} = 0.85$.

NB2: The realised algorithm attempts to reach a steady-state solution with enclosure pressure changing with time step not more than 0.001%.

NB3: The coefficient for the ignited case 22±1 was derived for the ignited releases in (Makarov et al., 2018b)

References:

- Molkov V., Shentsov, V., Quintiere, J., Passive ventilation of a sustained gaseous release in an enclosure with one vent, Int. Journal of Hydrogen Energy, Vol. 39, Issue 15, May 2014, pp 8158-8168.
- Brennan S., Molkov V. Safety assessment of unignited hydrogen discharge from onboard storage in garages with low levels of natural ventilation, Int. Journal of Hydrogen Energy, Vol. 38, Issue 19, June 2013, pp. 8159 – 8166
- Makarov, D., Shentsov, V., Kuznetsov, M., Molkov, V., 2018b. Pressure Peaking Phenomenon: Experiments and Model Validation. Int. Journal of Hydrogen Energy.

3.5.5.2.2 Input values

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Atmospheric pressure	p_{atm}	101325	Pa	$101325 - 90{,}000{,}000$	101325
Enclosure temperature	T_{encl}	293.15	K		293.15
Enclosure volume	V_{encl}	30.42	m^3		30.42
Vent height	H_{vent}	0.05	m		0.05
Vent width	W_{vent}	0.25	m		0.25
Mass flow rate of hydrogen	$\dot{m}_{H_2}$	0.39	kg/s		0.39
Coefficient of discharge	C_D	0.6	-		0.6
Time step for integration	Δt	1	s		1
Number of time steps for integrations	n_{last}	1000	-		1000
Coefficient for ignited release	C_I	1	-		1

Note: Input value for C_I highlighted in yellow should appear only for ignited case (when option for ignited release checked in section 3.5.5.1).

3.5.5.2.3 Calculation procedure

Model constants		
Parameter	**Value / Calculation**	**Unit**
Universal gas constant	R=8314.47	J/(kmol K)
H$_2$ molecular mass	M_{H_2}=2.016	kg/kmol
Air molecular mass	M_{air}=28.97	kg/kmol
Acceleration due to gravity	g=9.81	m/s^2
Coefficient of discharge (100%)	$C_{D\_100\%} = 0.85$	-
Initial air density in enclosure	$\rho_{air} = \left(p_{atm} M_{air}\right)/R\,T_{encl}$	kg/m^3
Initial hydrogen density in enclosure	$\rho_{H2} = (p_{atm} \cdot M_{H2})/(R \cdot T_{encl})$	kg/m^3
Vent area	$A_{vent} = H_{vent} \cdot W_{vent}$	m^2
Minimum mass flow rate which will lead to 100% hydrogen concentration in enclosure	$\dot{m}_{H2\_min} = C_{D\_100\%} \cdot A_{vent} \cdot \sqrt{H_{vent}}$ $\cdot \sqrt{\dfrac{8 \cdot g \cdot \rho_{H2} \cdot (\rho_{air} - \rho_{H2})}{9}}$	kg/m^3

Initial check if release is ignited.

If release is **ignited** (box checked in section 3.5.5.1) — YES → $\dot{m}_{H2} = \dot{m}_{H2} \times C_I$

NO ↓

Initial check if mass flow rate is sufficient to result in PPP.
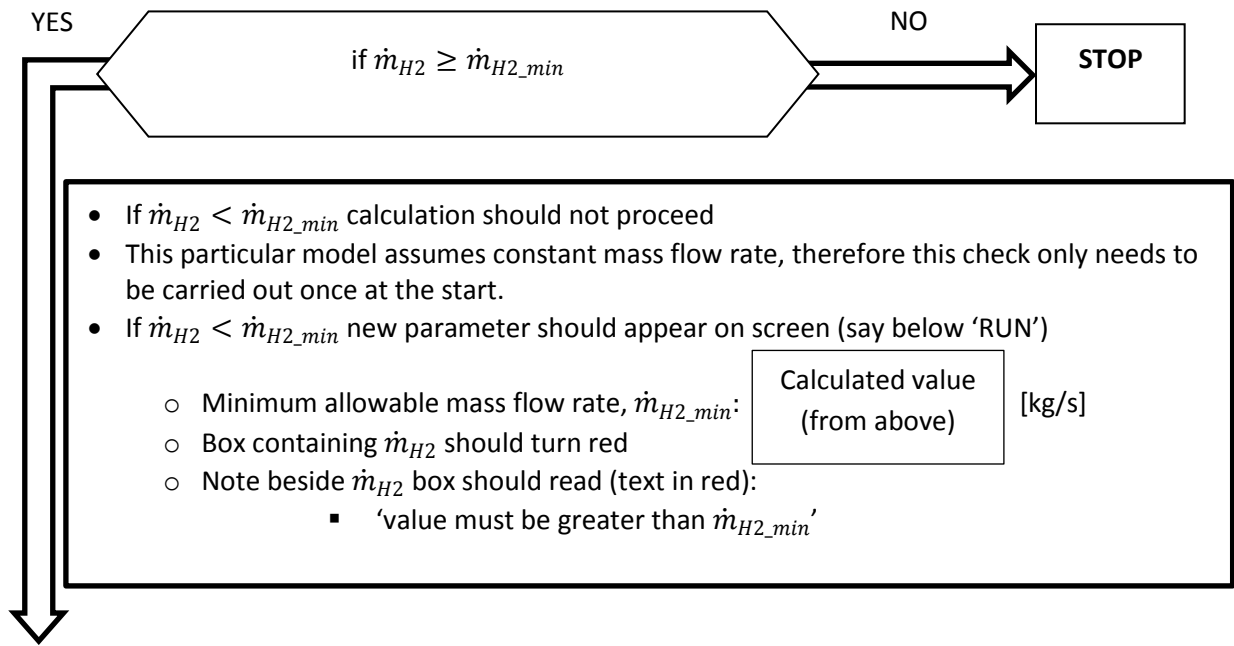
[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

YES   NO

$$\text{if } \dot{m}_{H2} \geq \dot{m}_{H2\_min}$$ **STOP**

- If $\dot{m}_{H2} < \dot{m}_{H2\_min}$ calculation should not proceed
- This particular model assumes constant mass flow rate, therefore this check only needs to be carried out once at the start.
- If $\dot{m}_{H2} < \dot{m}_{H2\_min}$ new parameter should appear on screen (say below 'RUN')

    o Minimum allowable mass flow rate, $\dot{m}_{H2\_min}$: | Calculated value (from above) | [kg/s]
    o Box containing $\dot{m}_{H2}$ should turn red
    o Note beside $\dot{m}_{H2}$ box should read (text in red):
        ▪ 'value must be greater than $\dot{m}_{H2\_min}$'

Mark 1

Initial mass of air in enclosure:	$m_{encl}^{0} = V_{encl}\rho_{air}$	[kg]
Initial mass flow in vent:	$\dot{m}_{vent}^{0} = 0$	[kg/s]
Initial quantity of gas in enclosure:	$n_{encl}^{0} = m_{encl}^{0}/M_{air}$	[kmol]
Initial time:	$t = 0$	[s]
Time step counter:	$n = 0$	[-]

INTEGRATION NEXT STEP

Time, t:	$t = t + \Delta t$	[s]
Time step counter, i:	$n = n + 1$	[-]
Mass of gases in enclosure, $m_{encl}^{t+\Delta t}$:	$m_{encl}^{t+\Delta t} = m_{encl}^{t} + \left(\dot{m}_{H2}^{t} - \dot{m}_{vent}^{t}\right) \cdot \Delta t$	[kg]
Quantity of gas in enclosure, $n_{encl}^{t+\Delta t}$:	$n_{encl}^{t+\Delta t} = n_{encl}^{t} + \left(\dfrac{\dot{m}_{H2}^{t}}{M_{H2}} - \dfrac{\dot{m}_{vent}^{t} n_{encl}^{t}}{m_{encl}^{t}}\right) \cdot \Delta t$	[kmol]
Pressure in enclosure, $p_{encl}^{t+\Delta t}$:	$p_{encl}^{t+\Delta t} = \dfrac{n_{encl}^{t+\Delta t} RT_{encl}}{V_{encl}}$	[Pa]

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

Overpressure in enclosure, $p_{g\,encl}^{t+\Delta t}$: $p_{g\,encl}^{t+\Delta t} = p_{encl}^{t+\Delta t} - p_{atm}$ [Pa]

Vent mass flow rate, $\dot{m}_{vent}^{t+\Delta t}$: $\dot{m}_{vent}^{t+\Delta t} = C \cdot \left(\dfrac{m_{encl}^{t+\Delta t}\, A_{vent}}{V_{encl}} \right) \left[\dfrac{2\left(p_{encl}^{t+\Delta t} - p_{atm} \right) V_{encl}}{m_{encl}^{t+\Delta t}} \right]^{1/2}$ [kg/s]

Output to file:

1)   Time step counter, n [-]

2)   Time, t [s]

3)   Mass of gases in enclosure, m_{encl} [kg]

4)   Vent mass flow rate, $\dot{m}_{vent}$ [kg/s]

5)   Overpressure, $p_{g_{encl}}$ [Pa/atm/bar/psi] (whichever has been chosen by the user)

Note to programmer:
Please include these column headings in produced 'Excel' output file.

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]
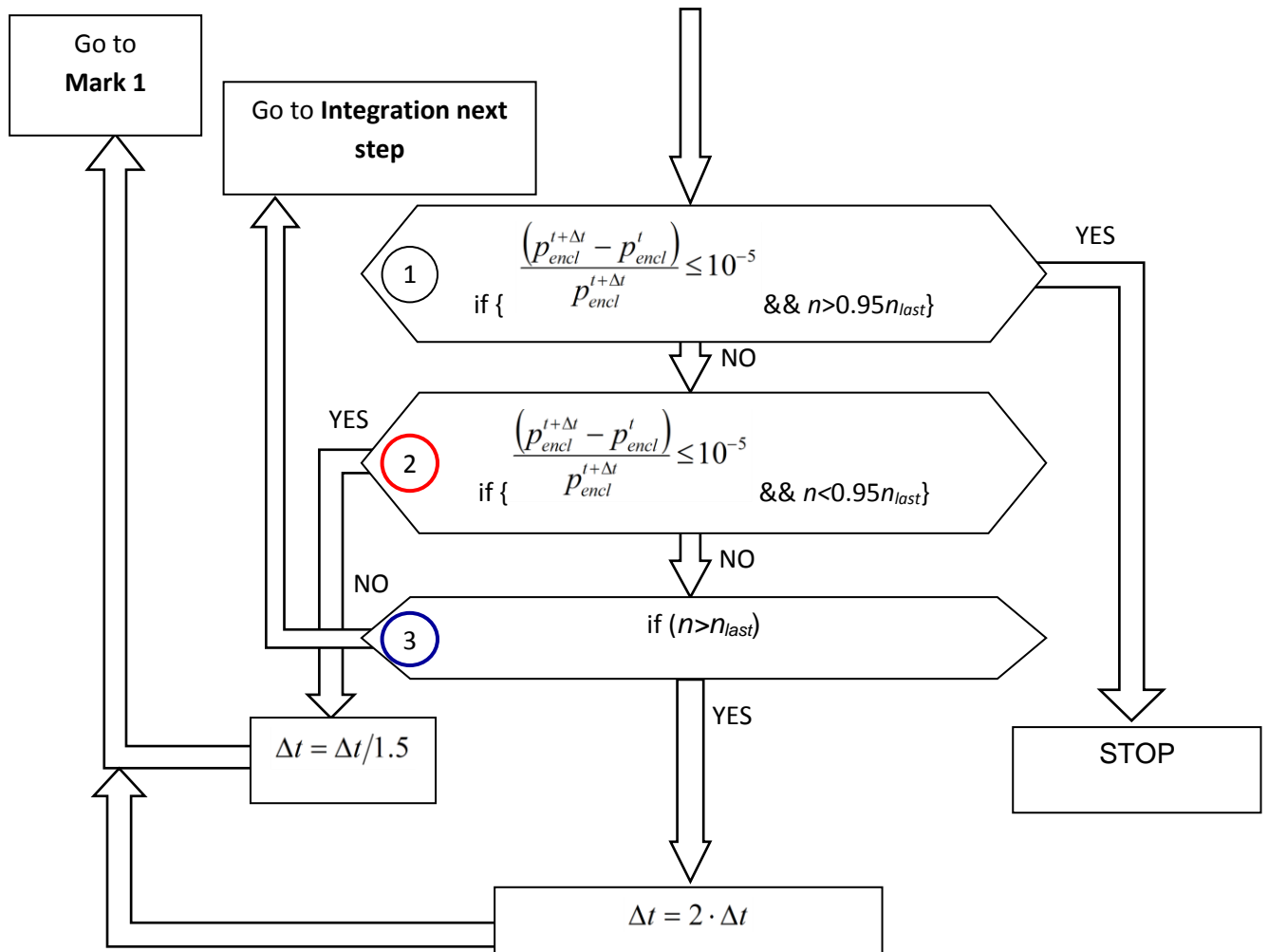
3.5.5.2.4 Output values

Upon calculation finished, the graph for the pressure **p_1** (Y-axis) against time **t** (X-axis) PPP should be plotted. The pressure axis should have axis title with respect to the pressure units chosen at the beginning e.g. Pressure (bar/Pa/kPa etc.).

The link to or SAVE button should be available for save excel file with results after calculation

3.5.5.3   Option 2: Pressure peaking phenomenon (tank blowdown)

3.5.5.3.1 Introduction

This model allows for the simulation of the pressure dynamics in a vented enclosure resulting from an *unignited* and **ignited** releases of hydrogen from a high-pressure reservoir through an orifice of specified diameter. The model is based on adiabatic release from a high-pressure reservoir, assuming fast release process and negligible heat transfer to the reservoir and piping.

The modelling approach is similar, in its major features, to that in the previous pressure peaking model, "Pressure peaking phenomenon (constant mass flow rate)" (Brennan and Molkov, 2013).

This model is valid for both expanded and under-expanded jet outflows.

When considering ratios of pressure in the reservoir, p_{res}, to the pressure in the enclosure, p_{encl}, larger than the critical value corresponding to chocked flow conditions in orifice:

$p_{res}/p_{encl} = \left[(\gamma+1)/2\right]^{\gamma/(\gamma-1)}$, which for hydrogen ($\gamma$ =1.405) is equal to $p_{res}/p_{encl} = 1.9$,

the calculation of outflow from this high-pressure reservoir into the enclosure is based on the model for under-expanded jet parameters (see references Molkov et al., 2009 and Molkov, 2012) realised in the "Adiabatic blowdown model"(please include hyperlink to this model) of this software suite and is derived based on:

- Abel-Noble equation of state for hydrogen.
- Conservation equation for mass.
- Conservation equation for energy.

Additionally if $p_{res}/p_{encl} < 1.9$, the jet is considered to be expanded, and the outflowing mass flow rate is then calculated using isentropic pressure and density relationships.

Calculation of outflow from the reservoir is based on:

- The assumption of initial pressure and temperature in the enclosure equal to those in atmosphere.
- The assumption of a perfectly stirred reactor (uniform mixture of gases in enclosure).
- Vent flow relation derived from Bernoulli's equation.

The model also assumes that there is uniform outflow velocity profile from the vent. However, at extremely low hydrogen mass flow rates the conditions for concurrent inflow-outflow in the vent

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

plane may be established. *Under such conditions this particular model cannot be applied.* Therefore the minimum mass flow rate ($\dot{m}_{H2\_min}$) which will lead to 100% hydrogen concentration in the enclosure is calculated. The entered value of mass flow rate ($\dot{m}_{H2}$) is then compared to this minimum value ($\dot{m}_{H2\_min}$).

The calculation process will only proceed if $\dot{m}_{H2} > \dot{m}_{H2\_min}$.

NB1: For the assessment of the lower limit of mass flow rate that leads to 100% of hydrogen concentration in an enclosure the characteristic discharge coefficient is set to $C_{D\_100\%} = 0.85$.

NB2: The realised algorithm attempts to determine blowdown time starting from an initial guess provided by the user as an input parameter.

NB3: Initial number of time steps for integration is chosen as *n* = 1000 to avoid prolonged calculations. Though *n* = 1000 is usually sufficient to provide precise integration, users are advised to use larger number of time steps (e.g. *n* = 2000) to check if pressure dynamics in the reservoir remains essentially the same (after blowdown time is determined using initial time step number *n* = 1000). Time step number should be increased until pressure dynamics is time step insensitive, i.e. time step convergence is reached.

References:

- Molkov V., Shentsov, V., Quintiere, J., Passive ventilation of a sustained gaseous release in an enclosure with one vent, Int. Journal of Hydrogen Energy, Vol. 39, Issue 15, May 2014, pp 8158-8168.
- Brennan S., Molkov V. Safety assessment of unignited hydrogen discharge from onboard storage in garages with low levels of natural ventilation, Int. Journal of Hydrogen Energy, Vol. 38, Issue 19, June 2013, pp. 8159 – 8166
- Molkov V., Makarov D. and Bragin M. Physics and modeling of under-expanded jets and hydrogen dispersion in atmosphere, in Fortov VE, et al. (eds.). Physics of extreme state of matter, 2009. Chernogolovka, Russia, pp.143-145. ISBN 978-5-901675-89-2.
- Molkov V. "Introduction to Hydrogen Safety Engineering", BookBoon, 2012, ISBN: 978-87-403-0226-4.

3.5.5.3.2 Input values

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Atmospheric pressure	p_{atm}	101325	Pa	101325 – 90,000,000	101325
Enclosure temperature	T_{encl}	293	K		
Enclosure volume	V_{encl}	30.42	m^3		
Vent height	H_{vent}	0.316	m		
Vent width	W_{vent}	0.316	m		
Coefficient of discharge	C_D	0.6	-		0.6
Initial hydrogen pressure in reservoir	p_{res}^{0}	20500000	Pa		

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

Initial hydrogen temperature in reservoir	T_{res}	288	K		
Reservoir volume	V_{res}	0.196	m^3		
Orifice diameter	d_3	0.0095	m		
Initial guess for integration time	t_{f0}	10	s		
Number of time steps for integrations	i_{last}	1000	-		
Coefficient for ignited release	C_I	1	-		1

Note: Input value for C_I highlighted in yellow should appear only for ignited case (when option for ignited release checked in section 3.5.5.1).

3.5.5.3.3 Calculation procedure

Model constants		
Parameter	**Value / Calculation**	**Unit**
Universal gas constant	$R=8314.47$	J/(kmol K)
H$_2$ molecular mass	$M_{H_2}=2.016$	kg/kmol
Air molecular mass	$M_{air}=28.97$	kg/kmol
Acceleration due to gravity	g=9.81	m/s^2
Coefficient of discharge (100%)	$C_{D\_100\%}=0.85$	-
Hydrogen specific gas constant	$R_{H2}=R/M_{H2}$	[J/ (kg K)]
H$_2$ co-volume constant	$b=0.007691$	[m^3/kg]
Adiabatic index	$\gamma=1.405$	-
Pressure in reservoir	p_{res}^0 - user input	Pa
Critical pressure, p_{crit}	$p_{crit}=p_{atm}\cdot\left[(\gamma+1)/2\right]^{\gamma/(\gamma-1)}$	Pa
Initial air density in enclosure	$\rho_{air}=\left(p_{atm}M_{air}\right)/R\,T_{encl}$	kg/m^3
Initial hydrogen density in enclosure	$\rho_{H2}=(p_{atm}\cdot M_{H2})/(R\cdot T_{encl})$	kg/m^3
Vent area	$A_{vent}=H_{vent}\cdot W_{vent}$	m^2
Minimum mass flow rate which will lead to 100% hydrogen concentration in enclosure	$\dot{m}_{H2\_min}=C_{D\_100\%}\cdot A_{vent}\cdot\sqrt{H_{vent}}$ $\cdot\sqrt{\dfrac{8\cdot g\cdot\rho_{H2}\cdot(\rho_{air}-\rho_{H2})}{9}}$	kg/m^3

Initial check if release is ignited.

If release is **ignited** (box checked in section 3.5.5.1) — YES → $\dot{m}_{H2}=\dot{m}_{H2}\times C_I$

NO

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

YES   NO

$$\text{if } \dot{m}_{H2} \geq \dot{m}_{H2\_min}$$

STOP

- If $\dot{m}_{H2} < \dot{m}_{H2\_min}$ calculation should not proceed
- This particular model assumes constant mass flow rate, therefore this check only needs to be carried out once at the start.
- If $\dot{m}_{H2} < \dot{m}_{H2\_min}$ new parameter should appear on screen (say below 'RUN')

  - Minimum allowable mass flow rate, $\dot{m}_{H2\_min}$: | Calculated value (from above) | [kg/s]
  - Box containing $\dot{m}_{H2}$ should turn red
  - Note beside $\dot{m}_{H2}$ box should read (text in red):
    - 'value must be greater than $\dot{m}_{H2\_min}$'

Mark 1

Initial mass of air in enclosure:	$m_{encl}^{0} = V_{encl}\rho_{air}$	[kg]
Initial mass flow in vent:	$\dot{m}_{vent}^{0} = 0$	[kg/s]
Initial quantity of gas in enclosure:	$n_{encl}^{0} = m_{encl}^{0}/M_{air}$	[kmol]
Initial time:	$t = 0$	[s]
Time step counter:	$n = 0$	[-]
Time step size:	$\Delta t = t_{f0}/i_{last}$	[s]
Initial H$_2$ density in reservoir:	$\rho_{res}^{0} = \dfrac{p_{res}^{0}}{\left(p_{res}b + R_{H2}T_{res}\right)}$	[kg/m³]
Initial H2 mass in reservoir:	$m_{H2} = V_{res}\rho_{res}$	[kg]
Initial H2 flow rate from reservoir:	$\dot{m}_{H2} = 0$	[kg]

INTEGRATION NEXT STEP

Time, t:	$t = t + \Delta t$	[s]
Time step counter, i:	$i = i + 1$	[-]
Reassigning pressure in reservoir:	$p_{res}^{t} = p_{res}^{t+\Delta t}$	[Pa]
Reassigning density in reservoir:	$\rho_{res}^{t} = \rho_{res}^{t+\Delta t}$	[kg/m³]

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

Parameters in enclosure

Mass of gases in enclosure:
$$m_{encl}^{t+\Delta t} = m_{encl}^{t} + \left(\dot{m}_{H2}^{t} - \dot{m}_{vent}^{t}\right)\cdot \Delta t \qquad \text{[kg]}$$

Quantity of gas in enclosure:
$$n_{encl}^{t+\Delta t} = n_{encl}^{t} + \left(\frac{\dot{m}_{H2}^{t}}{M_{H2}} - \frac{\dot{m}_{vent}^{t}\, n_{encl}^{t}}{m_{encl}^{t}}\right)\cdot \Delta t \qquad \text{[kmol]}$$

Pressure in enclosure:
$$p_{encl}^{t+\Delta t} = \frac{n_{encl}^{t+\Delta t}\, R T_{encl}}{V_{encl}} \qquad \text{[Pa]}$$

Overpressure in enclosure:
$$p_{g\,encl}^{t+\Delta t} = p_{encl}^{t+\Delta t} - p_{atm} \qquad \text{[Pa]}$$

Vent mass flow rate:
$$\dot{m}_{vent}^{t+\Delta t} = C_{vent}\cdot \left(\frac{m_{encl}^{t+\Delta t}\, A_{vent}}{V_{encl}}\right)\left[\frac{2\left(p_{encl}^{t+\Delta t} - p_{atm}\right)V_{encl}}{m_{encl}^{t+\Delta t}}\right]^{1/2} \qquad \text{[kg/s]}$$

Parameters in reservoir

New H_2 mass in the reservoir:
$$m_{H2}^{t+\Delta t} = m_{H2}^{t} - \dot{m}_{H2}^{t}\cdot \Delta t \qquad \text{[kg]}$$

Density in the reservoir:
$$\rho_{res}^{t+\Delta t} = m_{H2}^{t+\Delta t}/V_{res} \qquad \text{[kg/m}^3\text{]}$$

Pressure in reservoir:
$$p_{res}^{t+\Delta t} = p_{res}^{t}\left[\frac{\rho_{res}^{t+\Delta t}}{\rho_{res}^{t}}\frac{\left(1-b\rho_{res}^{t}\right)}{\left(1-b\rho_{res}^{t+\Delta t}\right)}\right]^{\gamma} \qquad \text{[Pa]}$$

Temperature in reservoir:
$$T_{res}^{t+\Delta t} = \frac{p_{res}^{t+\Delta t}}{\rho_{res}^{t+\Delta t} R_{H2}}\left(1-b\rho_{res}^{t+\Delta t}\right) \qquad \text{[K]}$$

Density at the orifice, ρ_3:   **Procedure for ρ_3, use jet parameters tool**   [kg/m^3]

Temperature at the orifice:
$$T_3^{t+\Delta t} = T_{res}^{t+\Delta t}/\left(1 + (\gamma-1)/2\left(1-b\rho_{res}^{t+\Delta t}\right)^2\right) \qquad \text{[K]}$$

Pressure in orifice:
$$p_3^{t+\Delta t} = \frac{\rho_3^{t} R_{H2} T_3^{t+\Delta t}}{1-b\rho_3} \qquad \text{[Pa]}$$

Velocity in orifice:
$$V_3^{t+\Delta t} = \sqrt{\gamma R_{H2} T_3^{t+\Delta t}/(1-b\rho_3)^2} \qquad \text{[m/s]}$$

Temperature in notional nozzle:
$$T_4^{t+\Delta t} = \frac{2T_3^{t+\Delta t}}{(\gamma+1)} + \frac{(\gamma-1)}{(\gamma+1)}\frac{p_3^{t+\Delta t}}{\rho_3^{t+\Delta t}(1-b\rho_3^{t+\Delta t})R_{H2}} \qquad \text{[K]}$$

Velocity in notional nozzle:
$$V_4^{t+\Delta t} = \sqrt{\gamma R_{H2} T_4^{t+\Delta t}} \qquad \text{[m/s]}$$

Density in notional nozzle:
$$\rho_4^{t+\Delta t} = \frac{p_{encl}^{t+\Delta t}}{\left(p_{encl}^{t+\Delta t} b + R_{H2} T_4^{t+\Delta t}\right)} \qquad \text{[kg/m}^3\text{]}$$

Notional nozzle diameter:
$$d_4^{t+\Delta t} = d_3^{t+\Delta t}(\rho_3^{t+\Delta t} V_3^{t+\Delta t}/\rho_4^{t+\Delta t} V_4^{t+\Delta t})^{1/2} \qquad \text{[m]}$$

Mass flow rate:
$$\dot{m}_{H2}^{t+\Delta t} = \rho_4^{t+\Delta t} V_4^{t+\Delta t}\cdot \pi\left(d_4^{t+\Delta t}\right)^2/4 \qquad \text{[kg/s]}$$

If statement (1):

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

$$\text{If } 1.0 < \frac{p_{res}}{p_{encl}} = \left(\frac{(\gamma-1)}{2}\right)^{\gamma/(\gamma-1)} < 1.9$$

Density at the orifice, ρ_3 :	$\rho_3 = \rho_1 \cdot \left(\dfrac{p_{res}}{p_{encl}}\right)^{(1/\gamma)}$	[kg/m^3]
Mach number at the orifice:	$M_3 = \sqrt{\dfrac{2\left[\left(\dfrac{p_{res}}{p_{encl}}\right)^{\frac{(\gamma-1)}{\gamma}} -1\right]}{(\gamma-1)}}$	[ND]
Temperature at the orifice:	$T_3 = T_1 \cdot \left(\dfrac{p_{encl}}{p_{res}}\right)^{(\gamma-1)/\gamma}$	[K]
Speed of sound at orifice:	$C_3 = \sqrt{\dfrac{\gamma \cdot R \cdot T_3}{M_{H_2}}}$	[m/s]
Velocity at the orifice (actual):	$V_3 = M_3 \times C_3$	[m/s]
Mass flow rate:	$\dot{m} = \rho_3 \times V_3 \times \dfrac{\pi \cdot d_3^2}{4}$	[kg/s]

Note to programmer:
Concerning output (excel file) - When this loop is active please print in each respective column
ρ_4 = N/A, T_4 = N/A and d_4 = N/A
If statement (2):

$$\text{If } \frac{p_{res}}{p_{encl}} = \left(\frac{(\gamma-1)}{2}\right)^{\gamma/(\gamma-1)} \leq 1.0$$

Stop calculation

Output to file:

1)   Time step counter, i [-]
2)   Time, t [s]
3)   H₂ mass in reservoir, m_{H_2} [kg]
4)   Mass flow rate from reservoir, $\dot{m}_{H_2}$ [kg/s]
5)   Density in notional nozzle, ρ_4 [kg/m^3]

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6)   Velocity in notional nozzle, V_4 [m/s]

7)   Notional nozzle diameter, d_4 [m]

8)   Mass of gas in enclosure, m_{encl} [kg]

9)   Vent mass flow rate, $\dot{m}_{vent}$ [kg/s]

10)   Overpressure, $p_{g_{encl}}$ [Pa/atm/bar/psi] (whichever has been chosen by the user)

Notes to programmer:
Please include these column headings in produced 'Excel' output file.
Procedure for changing time step and integration time is the same as for adiabatic blowdown model.
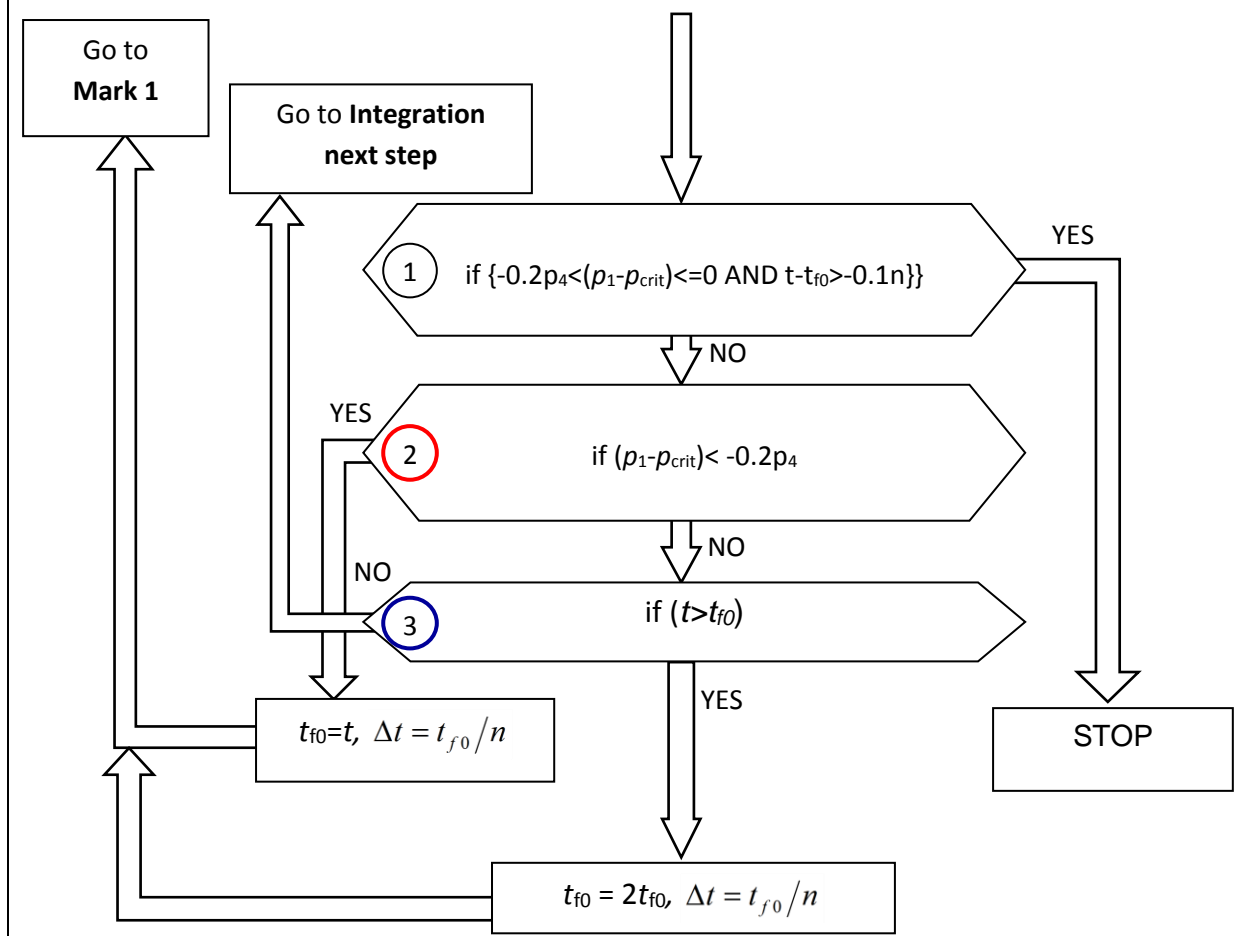
3.5.5.3.4 Output values

Upon calculation finished, the graph for the pressure **p_1** (Y-axis) against time **t** (X-axis) PPP should be plotted. The pressure axis should have axis title with respect to the pressure units chosen at the beginning e.g. Pressure (bar/Pa/kPa etc.).

The link to or SAVE button should be available for save excel file with results after calculation

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

3.5.5.4   Tool realisation

The snapshot of tool realisation is presented in Figure 15.

Figure 15 - Snapshot of PPP tool realisation.

3.5.6   Passive ventilation in an enclosure with one vent: uniform hydrogen concentration (UU)

3.5.6.1   Introduction

This model consists of three options to allow for the calculation of the three features:

1. Steady-state hydrogen uniform concentration for the given release rate and vent size
2. Parameters of the vent to get desired concentration for the given release
3. Calculation of the release rate to get desired concentration for the given vent sizes

3.5.6.2   Nomenclature

Parameter	Symbol	Unit
Area	A	m^2
Discharge coefficient	C_D	-
Gravity acceleration	g	m/s^2
Reduced gravity	g'	m/s^2
Vent height	H	m
Vent width	W	m
Molecular mass	M	kg/kmol
Pressure	p	Pa
Volumetric flow rate of gas leak	Q_0	m^3/s
Universal gas constant	R	J/K/kmol
Temperature	T	K
Volume fraction of hydrogen	X	-

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

Density	ρ	kg/m³

Note: Discharge coefficient C_D =0.6 is default value according to paper (V. Molkov, Shentsov, & Quintiere, 2014), but if user wants to adjust it, that it can be changed in input values.

3.5.6.3   Model description

Note: Model description should appear upon pressing the appropriate button on the home screen of the tool.

The neutral plane (NP) is a horizontal plane where pressure inside and outside an enclosure are equal. In general case of passive ventilation of the enclosure with release of gas lighter than air, the neutral plane is located at or below the half height of the vent for steady-state conditions. Below NP air enters the enclosure and above NP lighter hydrogen-air mixture exits the enclosure Figure 16.
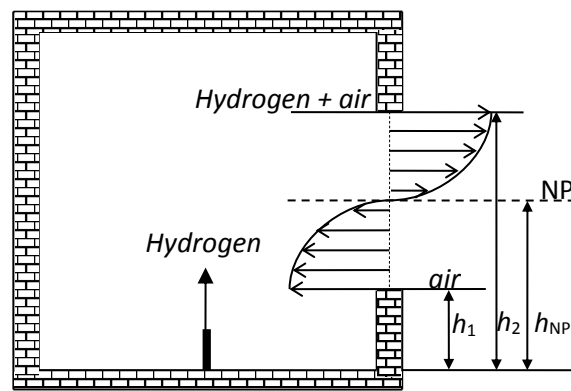
Figure 16 - Flow velocity through the vent for a case when neutral plane is between the lower edge and half height of the vent.

The model of passive ventilation of sustained gaseous leak in an enclosure with one vent is developed in the assumption of perfect mixing, described by (Eq.1) and reported in (V. Molkov et al., 2014).

$$X = f(X) \cdot \left[\frac{Q_0}{C_D A (g' H)^{1/2}} \right]^{2/3}, \tag{1}$$

where Q_0 is the volumetric flow rate of release (m³/s), and the reduced gravity is $g'=g(\rho_{air} - \rho_{H2})/\rho_{air}$ (m/s²), C_D=0.6 is the discharge coefficient, H is the height of the vent (m), $A=WxH$ is the area of the vent (m²), W is the width of the vent (m), function $f(X)$, which defines the difference between the approximate solution for volumetric fraction of hydrogen by natural ventilation (Cariteau & Tkatschenko, 2013) and the exact solution of the problem by passive ventilation theory presented here (Eq.2), is

$$f(X) = \left(\frac{9}{8} \right)^{1/3} \cdot \left\{ \left[1 - X \left(1 - \frac{\rho_{H_2}}{\rho_{air}} \right) \right]^{1/3} + (1-X)^{2/3} \right\}. \tag{2}$$

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

Density is calculated as $\rho = \dfrac{p_2 M}{R T_2}$ (kg/m3), where p is ambient pressure (Pa), M molecular mass of the gas (kg/kmol), T is the ambient temperature (K) and R=8314.4 is the universal gas constant (J/K/kmol).

3.5.6.4   Choice of the model

When the tool is selected the screen with the choice should appear prompting to select the option.

> **Please choose the option you want to calculate:**
>
> ○ 1. Steady-state hydrogen uniform concentration for the given release rate and vent size
>
> ○ 2. Parameters of the vent to get desired concentration for the given release
>
> ○ 3.Calculation of the release rate to get desired concentration for the given vent sizes

Note: Example of the model choice is the Option(radio) Button. When checked the screen with appropriate input parameters should appear below, together with button to initiate calculation (choice of RUN, CALCULATE, START etc. to be uniform across the e-Laboratory).

3.5.6.5   Option 1: Steady-state hydrogen uniform concentration for the given release rate and vent size

This option allows user to calculate the steady-state hydrogen uniform concentration by the given parameters of the release and ventilation size.

3.5.6.5.1 Input values

Test values to calculate hydrogen concentration.

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Hydrogen mass flow rate	$\dot{m}_{H2}$	1e-5	kg/s	0.0001-1	0.001
Ambient pressure	p_2	101325	Pa	33700-107900	101325
Ambient temperature	T_2	293	K	240-350	293
Vent height	H	0.2	m	0.001-10	2
Vent width	W	0.2	m	0.001-10	1
Discharge coefficient	C_D	0.6	-	0.4-1	0.6

Test values to get message "You reached 100% concentration!":

Parameter name	Symbol	Input value	Unit for calculation
Hydrogen mass flow rate	$\dot{m}_{H2}$	1e-5	kg/s
Ambient pressure	p_2	101325	Pa
Ambient temperature	T_2	293	K
Vent height	H	0.01	m
Vent width	W	0.01	m
Discharge coefficient	C_D	0.6	-

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

Example of input parameters panel which should appear after the option choice.

Parameter name	Symbol	Input value	Input Unit
Hydrogen mass flow rate	$\dot{m}_{H2}$	1e-5	kg/s
Ambient pressure	p_2	101325	Pa
Ambient temperature	T_2	293	K
Vent height	H	0.2	m
Vent width	W	0.2	m
Discharge coefficient	C_D	0.6	n/a

Calculate

3.5.6.5.2 Calculation procedure

Input parameters from user

Calculate Eq. 1-5 using input values and constants 6-10

Solve Eq. 12 to find **X** using algorithm of solution

1	Density of hydrogen, ρ_{H2}	$$\rho_{H2} = \frac{p_2 M_{H2}}{RT_2}$$	kg/m³
2	Density of air, ρ_{air}	$$\rho_{air} = \frac{p_2 M_{air}}{RT_2}$$	kg/m³
3	Vent area, A	$A = W \cdot H$	m²
4	Volumetric flow rate of gas leak, Q_0	$Q_0 = \dot{m}_{H2} / \rho_{H2}$	m³/s
5	Reduced gravity, g'	$g' = g(\rho_{air} - \rho_{H2})/\rho_{air}$	m/s²
6	Universal gas constant, R	$R=8314.47$	J/K/kmol
7	H2 molar mass M_{H2}	2.016	kg/kmol
8	Air molar mass M_{air}	29	kg/kmol
9	Coefficient of discharge, C_D	$C_D=0.6$	-
10	Gravity acceleration, g	$g=9.81$	m/s²
11	Function $f(X)$	$$f(X) = \left(\frac{9}{8}\right)^{1/3} \cdot \left\{ \left[1 - X\left(1 - \frac{\rho_{H_2}}{\rho_{air}}\right) \right]^{1/3} + (1 - X)^{2/3} \right\}$$	-
12	Volume fraction of hydrogen, X	$$X = f(X) \cdot \left[\frac{Q_0}{C_D A (g' H)^{1/2}} \right]^{2/3}$$	-

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

Algorithm of solution:

```
START
X=0; X<=1; ΔX=0.0001
```

$$X = 1 \text{ and } X \neq f(X)\cdot\left[\frac{Q_0}{C_D A(g^{'}H)^{1/2}}\right]^{2/3}$$

$$X + \Delta X$$

$$X = f(X)\cdot\left[\frac{Q_0}{C_D A(g^{'}H)^{1/2}}\right]^{2/3}$$

```
Return X
FINISH
```

```
Return message:
"You reached 100% hydrogen
concentration!" FINISH
```
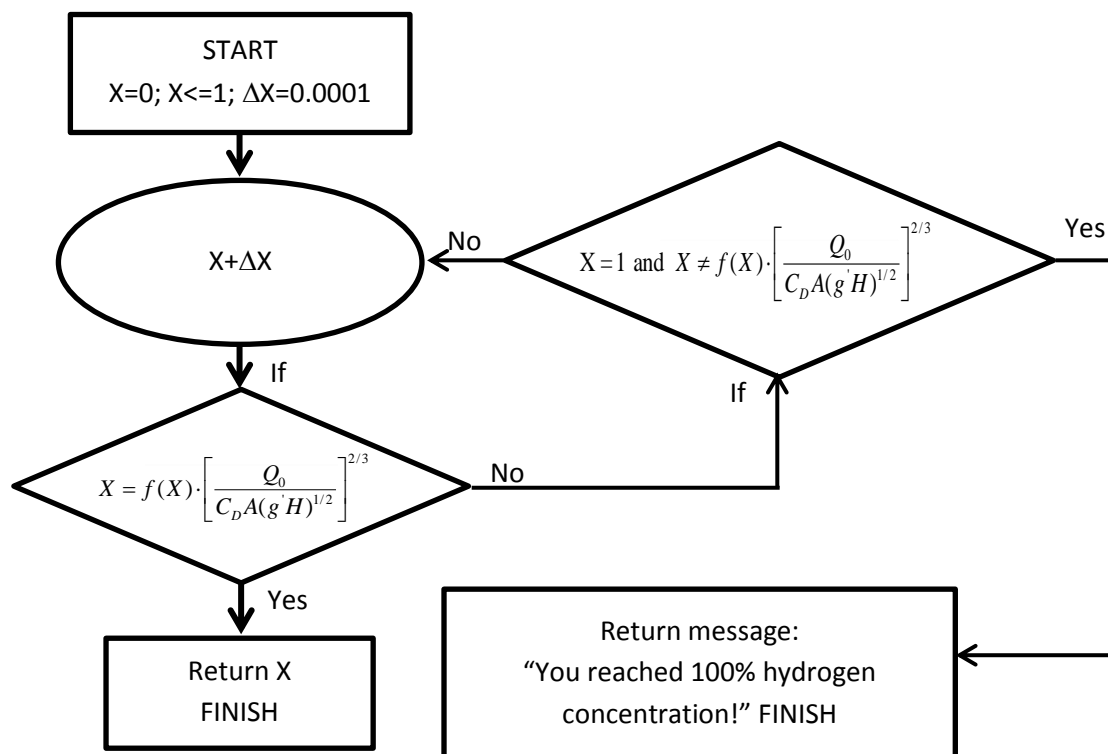
Note: Parameter ΔX is the volume fraction step that has value 1e-4 which means that this is precision of the model for the concentration.

3.5.6.5.3 Output values

Parameter name	Symbol	Output value	Unit
Hydrogen volume fraction	X	0.048393207	-

Example of results panel which should appear after calculation.

Parameter name	Symbol	Value	Unit
Hydrogen volume fraction	X	0.048393207	- ▼

New calculation	Save results	Print results	Share

3.5.6.6   Option 2: Parameters of the vent to get desired concentration

This option allows user calculating the parameters of the vent either width or height for the possible release in order not to exceed the required level of hydrogen concentration e.g. 25% from lower flammability limit of 4% (LFL).

3.5.6.6.1 Input values

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Hydrogen mass flow rate	$\dot{m}_{H2}$	1e-5	kg/s	0.0001-1	0.001
Ambient pressure	p_2	101325	Pa	33700-107900	101325
Ambient temperature	T_2	293	K	240-350	293

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

Choose an item.	H/W	0.2	m	0.001-10	2
Discharge coefficient	C_D	0.6	-	0.4-1	0.6
Desired mole fraction of hydrogen	X	0.048393207	-	0-1	0.04

Note: There should be an option ratio button or drop-down list to choose either height or width of the vent before proceed to calculation.

3.5.6.6.2 Calculation procedure

Input parameters from user

Calculate Eq. 1-6 using input values and constants 8-12 to get Width of the vent

Calculate Eq. 1-5&7 using input values and constants 8-12 to get Height of the vent

Result - vent Width

Result - vent Height

1	Density of hydrogen, ρ_{H2}	$$\rho_{H2} = \frac{p_2 M_{H2}}{R T_2}$$	kg/m³
2	Density of air, ρ_{air}	$$\rho_{air} = \frac{p_2 M_{air}}{R T_2}$$	kg/m³
3	Volumetric flow rate of gas leak, Q_0	$$Q_0 = \dot{m}_{H2} / \rho_{H2}$$	m³/s
4	Reduced gravity, g'	$$g' = g(\rho_{air} - \rho_{H2})/\rho_{air}$$	m/s²
5	Function, $f(X)$	$$f(X) = \left(\frac{9}{8}\right)^{1/3} \cdot \left\{\left[1 - X\left(1 - \frac{\rho_{H_2}}{\rho_{air}}\right)\right]^{1/3} + (1-X)^{2/3}\right\}$$	-
6	Width of the vent, W	$$W = \frac{Q_0}{C_D (g' H^3)^{1/2} \cdot \left[\dfrac{X}{f(X)}\right]^{3/2}}$$	m
7	Height of the vent, H	$$H = \left(\left[\frac{Q_0}{C_D W \left[\dfrac{X}{f(X)}\right]^{3/2}}\right]^2 / g'\right)^{1/3}$$	m
8	Universal gas constant, R	$R = 8314.47$	J/K/kmol
9	H2 molar mass, M_{H2}	2.016	kg/kmol
10	Air molar mass, M_{air}	28.97	kg/kmol
11	Coefficient of discharge, C_D	$C_D = 0.6$	-
12	Gravity acceleration, g	$g = 9.81$	m/s²

Note: regarding what was chosen for the input width or height appropriate equation should be solved and output values given.

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

3.5.6.6.3 Output values

For calculation of vent height based on vent width and mass flow rate:

Parameter name	Symbol	Output value	Unit
Vent height calculated	*H*	0.2	m

For calculation of vent width based on vent height and mass flow rate:

Parameter name	Symbol	Value	Unit
Vent width calculated	*W*	0.2	m

3.5.6.7   Option 3: Calculation of the release rate to get desired concentration for the given vent sizes

This option allows calculating the mass flow rate which could be allowed for the particular vent parameters in order not to exceed the required level of hydrogen concentration e.g. 25% from lower flammability limit of 4% (LFL).

3.5.6.7.1 Input values

Parameter name	Symbol	Input value	Unit	Limits (min-max)	Defaults
Ambient pressure	p_2	101325	Pa	33700-107900	101325
Ambient temperature	T_2	293	K	240-350	293
Vent height	H	0.2	M	0.001-10	2
Vent width	W	0.2	m	0.001-10	1
Discharge coefficient	C_D	0.6	-	0.4-1	0.6
Desired mole fraction of hydrogen	X	0.048393207	-	0-1	0.04

3.5.6.7.2 Calculation procedure

1	Density of hydrogen, ρ_{H2}	$$\rho_{H2} = \frac{p_2 M_{H2}}{R T_2}$$	kg/m³
2	Density of air, ρ_{air}	$$\rho_{air} = \frac{p_2 M_{air}}{R T_2}$$	kg/m³
3	Universal gas constant, R	$R=8314.47$	J/K/kmol
4	H2 molar mass, M_{H2}	2.016	kg/kmol
5	Air molar mass, M_{air}	28.97	kg/kmol
6	Coefficient of discharge, C_D	$C_D=0.6$	-
7	Gravity acceleration, g	$g=9.81$	m/s²
8	Reduced gravity, g'	$g'=g(\rho_{air} - \rho_{H2})/\rho_{air}$	m/s²
9	Volumetric flow rate of gas leak, Q_0	$$Q_0 = \left(\frac{X}{f(X)}\right)^{3/2} C_D A (g' H)^{1/2}$$	m³/s
10	Function, $f(X)$	$$f(X) = \left(\frac{9}{8}\right)^{1/3} \cdot \left\{ \left[1 - X\left(1 - \frac{\rho_{H_2}}{\rho_{air}}\right)\right]^{1/3} + (1-X)^{2/3} \right\}$$	-

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11	Mass flow rate, $\dot{m}_{H2}$	$\dot{m}_{H2} = Q_0 \rho_{H2}$	kg/s

3.5.6.7.3 Output values

Parameter name	Symbol	Output value	Unit
Hydrogen mass flow rate	$\dot{m}$	1e-5	kg/s

3.5.6.8   Tool realisation

The snapshot of tool realisation is presented in Figure 17.
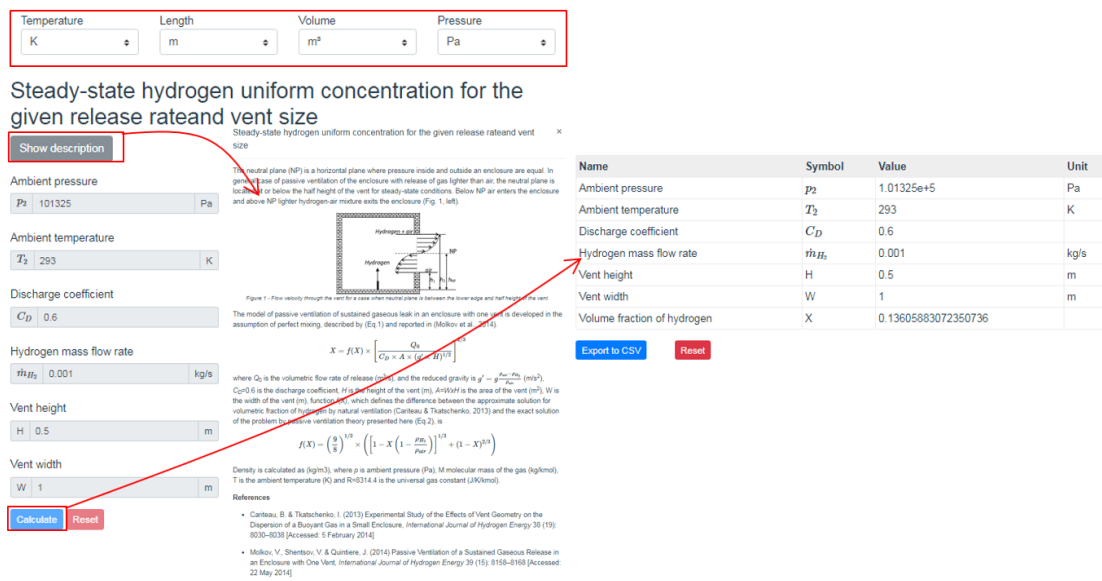
Figure 17 - Snapshot of PPP tool realisation.

3.5.7   Mitigation of uniform mixture deflagration by venting technique (UU)

3.5.7.1   Introduction

Note: Model description should appear upon pressing the appropriate button on the home screen of the tool.

The tool allows for:

- calculation of the vent area required to reduce deflagration overpressure to a given level, or
- estimate an overpressure for a vent of known area.

The model implemented in this tool is presented in (V. Molkov & Bragin, 2015) and validated against the widest range of experimental conditions available to date. The validation covers a wide range of test conditions: different shape enclosures of volume up to 120 m3; initially quiescent and turbulent hydrogen-air mixtures; hydrogen concentration in air from 6% to 30% by volume; ignition source location at enclosure centre, near and far from a vent; empty enclosures and enclosures with obstacles.

Figure 18 presents the vent sizing correlation (V. Molkov & Bragin, 2015) that can be used to calculate vent area required for the overpressure to remain below specified limit or to estimate an

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overpressure for a vent of known size. General expression for the dimensionless overpressure as a function of turbulent Bradley number Br_t was developed analytically and then coefficients were obtained using the best fit for 76 processed experiments, $\pi_{red} = 0.33 \cdot Br_t^{-1.3}$, see Figure 18. Note that the correlation is derived for deflagrations in a low strength equipment and buildings, with deflagration overpressure not exceeding 1 bar.

A conservative form of correlation is developed in such a way that the predicted reduced overpressure π_{red} is knowingly above the measured experimental value across the complete range of experimental conditions and is given by equation $\pi_{red} = 0.86 \cdot Br_t^{-1.3}$ (not shown in Figure 18).
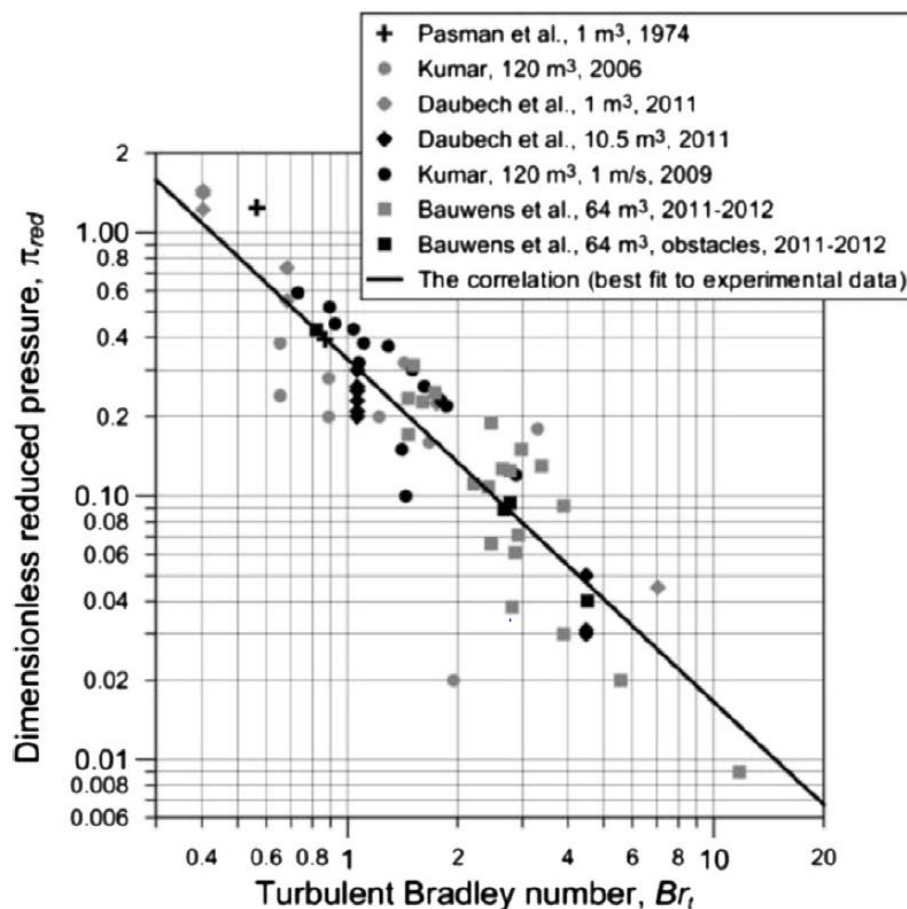
Figure 18 – Vent sizing correlation, best fit.

3.5.7.2   Nomenclature and model constants

Table 5 – Nomenclature and model constants

Parameter	Symbol	Unit
Enclosure volume	$V=H_E x W_E x L_E$	m^3
Enclosure height	H_E	m
Enclosure width	W_E	m
Enclosure length	L_E	m
Maximum absolute pressure	P_{max}	Pa
Vent area	F	m^2
Initial absolute pressure	P_i	Pa

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Initial turbulence	u'	m/s
Dimensionless reduced pressure	π_{red}	ND
Turbulent Bradley number	Br_t	ND
Factor to account for presence of obstacles in enclosure	Ξ_O	ND
Initial burning velocity	S_{ui}	m/s
Expansion coefficient	E_i	ND
Empirical coefficient	ψ	ND
Hydrogen volume fraction	X_{H2}	ND
Air volume fraction	$X_{air}=1-X_{H2}$	ND
Initial temperature	T_{ui}	K
Internal surface area of an enclosure	A_{EW}	m^3
Area of the sphere of the same volume as enclosure	A_S	m^3
Speed of sound	c_{iu}	m/s
Pi number	$\pi_0=3.1415...$	ND
Specific heat ratio	$\gamma_u=1.4$	ND
Universal gas constant	$R_g=8314.5$	J/(kmol K)
Radius of equivalent volume sphere	R	m
Characteristic flame radius	R_0	m
Theoretical maximum of wrinkling factor due to turbulence generated by the flame front itself	Ξ_K^{max}	ND
Wrinkling factor due to turbulence generated by the flame front itself	Ξ_K	ND
Maximum leading point wrinkling factor	Ξ_{LP}^{max}	ND
Leading point flame wrinkling factor	Ξ_{LP}	ND
Internal surface area of an enclosure	A_{EW}	m^2
Aspect ratio wrinkling factor	Ξ_{AR}	ND
Fractal wrinkling factor	Ξ_{FR}	ND
Factor to account for the presence of obstacles in the enclosure	Ξ_O	ND
Temperature index	m_0	ND
Laminar flame velocity	S_u	m/s
SGS wrinked flame burning velocity	S_u^{SGS}	m/s
Turbulent burning velocity	S_t	m/s
Wrinkling factor to account for initial turbulence	$\Xi_{u'}$	ND
Deflagration-outflow interaction number	χ/μ	ND
Speed of sound	c_{ui}	m/s
Molecular mass of mixture	M_{ui}	kg/kmol
H$_2$ molecular mass	$M_{H_2}=2$	kg/kmol
Air molecular mass	$M_{air}=28.97$	kg/kmol
Fractal dimension	$D=2.33$	ND

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

3.5.7.3   Choice of the option to calculate

When the tool is selected, the screen with the choice should appear prompting to select the option.

> **Please choose the option you want to calculate:**
>
> ⦿ 1. Vent area required to reduce deflagration pressure to a given level
>
> ○ 2. Estimate an overpressure for a vent of known size

3.5.7.4   Option 1: Calculation of vent area to reduce deflagration pressure to a given level

3.5.7.4.1 Input values

Please provide values for calculation and select the methodology.

Table 6 – Input values.

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Maximum absolute pressure	P_{max}	139828.5	Pa	33700 - 209225	
Initial absolute pressure in enclosure	P_i	101325	Pa	33700 - 107900	
Hydrogen volume fraction	X_{H2}	0.078	ND	0.04 - 0.75	
Initial turbulence	u'	1	m/s	≥0	
Factor to account for presence of obstacles in enclosure	Ξ_O	1	ND	≥1	
Initial temperature	T_{ui}	298	K	233 - 313	
Enclosure height	H_E	3	m		
Enclosure width	W_E	4	m		
Enclosure length	L_E	10	m		

Note:

- When the option is selected, the screen with input values should appear prompting to input values for calculation.
- If the input maximum absolute pressure is above the limits a warning message should appear that the model was not validated above specified value but allowing to calculate with higher values.
- The default value of factor to account for presence of obstacles in enclosure is 1 means absence of obstacles. The model was validated against experiments without obstacles. User may choose any value above 1.
- There should be an option to choose either conservative or best fit methodology for calculation for example as below.

> **Please select methodology:**
> ○ 1. BEST FIT
>
> ○ 2. CONCERVATIVE

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

3.5.7.4.2 Output values

Table 7 – Model outputs.

Parameter	Value	Symbol	Unit
Maximum absolute pressure	139828.5	P_{max}	Pa
Hydrogen volume fraction in an enclosure	0.078	X_{H2}	ND
Volume of enclosure	120	V	m^3
Vent area required not to exceed maximum pressure	**0.55**	**F**	**m^2**

3.5.7.5   Option 2: Calculation of an overpressure for a vent of known size

3.5.7.5.1 Input values

Please provide values for calculation and select the methodology.

Table 8 – Input values.

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Initial absolute pressure	P_i	101325	Pa	33700 - 107900	
Hydrogen volume fraction	X_{H2}	0.078	ND	0.04 - 0.75	
Initial temperature	T_{ui}	298	K	233 - 313	
Initial turbulence	u'	1	m/s	≥0	
Factor to account for presence of obstacles in enclosure	Ξ_O	1	ND	>1	
Enclosure height	H_E	3	m		
Enclosure width	W_E	4	m		
Enclosure length	L_E	10	m		
Vent area	F	0.55	m^2		

When the option is selected, the screen with input values as in Table 3 should appear prompting to input values for calculation. There should be an option to choose either conservative or best fit methodology for calculation.

Please select methodology:

○ 1. BEST FIT

○ 2. CONCERVATIVE

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

3.5.7.5.2 Output values

Table 9 – Model outputs.

Parameter	Value	Symbol	Unit
Vent area	0.55	F	m^2
Hydrogen volume fraction in an enclosure	0.078	X_{H2}	ND
Volume of enclosure	120	V	m^3
Maximum absolute pressure	139828.5	P_{max}	**Pa**

3.5.7.6   Calculation procedure

Follow procedure as per Table 3.

Table 10 – Calculation procedure.

	General calculations for Option 1 and Option 2		
1	Initial burning velocity, S_{ui}	$Sui = 997.96 \cdot X_{H_2}^5 - 1677.3 \cdot X_{H_2}^4 + 774.7 \cdot X_{H_2}^3 - 102.51 \cdot X_{H_2}^2 + 6.0408 \cdot X_{H_2}^1 - 0.0906$	m/s
2	Expansion coefficient, E_i	$Ei = 8775.5185528 \cdot X_{H_2}^6 - 12712.180895 \cdot X_{H_2}^5 + 6167.6542811 \cdot X_{H_2}^4 - 1364.5614133 \cdot X_{H_2}^3 + 124.27324034 \cdot X_{H_2}^2 + 19.766929968 \cdot X_{H_2}^1 + 1.147791802$	ND
3	Empirical coefficient, ψ	**If 4% ≤ X_{H_2} < 20%** $\psi = 1$ **If 20% ≤ X_{H_2} < 30%** $\psi = -5 X_{H_2} - 2$ **If 30% ≤ X_{H_2} ≤ 75%** $\psi = 0.5$	ND
4	Enclosure volume, V	$V = W_E \cdot H_E \cdot L_E$	m^3
5	Radius of equivalent volume sphere , R	$R = \sqrt[3]{3V/4\pi}$	m
6	Characteristic flame radius, R_0	**If 4% < X_{H_2} <20%** $R_0 = 6.7515 X_{H_2} - 0.1215$ **If 29.5% ≤ X_{H_2} < 75%** $R_0 = 1.2$	m
7	Theoretical maximum of wrinkling factor due to turbulence generated by the flame front itself,	$\Xi_K^{\max} = (E_i - 1)/\sqrt{3}$	

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8	Wrinkling factor due to turbulence generated by the flame front itself, Ξ_K	$\Xi_K = 1 + \left(\psi \cdot \Xi_K^{\max} - 1\right) \cdot \left[1 - \exp\left(-R/R_0\right)\right]$	ND
9	Maximum leading point wrinkling factor, Ξ_{LP}^{max}	**If 6% ≤ X_{H_2} < 17.42%** $\Xi_{LP}^{max} = -14359602.023 \cdot X_{H_2}^6$ $+ 10123867.773 \cdot X_{H_2}^5$ $- 2916887.3772 \cdot X_{H_2}^4$ $+ 440588.70586 \cdot X_{H_2}^3$ $- 36817.553635 \cdot X_{H_2}^2$ $+ 1602.0558168 \cdot X_{H_2}^1$ $- 25.461905777$ **If 17.42% ≤ X_{H_2} < 29.66%** $\Xi_{LP}^{max} = -51.456479236 \cdot X_{H_2}^2$ $+ 17.427219398 \cdot X_{H_2}^1$ $+ 0.63502119987$ **If 29.66% ≤ X_{H_2} < 71.27%** $\Xi_{LP}^{max} = -143.23023003 \cdot X_{H_2}^5$ $+ 425.62891627 \cdot X_{H_2}^4$ $- 496.19245746 \cdot X_{H_2}^3$ $+ 286.05307157 \cdot X_{H_2}^2$ $- 82.455320688 \cdot X_{H_2}^1$ $+ 10.550603906$ **If 71.27% ≤ X_{H_2} ≤ 75%** $\Xi_{LP}^{max} = 0.9333$	ND
10	Leading point flame wrinkling factor	IF R ≤ R$_0$/2 $\Xi_{LP} = 1 + \dfrac{\left(\Xi_{LP}^{\max} - 1\right) \cdot 2R}{R_0}$ ELSE $\Xi_{LP} = \Xi_{LP}^{\max}$	ND
11	Internal surface area of an enclosure, A_{EW}	$A_{EW} = 2 \cdot \left(E_W \cdot E_L + E_H \cdot E_L + E_H \cdot E_W\right)$	m²
12	Area of the equivalent volume, A_S	$A_S = 4\pi \cdot R^2$	m²
13	Aspect ratio wrinkling factor	$\Xi_{AR} = \dfrac{A_{EW}}{A_S}$	ND
14	Fractal wrinkling factor	**If $R>R_0$** $\Xi_{FR} = \left(\dfrac{R}{R_0}\right)^{D-2}$ **If $R<R_0$** $\Xi_{FR} = 1$	ND

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15	Factor to account for the presence of obstacles in the enclosure	$\Xi_O = 1$	ND
16	Temperature index	$m_0 = -25.945589631 \cdot X_{H_2}^5 + 67.152094773 \cdot X_{H_2}^4 - 66.699205247 \cdot X_{H_2}^3 + 44.328192289 \cdot X_{H_2}^2 - 18.547832349 \cdot X_{H_2}^1 + 4.5752821336$	ND
17	Laminar flame velocity	$S_u = S_{ui} \cdot \left(\dfrac{T_{ui}}{298} \right)^{m_0}$	m/s
18	SGS wrinked flame burning velocity	$S_u^{SGS} = S_u \cdot \Xi_K \cdot \Xi_{LP} \cdot \Xi_{FR} \cdot \Xi_{AR} \cdot \Xi_O$	m/s
19	Turbulent burning velocity	**Solve transcendental equation to find S_t using procedure in section 3.5.7.7** $S_t = S_w^{SGS} \cdot \exp(u'/S_t)^2$	m/s
20	Wrinkling factor to account for initial turbulence	$\Xi_{u'} = S_t / S_w^{SGS}$	ND
21	Deflagration-outflow interaction number	$\chi/\mu = \Xi_K \cdot \Xi_{LP} \cdot \Xi_{FR} \cdot \Xi_{u'} \cdot \Xi_{AR} \cdot \Xi_O$	ND
22	Molecular mass of mixture	$M_{ui} = M_{air} \cdot X_{air} + M_{H_2} \cdot X_{H_2}$	kg/kmol
23	Speed of sound	$c_{ui} = \sqrt{\dfrac{\gamma R_g T_{ui}}{M_{ui}}}$	m/s
IF Option 1			
1	Dimensionless reduced pressure, π_{red}	$\pi_{red} = (P_{max} - P_i)/P_i$	ND
2	Based on methodology selected in section 3.5.7.4.1 calculate turbulent Bradley number, Br_t	**If BEST FIT** $Br_t = \left(\dfrac{\pi_{red}}{0.33} \right)^{-1/1.3}$ **If CONCERVATIVE** $Br_t = \left(\dfrac{\pi_{red}}{0.86} \right)^{-1/1.3}$	ND
3	**Vent area**	$F = Br_t \cdot \dfrac{\chi}{\mu} \cdot \sqrt[3]{36\pi_0} \cdot V^{2/3} \cdot \dfrac{S_{ui} \cdot (E_i - 1)}{c_{ui} \cdot \sqrt{E_i / \gamma_u}}$	m^2
IF Option 2			
1	Calculate turbulent Bradley number, Br_t	$Br_t = \dfrac{F}{\dfrac{\chi}{\mu} \cdot \sqrt[3]{36\pi_0} \cdot V^{2/3} \cdot \dfrac{S_{ui} \cdot (E_i - 1)}{c_{ui} \cdot \sqrt{E_i / \gamma_u}}}$	ND
2	Based on methodology selected in section 3.5.7.5.1 calculate	**If BEST FIT** $\pi_{red} = 0.33 \cdot Br_t^{-1.3}$	ND

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	dimensionless reduced pressure, π_{red}	**If CONCERVATIVE** $$\pi_{red} = 0.86 \cdot Br_t^{-1.3}$$	
3	**Maximum absolute pressure, P_{max}**	$$P_{\max} = \pi_{red} \cdot P_i + P_i$$	Pa

3.5.7.7 Procedure to calculate S_t: Newton-Raphson Method

START

St_iter=0

S_t=Sui+0.5u'

Initialisation

WHILE St_iter < 100 **AND** f_xn ≥ 1.e-6

St_iter++

$$f\_xn = S_t - S_w^{SGS} \cdot \exp\left[(u'/S_t)^2\right]$$

$$df\_xn = 1 + 2*(S_w^{SGS} \cdot \exp\left[(u'/S_t)^2\right]*\frac{u'^2}{S_t^3})$$

$$S_t = S_t - \frac{f\_xn}{df\_xn}$$

IF St_iter = 100

Show message: S_t error St_iter=100

EXIT

3.5.8 Forced ventilation system parameters (UU)

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]
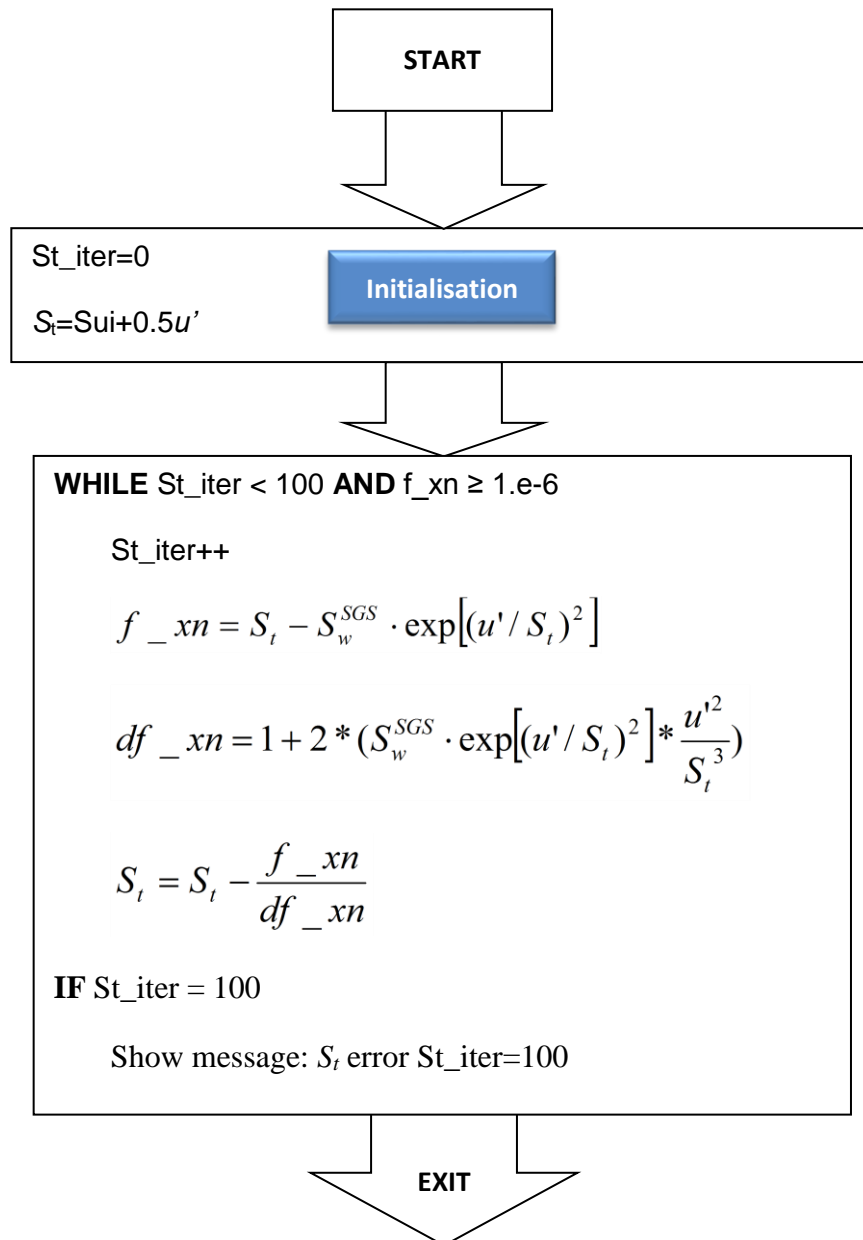
3.5.8.1   Introduction

This model calculates the ventilation flow rate of air required in steady state regime to get desired uniform concentration of hydrogen based on the gas release rate.

According to (ATEX, 2001), (CEI EN-60079-10., 2004) and (Cerchiara, Mattei, Schiavetti, & Carcassi, 2011) in the case of an accidental hydrogen release the ventilation system should maintain concentration of the hydrogen in an enclosure below 2% v/v. In most situations with passive ventilation, this could lead to the drastic increase of the ventilation opening. For this reason, in order to reduce the heat losses from the buildings and activate the necessary ventilation only when the sensor has detected a leak it is sensible to apply forced ventilation.

The model used in this tool is based on the model for passive ventilation of sustained gaseous leak in an enclosure with one vent (V. Molkov et al., 2014). It was developed in the assumption of perfect mixing, described by Eq. (3-1) and reported in (Shentsov, 2015).

$$X = f(X) \cdot \left[\frac{Q_0}{C_D A (g' H)^{1/2}} \right]^{2/3}, \tag{3-1}$$

where Q_0 is the volumetric flow rate of release (m^3/s), and the reduced gravity is $g' = g(\rho_{air} - \rho_{H2})/\rho_{air}$ (m/s^2), C_D=0.6 is the discharge coefficient, H is the height of the vent (m), $A=WxH$ is the area of the vent (m^2), W is the width of the vent (m), function $f(X)$, which defines the difference between the approximate solution for volumetric fraction of hydrogen by natural ventilation and the exact solution of the problem by passive ventilation theory presented Eq. (3-2).

$$f(X) = \left(\frac{9}{8} \right)^{1/3} \cdot \left\{ \left[1 - X \left(1 - \frac{\rho_{H_2}}{\rho_{air}} \right) \right]^{1/3} + (1-X)^{2/3} \right\}. \tag{3-2}$$

3.5.8.2   Nomenclature

Parameter	Symbol	Unit
Area	A	m^2
Discharge coefficient	C_D	-
Gravity acceleration	g	m/s^2
Reduced gravity	g'	m/s^2
Vent height	H	m
Vent width	W	m
Molecular mass	M	kg/kmol
Pressure	p	Pa
Volumetric flow rate of gas leak	Q_0	m^3/s
Universal gas constant	R	J/K/kmol
Temperature	T	K
Volume fraction of hydrogen	X	-
Density	ρ	kg/m^3

Note: Discharge coefficient C_D =0.6 is default value according to paper (V. Molkov et al., 2014), but if user wants to adjust it, that it can be changed in input values.

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3.5.8.3   Input values

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Hydrogen mass flow rate	$\dot{m}_{H2}$	1e-5	kg/s	0.0001-1	0.001
Ambient pressure	p	101325	Pa	33700-107900	101325
Ambient temperature	T	293	K	240-350	293
Desired mole fraction of hydrogen	X	0.048393207	-	0-1	0.04

3.5.8.4   Calculation procedure

Calculate Eq. 6-15 using input values and constants 1-5 to get ventilation flow rate

1	Universal gas constant, R	$R=8314.47$	J/K/kmol
2	H2 molar mass, M_{H2}	$M_{H2}=2.016$	kg/kmol
3	Air molar mass, M_{air}	$M_{air}=28.97$	kg/kmol
4	Coefficient of discharge, C_D	$C_D=0.6$	-
5	Gravity acceleration, g	$g=9.81$	m/s^2
6	Density of hydrogen, ρ_{H2}	$\rho_{H2} = \dfrac{pM_{H2}}{RT}$	kg/m^3
7	Density of air, ρ_{air}	$\rho_{air} = \dfrac{pM_{air}}{RT}$	kg/m^3
8	Density of H2-air mixture, ρ_{mix}	$\rho_{mix} = X\rho_{H_2} + (1-X)\rho_{air}$	kg/m^3
9	Volumetric flow rate of gas leak, Q_{gas}	$Q_{gas} = \dot{m}_{H2} / \rho_{H2}$	m^3/s
10	Reduced gravity, g'	$g' = g(\rho_{air} - \rho_{H2})/\rho_{air}$	m/s^2
11	Function, $f(X)$	$f(X) = \left(\dfrac{9}{8}\right)^{1/3} \cdot \left\{ \left[1 - X\left(1 - \dfrac{\rho_{H_2}}{\rho_{air}}\right)\right]^{1/3} + (1-X)^{2/3} \right\}$	-
12	Height of the vent, H	$H = \left(\left[\dfrac{Q_0}{C_D\left[\dfrac{X}{f(X)}\right]^{3/2}} \right]^{2} \Big/ g' \right)^{1/3}$	m

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13	Height of the neutral plane	$$h_{NP} = \dfrac{H \cdot \left(1 - \dfrac{X\rho_{H_2}}{\rho_{mix}}\right)^{2/3} \left(\dfrac{\rho_{mix}}{\rho_{air}}\right)^{1/3}}{1 + \left(1 - \dfrac{X\rho_{H_2}}{\rho_{mix}}\right)^{2/3} \left(\dfrac{\rho_{mix}}{\rho_{air}}\right)^{1/3}}$$	m
14	Mass flow rate of air	$$\dot{m}_{air} = (h_{NP})^{3/2} \frac{2}{3} \sqrt{2\rho_{air} g(\rho_{air} - \rho_{mix})}$$	kg/s
15	Volume flow rate of air, Q_{air}	$$Q_{air} = \dot{m}_{air} / \rho_{air}$$	m³/s

Note: regarding what was chosen for the input width or height appropriate equation should be solved and output values given.

3.5.8.5   Output values

Parameter name	Symbol	Output value	Unit
Volume flow rate of air	Q_{air}	0.003908561	m³/s

3.5.9   Blast wave from high-pressure tank rupture without and with combustion (UU)

3.5.9.1   Introduction

This tool allows calculating Blast wave decay, Impulse and hazarding distances for several options:

3. Stand-alone (tank located on the ground)
    a) With combustion
    b) Without combustion
4. Under-vehicle tank location
    a) With combustion
    b) Without combustion
5. Stand-alone (tank located in air – no effect of the ground)
    a) With combustion
    b) Without combustion

3.5.9.2   Nomenclature

Parameter	Symbol	Unit
Area	A	m²
speed of sound in compressed gas	a_g	m/s
speed of sound in surrounding gas	a_s	m/s
ratio of specific heats	γ	ND
Pressure of gas in a vessel	p_g	Pa
Pressure of surrounding air	p_s	Pa
Molecular mass of air	M_a	kg/kmol
Molecular mass of hydrogen	M_g	kg/kmol
Universal gas constant	R	J/K/kmol
Temperature	T	K
Hydrogen co-volume constant	$b=0.007691$	m³/kg

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Mass of compressed gas in tank	m_g	kg
Mechanical energy coefficient	α	ND
Chemical energy coefficient	β	ND
Hydrogen heat of combustion	$H_c=1.1993\times10^8$	J/kg
Density of air	ρ_s	kg/m^3
Density of H2	ρ_g	kg/m^3
Non-dimensional starting shock	$\overline{P}_{st}$	ND
Radius of spherical tank	r_v	m
Dimensionless radius of spherical tank	$\bar{r}_v$	ND
Fireball radius	r_b	m
Mechanical energy	ΔE_m	J
Total chemical energy	E_{ch}	J
Total mechanical energy	E_m	J
Dimensionless overpressure	$\overline{P}$	ND
Dimensional overpressure	ΔP	Pa
Dimensionless distance for finding non-dimensional impulse $\overline{I}$	$\overline{r}_i$	ND
Dimensionless impulse	$\overline{I}$	ND

3.5.9.3   Model description

Note: Model description should appear upon pressing the appropriate button on the home screen of the tool.

The model employed is based on the work by (Baker, 1983) and is fully described in details in (Molkov and Kashkarov, 2015), and accounts for non-ideal gas effects. It allows the estimation of overpressure and impulse in a blast wave at different distances from the tank. The methodology can be used to calculate deterministic hazard distances in the case of high-pressure gas tank physical explosion (rupture without combustion of released gas) by whatever reason.

The overall process of estimation of the blast wave characteristics involves calculation of the initial shock and calculation of the blast wave in the near/far field. The initial shock (also called sometimes as the contact pressure) is assumed to take place when the vessel wall disappears instantaneously (Ineris, Accident Risks Division, 2012).

The original methodology for calculation of overpressure and impulse in a blast wave from a high-pressure gas storage tank rupture in a fire is used in this. The methodology is built up using the novel model of combustion of hydrogen in air at the contact surface and behind it in the wake of the outward propagating shock. The Abele Noble equation of state for real gas is applied to calculate parameters of hydrogen in a tank, including the amount of stored mechanical (internal) energy similar to the Brode's model. The dimensionless starting shock is calculated in the model using the speed of sound in the real gas.

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

3.5.9.4   Choice of the model

When the tool is selected the screen with the choice should appear prompting to select the option.

Please select the option you would like to calculate:

☐ 1. Stand-alone tank location (on ground)   ☐ 2. Under-vehicle tank location   ☐ 3. Stand-alone tank location (air)

◉ a) Without combustion   ○ b) With combustion

Note: Example of the model choice is the Option(radio) Button. When checked the screen with appropriate input parameters should appear below, together with button to initiate calculation (choice of RUN, CALCULATE, START etc. to be uniform across the e-Laboratory).
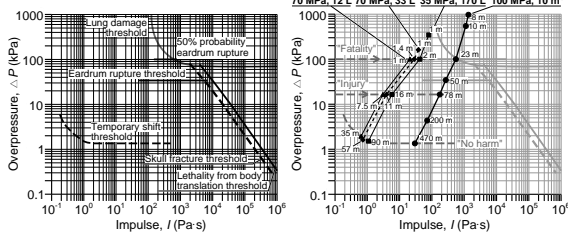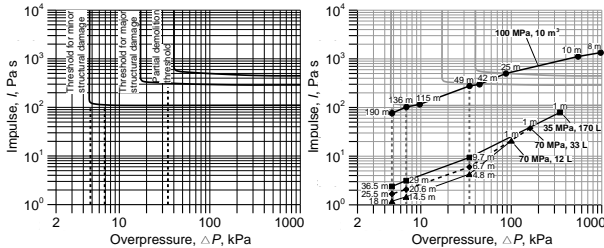
3.5.9.5   Input values

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Ambient pressure	p_s	101325	Pa	33700-107900	101325
Ambient temperature	T_s	293	K	240-350	293
Pressure in a tank	p_g	35000000	Pa	101325-100000000	35000000
Temperature in a tank	T_g	293	K	240-350	293
Tank volume	V	0.0724	m^3	0.001-10	0.0724
Mechanical energy constant	α	Based on option chosen in 7	ND	0-2	Based on option chosen
Chemical energy constant	β	Based on option chosen in 8	ND	0-1	Based on option chosen

3.5.9.6   Calculation procedure

	Constants		
1	Specific heat ratio of air	$\gamma_s = 1.4$	ND
2	Specific heat ratio of hydrogen	$\gamma_g = 1.39$	ND
3	Molecular mass of air	$M_a = 28.97$	kg/kmol
4	Molecular mass of hydrogen	$M_g = 2.016$	kg/kmol
5	Hydrogen co-volume constant	$b = 0.007691$	m^3/kg
6	Universal gas constant	$R = 8314.47$	J/(kmol·K)
7	Define alpha constant **NB: The user should be able to change default value of alpha**	**IF** option 1: alpha value for stand-alone tank $\alpha = 1.8$; **IF** option 2: alpha value for under-vehicle tank $\alpha = 0.12$	ND Limit:0-2

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		IF option 2: alpha value for under-vehicle tank $\alpha=1$	
8	Define beta constant **NB: The user should be able to change default value of betta**	**IF** option 1: stand-alone tank (ground) $\beta=0.052$; **IF** option 2: under-vehicle tank $\beta=0.09$ IF option 3: stand-alone tank (air) $\beta=0.052$; **IF** option 1a **OR** 2a **OR** 3a: $\beta=0$ (no combustion)	ND Limit:0-1
9	Hydrogen heat of combustion	$H_c=1.1993\times10^8$	J/kg
Calculation			
10	Density of air	$\rho_s=p_s M_a/RT_s$	kg/m³
11	Density of H2	$\rho_g=p_g M_g/RT_g$	kg/m³
12	Speed of sound air	$a_s = \sqrt{\gamma_s \dfrac{p_s}{\rho_s}}$	m/s
13	Speed of sound tank	$a_g = \sqrt{\gamma_g \dfrac{p_g}{\rho_g}}$	m/s
14	Mach number finding	$\dfrac{p_g}{p_s}=\left(1+\dfrac{2\gamma_s}{\gamma_s+1}\left(M_{sh}^2-1\right)\right)\Big/\left(1-\dfrac{\gamma_g-1}{\gamma_s+1}\cdot\dfrac{a_s}{a_g}\cdot\dfrac{M_{sh}^2-1}{M_{sh}}\right)^{\frac{2\gamma_g}{\gamma_g-1}}$ **Use** Algorithm of solution for the Mach number M_{sh}:	ND
15	Define non-dimensional starting shock	$\bar{P}_{st} = \left(\dfrac{2\gamma_s M_{sh}^2}{\gamma_s+1}-\dfrac{\gamma_s-1}{\gamma_s+1}\right)$	ND
16	Mass of stored gas in tank	$m_g=\rho_{greal}V$ where ρ_{greal} **is real gas EOS!** $\rho_{greal} = \dfrac{p_g}{p_g + R_{H2}\cdot T_g}$	kg
17	Find mechanical energy (for dimensionless distance equation)	$E_m = \dfrac{\left(p_g-p_s\right)\cdot\left(V-m_g b\right)}{\gamma_g-1}$	J
18	Find the radius of spherical tank	$r_v = \left(\dfrac{3V}{4\pi}\right)^{1/3}$	m
19	Dimensionless radius of spherical tank	$\bar{r}_v=r_v(p_s/E_m)^{1/3}$	ND
20	Using dimensionless starting shock eq.15 (Y-axis) and dimensionless sphere radius eq.19 (X-axis) find a point (in intersection) and build	**Use Algorithm of solution for dimensionless overpressure $\bar{P}$ as a function of $\bar{r}_v$:**	

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	a new curve (function $\bar{P}=f(\bar{r}_v)$) parallel to nearest existing curve. This will be new curve to find dimensionless overpressure.		
21	Define chemical energy of combusted gas	$E_{ch}=m_g\times H_c$	J
22	Define fireball radius	Calculate fireball stand-alone radius using fireball size tool description: $r_b=D_{SA}$	m
23	Use Algorithm of solution for the blast wave overpressure $\varDelta$P, impulse I, and distance r:		
24	Put distance points r on the graph with 2m step using overpressure and impulse to define hazard distance to human	Example	
25	Put distance points r on the graph with 2m step using overpressure and impulse to define hazard distance to building	Example	

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

Algorithm of solution for the Mach number M_{sh}:

$\Delta=0.1$ /* Δ Index (Required within 'If' loop) */

$i_{\Delta}=0$

$M_{sh}=1$ /* first guess for M_{sh}*/

$$LHS = \frac{p_g}{p_s}$$ /* Left hand side of equation */

$$RHS = \left(1+\frac{2\gamma_s}{\gamma_s+1}\left(M_{sh}^2-1\right)\right) \bigg/ \left(1-\frac{\gamma_g-1}{\gamma_s+1}\cdot\frac{a_s}{a_g}\cdot\frac{M_{sh}^2-1}{M_{sh}}\right)^{\frac{2\gamma_g}{\gamma_g-1}}$$ /* Right hand side of eq */
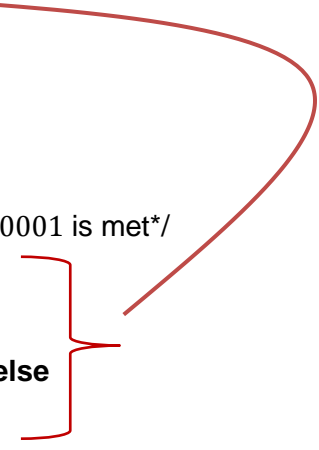
Loop:

WHILE   (LHS-RHS)/LHS≥0.00001   **DO**

/* This loop should continue until condition $\left|\frac{(LHS-RHS)}{LHS}\right| < 0.00001$ is met*/

If (RHS < LHS)   { $i_{\Delta}=0$; $M_{sh}=M_{sh}+\Delta$ } **else**

If (RHS > LHS and $i_{\Delta}=0$)   { $\Delta=\Delta/2$; $i_{\Delta}=1$; $M_{sh}=M_{sh}-\Delta$ } **else**

If (RHS > LHS and $i_{\Delta}=1$)   {$M_{sh}=M_{sh}-\Delta$}

/* Purpose of this loop is to iterate M_{sh} calculation until LHS = RHS (to specified accuracy)*/

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

Algorithm of solution for dimensionless overpressure $\bar{P}$ as a function of $\bar{r}_v$:

$$\bar{P}_{st} = \left(\frac{2\gamma_s M_{sh}^2}{\gamma_s + 1} - \frac{\gamma_s - 1}{\gamma_s + 1} \right)$$ /* dimensionless starting shock from point 15*/

$\bar{r}_v = r_v (p_s / \Delta E_m)^{1/3}$ /*dimensionless radius of spherical tank from point 19*/

/*Plot the graph with 11 curves using data from the excel file provided **Microsoft Excel 97-2003 Worksheet** */
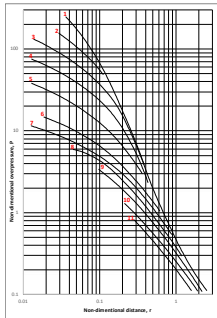
/*Graph should contain the point (r_v, P_{st}) represented by values obtained from 15 and 19*/

/*Message should prompt user to select the curves number between which the point is located from the dropdown lists. Message above the graph: "Please select the curve numbers from the dropdown list in between which the point is located Choose an item."/

/*When the curves are selected procedure to calculate new array for the curve located in between those selected preserving the aspect ratio as per point should be executed based on the data presented in an input file*/

Function new_Pr;

n=262 /*number of rows in the file containing the curves*/

m1= M1 /*first number from dropdown list selection representing corresponding column*/

m2= M2 /*second number from dropdown list selection representing corresponding column */

P=log₁₀(P_{st});

r=log₁₀(r_{rv}); /*taking logarithm since the graph is in log scale*/

Pr=array [1..n, 1..m] /*array of curves from the file representing matrix n x m = 262 x 12 see excel file*/

L=array[1..n, 1..2] /*array of difference between Pr[i,m2] and Pr[i, m1] */

Pr_new=array[**1..n+1, 1..n+1**] /* +1 due to adding of new point into array*/

begin

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

```
    for i = 1 to n do

/*find location of point (r,P) in array in between existing points and extrapolate new value for the P
from existing positions of i and i+1*/

    if Pr[i+1, m1] => r  and Pr[i, m1] <= r then

/*add new calculated element for P into array in between i and i+1 for each curve m1 and m2*/

Pr[i,m1]= Pr[i-1,m1]+((Pr[i]-Pr[i-1])(Pr[i+1,m1]-Pr[i-1,m1))/(Pr[i+1]-Pr[i-1]);

Pr[i,m2]= Pr[i-1,m2]+((Pr[i]-Pr[i-1])(Pr[i+1,m2]-Pr[i-1,m2))/(Pr[i+1]-Pr[i-1]);

/*Find distance l at this point between Pr[i,m1] and P*/

l=Pr[i,m1]-P

/*find coefficient of proportionality for new curve array lambda*/

λ=( Pr[i, m1] - Pr[i,m2])/ l

End


Begin

    for i = 1 to n+1 do /* +1 because of additional point added in previous step*/

/*Find the difference between Pr[i, m1] and Pr[i,m2]*/

L[i]= Pr[i,m2] - Pr[i, m1];

End


/*Calculation of new curve*/

Begin

For i=1 to n+1 do

Pr_new[i,m+1]= 10^(Pr[i,m1]+ λL);

end;
```

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

Algorithm of solution for the blast wave overpressure ΔP, impulse _I_, and distance _r_:

Initialise

r=2r$_v$ /* first guess for initial distance from the tank*/

r$_{sh}$=r   /*initial shock distance*/

Δ=0.1   /* Δ Index (Required within 'If' loop) */

i$_\Delta$=0

ΔP=4000   /* first guess for the overpressure*/

Mark 1

Begin

WHILE ΔP<=3000   **DO**

$$\bar{r}_P = r\left(\frac{p_s}{\alpha \cdot E_m + \beta \cdot \left(\frac{r_{sh}}{r_b}\right)^3 \cdot E_{ch}}\right)^{1/3}$$ /* Dimensionless distance*/

/*Find Dimensionless overpressure from newly defined curve **Pr_new** in **Algorithm of solution for dimensionless overpressure $\bar{P}$ as a function of $\bar{r}_v$:**

*/

/*find location of point (r,P) in array in between existing points and extrapolate new value for the P from existing positions of i and i+1*/

begin

  for i = 1 to n+1 **do**

    if Pr_new[i+1, m+1] => $\bar{r}_P$ **and** Pr_new[i, m+1] <= $\bar{r}_P$ **then**

/*add new calculated element for P_new into array in between i and i+1 increasing n respectively same as for calculation of impulse*/

Pr_new[i,1]= $\bar{r}_P$;

Pr_new[i,m+1]=Pr_new[i-1,m+1]+((Pr_new[i,1]-Pr_new[i-1,1])(Pr_new[i+1,m+1]-Pr_new[i-1,m+1]))/((Pr_new[i+1,1]-Pr_new[i-1,1]));

ΔP=Pr_new[i,m+1]*p_s /*Dimensionalise found in figure dimensionless overpressure*/

$$\bar{r}_i = r\left(\frac{p_s}{\alpha \cdot E_m}\right)^{1/3}$$ /*Find dimensionless distance r_I for finding impulse */

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

$$I = \frac{\bar{I} \cdot \left[(\alpha \cdot E_m)^{1/3} \, p_s^{2/3} \right]}{a_s}$$ /*Dimensionalise impulse*/

End;

> ***Loop: /*Calculate new value for r */***
>
> **WHILE** $(r_b - r_{sh})/r_b \leq 0.001$ **DO**
>
> /* This loop should continue until condition $\left| \frac{(r_{sh} - r_b)}{r_b} \right| < 0.001$ is met*/
>
> **If** $(r_{sh} < r_b)$ { iΔ=0; r=r+Δ; r$_{sh}$=r;} **ELSE**
>
> **If** $(r_{sh} > r_b$ and iΔ=0)   { Δ=Δ/2; iΔ=1; r=r-Δ; r$_{sh}$=r;} **ELSE**
>
> **If** $(r_{sh} > r_b$ and iΔ=1)   { r=r-Δ; r$_{sh}$=r;}
>
> **END**

/* Purpose of this loop is to iterate r_{sh} calculation until $r_{sh} = r_b$ (to specified accuracy)*/

> **IF** $(r_{sh}$-$r_b)/r_b$>0.001 **TRUE** {r$_{sh}$=r$_b$};
>
> r=r+0.1

Write output to file:

> 1) Distance, r [m]
>
> 2) Overpressure, ΔP [Pa]
>
> 3) Impulse, I [Pa·s]

/*go to Mark 1*/
END;
Note to programmer:
Please include these column headings in produced 'Excel' output file.

Algorithm of solution for non-dimensional impulse $\bar{I}$:

rI_array=[1..n, 2]   /*array of known dimensionless distances $\bar{r_I}$ and known dimensionless

Microsoft Excel
97-2003 Worksheet

impulses $\bar{I}$, input from file */

$$\bar{r_i} = r\left(\frac{p_s}{\alpha \cdot E_m}\right)^{1/3}$$ /* As per point 25 above*/

n=419; /*as per excel*/

Function Search_I$_n$;

begin

  for i = 1 to n **do**

    if rI_array[i+1,1..2] => $\bar{r_I}$ **and** rI_array[I,1] <= $\bar{r_I}$ then

I$_n$=rI_array[i-1,2]+((rI_array[i,1]-rI_array[i-1,1])(rI_array[i+1,2]-rI_array[i-1,2]))/((rI_array[i+1,1]-rI_array[i-1,1]));

    return I$_n$

$$\bar{I}_n = \bar{I}_{n-1} + \frac{(\bar{r}_n - \bar{r}_{n-1})(\bar{I}_{n+1} - \bar{I}_{n-1})}{(\bar{r}_{n+1} - \bar{r}_{n-1})}$$

end;

3.5.10 Effect of buoyancy on hazard distance for unignited releases (UU)

3.5.10.1 Introduction

This tool shows effect of the hazard distance decrease due to buoyancy in unignited releases. It allows to calculate the distance from the release nozzle to the concentration at which release changes from momentum-controlled regime to buoyancy–controlled, as well as the hazard distance to concentration of 4% by volume of hydrogen.

All jets can be divided into three types based on the effect of buoyancy. These jet types are shown schematically in Figure 19 for a horizontal jet (Molkov, 2012). Fully momentum-controlled jets are not affected by buoyancy. Fully buoyancy-controlled jets are quickly diverted from the horizontal to vertical flow direction. Third type of jets that can be called transitional have momentum-dominated part closer to the nozzle and buoyancy-controlled flow further downstream when jet velocity drops and jet diameter increases. For hydrogen safety engineering it is important to know when this transition takes place. This has direct implication on the separation distance and thus safety and costs of hydrogen system or infrastructure.

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]
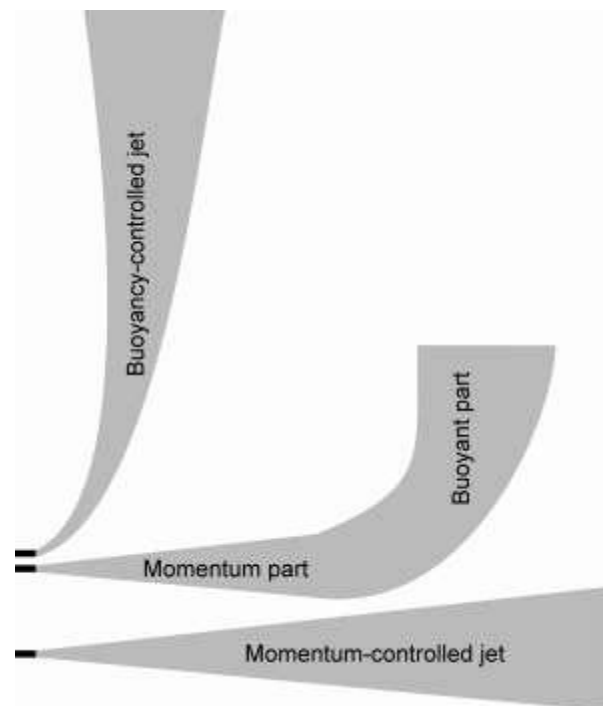
Figure 19 - Fully momentum-controlled jet (bottom), transitional jet (middle), and fully buoyancy-controlled jet.

The engineering tool presented here to qualify a hydrogen jet (both expanded and under-expanded) or its part as momentum-controlled, and the rest of the jet downstream as buoyancy controlled, is based on the work by (Shevyakov & Savelyeva, 2004; Shevyakov, Tomilin, & Kondrashkov, 1980) that was carried out with expanded jets only. Figure 5-8 shows in logarithmic coordinates the dependence of the distance to nozzle diameter ratio x/D (ordinate) for particular concentration of hydrogen in air on the Froude number (abscissa) in its classical form $Fr = \frac{U^2}{gD}$, where U is the velocity at the nozzle exit (notional nozzle exit for under-expanded jets) in m/s, g is the gravitational acceleration (standard acceleration of gravity on Earth is 9.80665 m/s2), and D is the nozzle diameter (notional nozzle exit diameter for under-expanded jet) in meters. For under-expanded jets in Figure 20 the notional nozzle exit diameter and velocity at the notional nozzle exit were calculated by the under-expanded jet theory (V. Molkov et al., 2009). Both expanded and under-expanded jets obey the same functional dependence with accuracy 20% acceptable for engineering applications.

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]
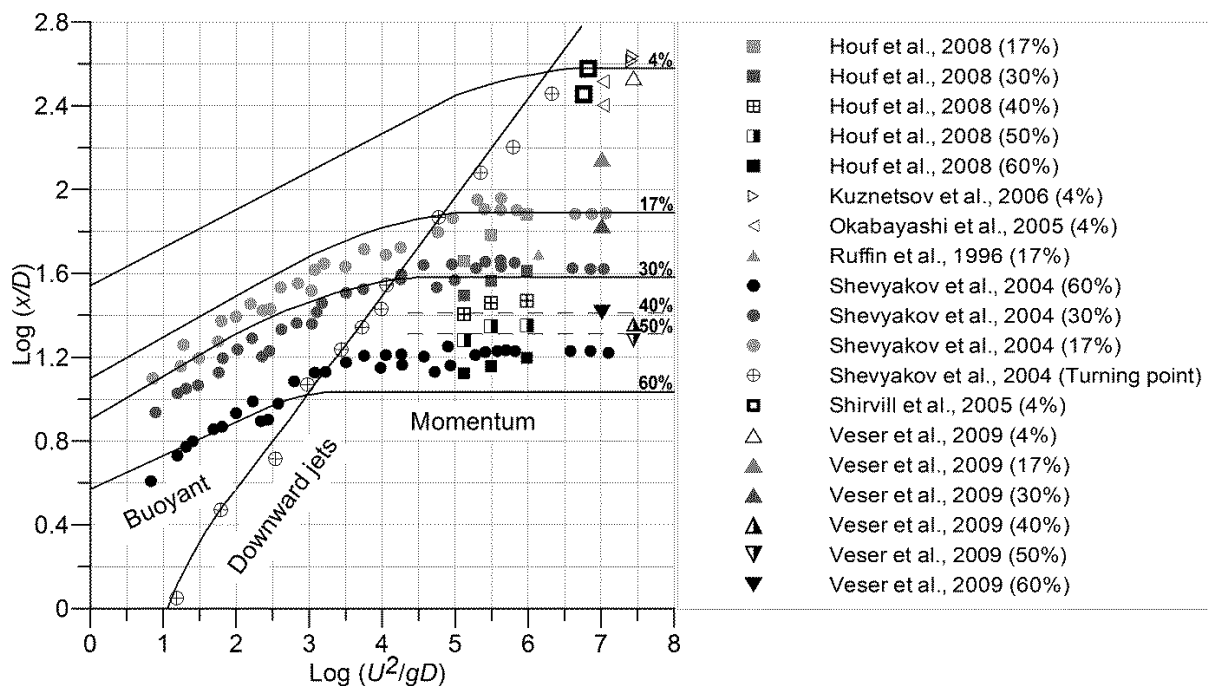
Figure 20 - The dependence of the distance to nozzle diameter ratio for particular concentration of hydrogen in air on the Froude number.

Five theoretical curves (solid lines) by (Shevyakov & Savelyeva, 2004; Shevyakov et al., 1980), experimental data for expanded jets (Shevyakov & Savelyeva, 2004; Shevyakov et al., 1980), and data of other researchers for under-expanded jets are shown in Figure 20. Practically all under-expanded jets in hydrogen incidents/accidents will be in the momentum-controlled regime as follows from available tests applied to validate the correlation in Figure 20. Four of five theoretical curves in the graph are related to hydrogen concentrations of 4%, 17%, 30%, and 60% by volume respectively. Each of these four curves has an ascending buoyant part and a momentum "plateau" part.

It is important to stress that the Froude number at transition from the buoyant part of the curve to the momentum part depends on the concentration of hydrogen under consideration. For example, at axial concentration of hydrogen 60% by volume the jet stays in momentum-controlled regime until Log (Fr)>3.5, while for the jet to be in the momentum-controlled regime at axial location where hydrogen concentration drops to 4% by volume (LFL) the nozzle exit Froude number has to be much higher, i.e. Log (Fr)>6.5 (three orders of magnitude higher).

The fifth curve in Figure 20 "Downward jets" is of special interest for hydrogen safety engineering. It gives for a jet directed vertically downward a dimensionless distance from the nozzle to the turning point, where the jet changes direction of flow from downward to upward. To calculate the distance to turning point only knowledge of the Froude number at the nozzle (notional nozzle) is required. The fifth curve intersects each of the four other curves in Figure 20 in the region of transition from momentum-dominated to buoyancy-controlled flow as expected.

The following sequence is applied in use of the correlation in Figure 20. Firstly, the nozzle exit Froude number is calculated and its logarithm. The under-expanded theory is applied to calculate the notional nozzle exit diameter and the velocity in the notional nozzle exit when applicable. Then, a vertical line is drawn upward from a point on the abscissa axis equal to the calculated Froude

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

number logarithm. The intersection of this vertical line with the line marked "Downward jets" on the graph indicates the concentration above which the jet is momentum-dominated and below which the jet is buoyancy-controlled.

For example, if a jet exit Froude number is Log (Fr)=4.25 (intersection of the vertical line with line "Downward jets" is at location of the theoretical curve corresponding to 30% by volume of hydrogen) then the jet is in momentum-dominated regime while the concentration in the jet is above 30% by volume and it becomes buoyant when the concentration on the jet axis is below 30% (further downstream of the axial concentration of 30% by volume).

This technique is quite simple to apply and at the same time can be very useful to develop cost-effective hydrogen safety solutions. For instance, the separation distance for a horizontal jet release can be essentially reduced as only a length of the momentum-dominated part of the jet can be taken as an indication of the separation distance rather than aggregated (both momentum- and buoyancy-controlled parts of the jet) distance to 4% by volume (LFL).

3.5.10.2 Nomenclature

Parameter	Symbol	Unit
Hydrogen pressure in reservoir	p_1	Pa
Hydrogen temperature in reservoir	T_1	K
Orifice diameter	D	m
Ambient pressure	p_4	Pa
Froude number	$Fr = \dfrac{V_3^2}{gD_3}$	ND
Velocity at the notional nozzle	V_3	m/s
Gravity acceleration	g=9.80665	m^2/s^2
Notional nozzle diameter	D_3	m
Logarithm of Froude number	Log_{Fr}	ND
Axial distance to nozzle ratio	X_over_D	-
Logarithm of axial distance to nozzle ratio	$Log_{X/D}$	-
Axial distance to concentration	X	m
Concentration at which release becomes buoyant	C_B	%

3.5.10.3 Input values

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Hydrogen pressure in reservoir	p_1	20500000	Pa	190000-100000000	20500000
Hydrogen temperature in reservoir	T_1	288	K	230-330	288
Orifice diameter	D	0.0095	m	0.0001-0.1	0.0095
Ambient pressure	p_4	101325	Pa	33700-107900	101325

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

3.5.10.4 Calculation procedure

Use input values calculate velocity in the notional nozzle, V_3, and its diameter D_3, as per methodology provided in Section 3.5.1"Jet Parameters Tool".

Two options can be calculated:

Option 1: For horizontal release the distance and concentration at which release becomes buoyant and hazard distance to 4% v/v along the jet central line.

Option 2: For vertical downward release the distance and concentration at which flow start to go up due to buoyancy.

When the tool is selected the screen with the choice should appear prompting to select the option.

Please choose the option you want to calculate:

○ 1. The distance and concentration at which release becomes buoyant and hazard distance for horizontal release

○ 2. The distance from the nozzle to the turning point, where the jet changes direction and concentration for vertical release

---

Note: Example of the model choice is the Option(radio) Button. When checked the screen with appropriate input parameters should appear below, together with button to initiate calculation (choice of RUN, CALCULATE, START etc. to be uniform across the e-Laboratory).

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

START

Calculating logarithm of Froude number: $Log_{Fr} = \log(Fr) = \log(\frac{V_3^2}{gD_3})$

Finding distance X (m) to concentration at which release turns into buoyant regime:

IF Log_{Fr} > 2.0034495 **THEN** $Log_{X/D}$ = 0.4628 Log_{Fr} -0.3349

 ELSE IF 1.05 <= $LogFr$ < 2.0034495 **THEN**

 $Log_{X/D}$=-0.2313 Log_{Fr}^4+1.447 Log_{Fr}^3-3.548 Log_{Fr}^2+4.5974 Log_{Fr}–2.3087

X_over_D=10^$Log_{X/D}$

X=X_over_D * D_3

Finding the concentration C_B (%) at which release switches to buoyant regime:

IF 1.89<$Log_{X/D}$<=2.57 **THEN** C_B=(17-(13*($Log_{X/D}$ -1.89))/(2.57-1.89) **ELSE**

IF 1.5837<$Log_{X/D}$<=1.89 **THEN** C_B =(30-(13*($Log_{X/D}$-1.5837))/(1.89-1.5837) **ELSE**

IF 1.4135< $Log_{X/D}$ <=1.5837 **THEN** C_B =(40-(10*($Log_{X/D}$-1.4135))/(1.5837-1.4135) **ELSE**

IF 1.3115< $Log_{X/D}$ <=1.4135 **THEN** C_B =(50-(10*($Log_{X/D}$-1.3115))/(1.4135-1.3115) **ELSE**

IF 1.03148<$Log_{X/D}$<=1.3115 **THEN** C_B =(60-(10*($Log_{X/D}$-1.0315))/(1.3115-1.03115) **ELSE**

IF $Log_{X/D}$ >2.57) **THEN Show Message:** «Release is fully momentum and becomes buoyant beyond flammable concentration of 4% v/v at distance "X"» **ELSE**

IF $Log_{X/D}$ <1.03148 **THEN Show Message:** «Release becomes buoyant at concentration above 60% v/v at distance "X"»

Finding distance X (m) to 4% concentration at buoyant regime:

IF 0<= Log_{Fr} < 5 **THEN** $Log_{X/D}$=0.01814 Log_{Fr}+1.5434 **ELSE**

 IF 5<= Log_{Fr} <= 6.27 $Log_{X/D}$= -0.0327 Log_{Fr}^2 + 0.4581 Log_{Fr} + 0.975 **ELSE**

 IF 6.27< Log_{Fr} **THEN Show Message:** «Release is fully momentum and becomes buoyant beyond flammable concentration of 4% v/v at distance "X"»

Finding distances to concentrations at momentum regime:

$X_{60\%}$=10^{1.03148}D_3; $X_{50\%}$=10^{1.3115}D_3; $X_{40\%}$= 10^{1.4135}D_3; $X_{30\%}$= 10^{1.5837}D_3; $X_{17\%}$=10^{1.89}D_3; $X_{4\%}$=10^{2.57}D_3;

Writing output values:

IF Option 1 THEN

IF $X_{4\%}$ <X **Write values** $X_{4\%}$ - $X_{60\%}$ **AND** Message: «Release is fully momentum and becomes buoyant beyond flammable concentration of 4% v/v at distance "X"»

IF X< $X_{4\%}$ **Write values** X **AND** $X_{4\%}$ - $X_{60\%}$

IF Option 2 THEN

Message "The distance from the nozzle to the turning point is" X "concentration for vertical release is " C_B

EXIT

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

3.5.10.5 Output values

Option 1:

Parameter name	Symbol	Output value	Unit
Axial distance from nozzle to C_B% by vol. H_2 where release becomes buoyant	X		m
Axial distance from nozzle to 4% by vol. H_2	$X_{4\%}$		m
Axial distance from nozzle to 17% by vol. H_2	$X_{17\%}$		m
Axial distance from nozzle to 30% by vol. H_2	$X_{30\%}$		m
Axial distance from nozzle to 40% by vol. H_2	$X_{40\%}$		m
Axial distance from nozzle to 50% by vol. H_2	$X_{50\%}$		m
Axial distance from nozzle to 60% by vol. H_2	$X_{60\%}$		m

Option 2:

Show message "The distance from the nozzle to the turning point is" X "concentration for vertical release is " C_B**"**

Note to programmer: An example of the interactive graph is shown in Figure 21 below. The similar graph if possible should be drawn based on calculation results, where the release is shown with concentration contours at appropriate distances. Semi-transparent contours of the concentration and distance at which the release becomes buoyant should be drawn and shown in the legend.

Figure 21 - Interactive graph example

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

3.5.11 Pressure peaking phenomenon for ignited releases (UU)
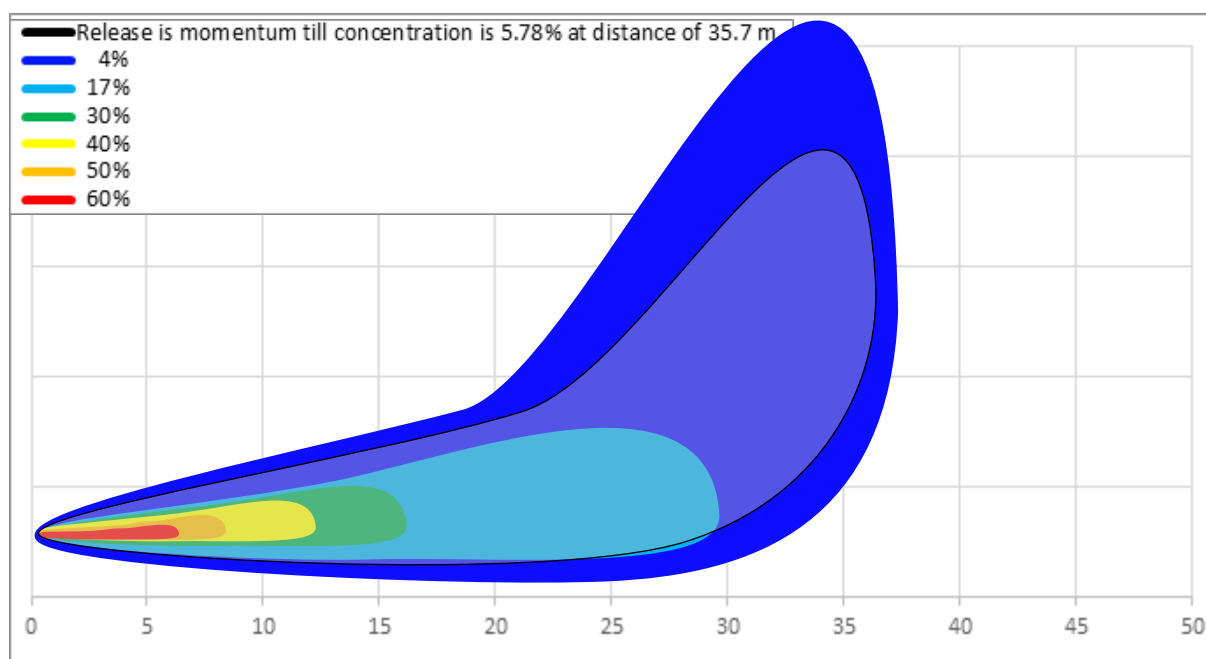
The tool description for ignited releases is based on the methodology for un-ignited and included into section 3.5.5

3.5.12 Upper limit of hydrogen inventory in closed space (UU)

3.5.12.1 Introduction

A thermodynamic model was developed (2014) to predict maximum mass of hydrogen, which may be allowed to be released in an enclosure without causing destructive overpressure in case of its combustion. The model presumes that enclosure is partially filled with air, volume fraction of air is x_a, and partially – with unburnt hydrogen-air mixture, volume fraction x_u, initial pressure p_0. If this hydrogen-air mixture is burnt in a sealed enclosure, the solution for resulting absolute pressure p_2 may be found from the following equation:

$$p_2 = x_u p_{b1} \left(\frac{p_2}{p_{b1}} \right)^{\frac{\gamma_b - 1}{\gamma_b}} + x_a p_0 \left(\frac{p_2}{p_0} \right)^{\frac{\gamma_a - 1}{\gamma_a}} ,$$

where p_{b1} – absolute pressure for combustion of unburnt hydrogen-air mixture in constant volume (as though after combustion it occupied the same fraction of the enclosure x_u). The given above model was validated against experiments by Stamps et al. (Stamps, Slezak, & Tieszen, 2006) and gave a good agreement with experimental data.

The transcendental equation above, was solved for overpressure in a sealed enclosure equal (p_2-p_0)=10kPa, which corresponds to the typical threshold value causing structural damage to civil structures. The range of studied hydrogen vol. fractions is 4-20%. Resulting solution is given in the Table 11. The table presents hydrogen vol. fraction in unburnt mixture x_{uH2}, volume fraction the unburnt mixture in the entire enclosure x_u, and "overall" volume fraction of hydrogen contained within flammability limits in entire enclosure $x_{H2} = x_{uH2} \cdot x_u$, which is a measure of hydrogen allowable to be safely released. The minimum for safely released hydrogen fraction is $x_{H2} = 0.314\%$ of total enclosure volume, assuming that all released hydrogen is at low flammability limit 4%.

Table 11. Solution of equation (3.1) for (p2-p0)=10 kPa.

x_{uH2}	x_u	$x_{H2} = x_{uH2} \cdot x_u$
0.04	0.0786	$3.14 \cdot 10^{-3}$
0.08	0.0474	$3.79 \cdot 10^{-3}$
0.12	0.0355	$4.26 \cdot 10^{-3}$
0.16	0.0293	$4.69 \cdot 10^{-3}$
0.20	0.0253	$5.06 \cdot 10^{-3}$

The maximum hydrogen inventory for non-destructive deflagration in enclosure may be calculated based on the conservative values of overall hydrogen fraction in enclosure 0.314% (vol.).

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

3.5.12.2 Nomenclature

Parameter	Symbol	Unit
Universal gas constant	$R=8314$	J/(kmol K)
Molecular mass of H2	$M_{H2}=2.016$	kg/kmol
Molecular mass of air	$M_{air}=29$	kg/kmol
Molecular mass of H2O	$M_{H2O}=18$	kg/kmol
Molecular mass of O2	$M_{O2}=32$	kg/kmol
Molecular mass of N2	$M_{N2}=28$	kg/kmol
Molecular mass of unburnt mixture	M_U	kg/kmol
Molecular mass of burnt mixture	M_b	kg/kmol
Density of hydrogen	ρ_{H2}	kg/m^3
Adiabatic index of unburnt mixture	$G_U=1.4$	ND
Adiabatic index of burnt mixture	G_b	ND
Adiabatic index H2O	G_{H2O}	ND
Adiabatic index O2	G_{O2}	ND
Adiabatic index N2	G_{N2}	ND
Allowable volume fraction of H2	X_{H2}	ND
Volume fraction of H2-air mixture in enclosure	X_U	ND
Volume fraction of air in H2-air mixture in enclosure	X_{air}	ND
Volume fraction of H2 in H2-air mixture	X_{U_H2}	ND
Volume fraction of air in unburnt mixture	X_{U_air}	ND
Initial temperature in enclosure	T_0	K
Assumed burnt temperature	T_{b1}	K
Burnt mixture temperature for V-Const combustion	Tv_{b1}	K
Burnt mixture pressure for V=Const combustion	p_{b1}	Pa
Initial pressure in enclosure	p_0	Pa
Absolute pressure in enclosure	p_2	Pa
Overpressure in enclosure	p_{2g}	Pa
Volume fraction of H2O	X_{H2O}	ND
Volume fraction of O2	X_{O2}	ND
Volume fraction of N2	X_{N2}	ND
Mass fraction of H2O	Y_{H2O}	ND
Mass fraction of O2	Y_{O2}	ND
Mass fraction of N2	Y_{N2}	ND
Specific heat of H2O	Cp_{H2O}	J/kg/K
Specific heat of O2	Cp_{O2}	J/kg/K
Specific heat of N2	Cp_{N2}	J/kg/K
Specific heat of combustion products at p=Const	Cp_b	J/kg/K
Specific heat of combustion products at V=Const	Cv_b	J/kg/K
Heat of reaction of H2	H_C	J/mol
Mass of products as per reaction	m_b	kg
Allowable mass of H2	m_{H2}	kg
Heat of reaction of products	h_C	J/kg

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Enclosure volume	V	m^3

3.5.12.3 Choice of the model option

When the tool is selected the screen with the choice should appear prompting to select the option.

> **Please choose the option you want to calculate:**
>
> ○ 1. Calculate inventory mass for the given overpressure and enclosure volume
>
> ○ 2. Calculate volume of enclosure for the given overpressure and inventory mass

Note: Example of the model choice is the Option(radio) Button. When checked the screen with appropriate input parameters should appear below, together with button to initiate calculation (choice of RUN, CALCULATE, START etc. to be uniform across the e-Laboratory).

3.5.12.4 Input values

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Initial temperature in enclosure	T_0	293	K		
Initial pressure in enclosure	p_0	101325	Pa		
Overpressure in enclosure	p_{2g}	10000	Pa		
Enclosure volume (Option 1)	V	1	m^3		
Mass of H2 (Option 2)	m_{H2}	0.000231	kg		

Note: Whichever option chosen the other field should go blank on the screen of input values.

3.5.12.5 Calculation procedure

Input parameters from user

Solve Eq. 1-33 to find allovable mass of H2 when Option 1 chosen

Solve Eq. 1-32 and 34 to find enclosure volume when Option 2 chosen
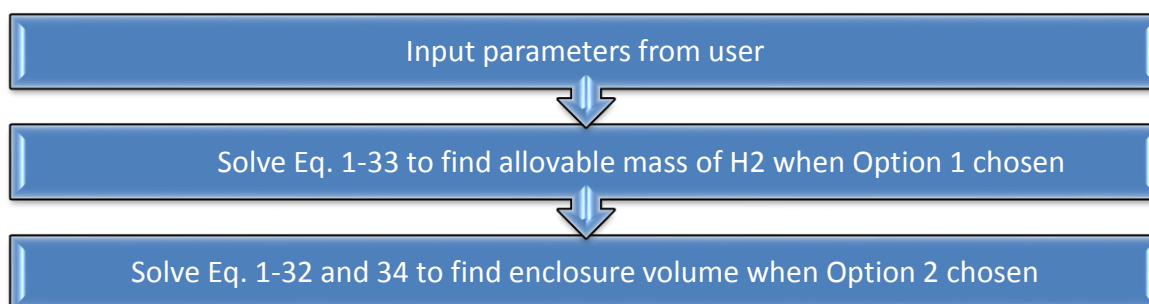
Constants		
1	Universal gas constant	$R=8314$	J/(kmol K)
2	Molecular mass of H2	$M_{H2}=2.016$	kg/kmol
3	Molecular mass of air	$M_{air}=29$	kg/kmol
4	Molecular mass of H2O	$M_{H2O}=18$	kg/kmol
5	Molecular mass of O2	$M_{O2}=32$	kg/kmol
6	Molecular mass of N2	$M_{N2}=28$	kg/kmol
	Heat of reaction of H2	$H_C=-244000$	J/mol

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	Calculation of unburnt mixture composition and properties (state "0")		
7	Adiabatic index of unburnt mixture	$G_U=1.4$	ND
8	Volume fraction of H2 in H2-air mixture	$X_{U\_H2}=0.04$	ND
9	Volume fraction of air in unburnt mixture	$X_{U\_air}=1- X_{U\_H2}$	ND
10	Molecular mass of unburnt mixture	$M_U= M_{air} \times X_{U\_air}+ M_{H2} \times X_{U\_H2}$	kg/kmol
	Calculation of burnt mixture composition and properties (state "1")		
11	Volume fraction of H2O	$X_{H2O}= X_{U\_H2}/(1-0.5 \times X_{U\_H2})$	ND
12	Volume fraction of O2	$X_{O2}=(0.21-0.71 \times X_{U\_H2})/(1-0.5 \times X_{U\_H2})$	ND
13	Volume fraction of N2	$X_{N2}=(0.79*(1-X_{U\_H2}))/(1-0.5 \times X_{U\_H2})$	ND
14	Molecular mass of burnt mixture	$M_b= X_{H2O} \times M_{H2O}+ X_{O2} \times M_{O2}+ X_{N2} \times M_{N2}$	kg/kmol
15	Mass fraction of H2O	$Y_{H2O}= X_{H2O} \times M_{H2O}/M_b$	ND
16	Mass fraction of O2	$Y_{O2}= X_{O2} \times M_{O2}/M_b$	ND
17	Mass fraction of N2	$Y_{N2}= X_{N2} \times M_{N2}/M_b$	ND
18	Initial guess (assumed burnt temperature)	$T_{b1}= T_0$	K
19	Specific heat of H2O	**IF $T_{b1}<1000$ THEN** $Cp_{H2O}=1563.077+1.603755 \times T_{b1}-0.002932784 \times T_{b1}^2+0.000003216101 \times T_{b1}^3-0.000000001156827 \times T_{b1}^4$ **ELSE** $Cp_{H2O}=1233.234+1.410523 \times T_{b1}-0.0004029141 \times T_{b1}^2+0.00000005542772 \times T_{b1}^3-0.000000000002939824 \times T_{b1}^4$	J/kg/K
20	Specific heat of O2	**IF $T_{b1}<1000$ THEN** $Cp_{O2}=834.8265+0.292958 \times T_{b1}-0.0001495637* \times T_{b1}^2+0.0000003413885 \times T_{b1}^3-0.0000000002278358 \times T_{b1}^4$ **ELSE** $Cp_{O2}=960.7523+0.1594126 \times T_{b1}-0.00003270885 \times T_{b1}^2+0.000000004612765 \times T_{b1}^3-0.0000000000002952832 \times T_{b1}^4$	J/kg/K
21	Specific heat of N2	**IF $T_{b1}<1000$ THEN** $Cp_{N2}=979.043+0.4179639 \times T_{b1}-0.001176279 \times T_{b1}^2+0.000001674394 \times T_{b1}^3-0.0000000007256297 \times T_{b1}^4$ **ELSE** $Cp_{N2}=868.6229+0.4416295 \times T_{b1}-0.000168273 \times T_{b1}^2+0.00000002996788 \times T_{b1}^3-0.000000000002004386 \times T_{b1}^4$	J/kg/K
22	Specific heat of combustion products at p=Const	$Cp_b= Y_{H2O} \times Cp_{H2O}+Y_{O2} \times Cp_{O2}+Y_{N2} \times Cp_{N2}$	J/kg/K
23	Specific heat of combustion products at V=Const	$Cv_b= Cp_b-R/ M_b$	J/kg/K

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24	Adiabatic index of burnt mixture	$G_b = Cp_b/Cv_b$	ND
Calculation of pressure and temperature at state "1"				
25	Mass of products as per reaction	$m_b = (X_{U\_H2} \times 18 + (0.21 - 0.71 \times X_{U\_H2}) \times 32 + (1 - X_{U\_H2}) \times 0.79 \times 28) \times 0.001$	kg
26	Heat of reaction of products	$h_C = X_{U\_H2} \times H_C/m_b$	J/kg
27	Burnt mixture temperature for V-Const combustion	$Tv_{b1} = (T_0 \times (Cp_b - R/M_U) - h_C)/(Cp_b - R/M_b)$	K
28	Tb1 update	**IF** $abs(Tv_{b1} - T_{b1}) < 0.01$ **THEN proceed to** 29 **ELSE** $Tb1 = Tvb1$ **go to** 19	ND
29	Burnt mixture pressure for V=Const combustion	$p_{b1} = p_0 \times M_U/M_b \times Tv_{b1}/T_0$	Pa
Calculation of pressure and mass of H2 at state "2"				
30	Absolute pressure in enclosure	$p_2 = p_{2g} + p_0$	Pa
31	Volume fraction of H2-air mixture in enclosure	$$X_U = \frac{p_0\left(\dfrac{p_2}{p_0}\right)^{\frac{G_U-1}{G_U}} - p_2}{p_0\left(\dfrac{p_2}{p_0}\right)^{\frac{G_U-1}{G_U}} - p_{b1}\left(\dfrac{p_2}{p_{b1}}\right)^{\frac{G_b-1}{G_b}}}$$	ND
32	Allowable volume fraction of H2	$X_{h2} = X_U \times X_{U\_H2}$	ND
33	Density of hydrogen	$\rho_{H2} = (M_{H2} \times p_0)/(R \times T_0)$	kg/m^3
34	Allowable mass of H2: (Option 1)	$m_{H2} = X_{h2} \times \rho_{H2} \times V$	kg
35	Volume of enclosure for the given mass: (Option 2)	$V = m_{H2}/(X_{h2} \times \rho_{H2})$	

Note: Appropriate option should be calculated based on the chosen one.

3.5.12.6 Output values

Parameter name	Symbol	Output value	Unit
Initial temperature in enclosure	T_0	293	K
Initial pressure in enclosure	p_0	101325	Pa
Enclosure volume	V	1	m^3
Overpressure in enclosure	p_{2g}	10000	Pa
Allowable mass of H2 (Option 1)	m_{H2}	0.000231	Kg
Volume of the enclosure (Option 2)	V	1	m^3

Note: Whichever option chosen the other field should go blank on the screen of output values.

3.5.13 Mitigation of localised non-uniform deflagration by venting technique (UU)

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

3.5.13.1 Introduction

Note: Model description should appear upon pressing the appropriate button on the home screen of the tool.

The tool allows for:

- Calculate vent area required to reduce deflagration overpressure to a given level
- Calculate an overpressure for a vent of known area.

Figure 22a shows a schematic physical layout for localised mixture deflagration in a vented enclosure at initial moment: a layer of flammable fuel-air mixture is located under the ceiling of the enclosure. Figure 22b demonstrates a conceptual calculation scheme corresponding to the same arrangement and used for the model (Makarov et al., 2018a) development: the flammable mixture contains fuel of mass m_f occupying volume V_f, and air with mass m'_{air} occupying volume V'_{air}. Total mass of air in the enclosure, including air in flammable mixture, is m_{air} and volume is V_{air}. It makes volumetric fraction of fuel in the flammable mixture $\varphi = V_f / (V_f + V'_{air})$, and fraction of flammable mixture in the vessel volume $\Phi = (V_f + V'_{air}) / (V_f + V_{air})$.
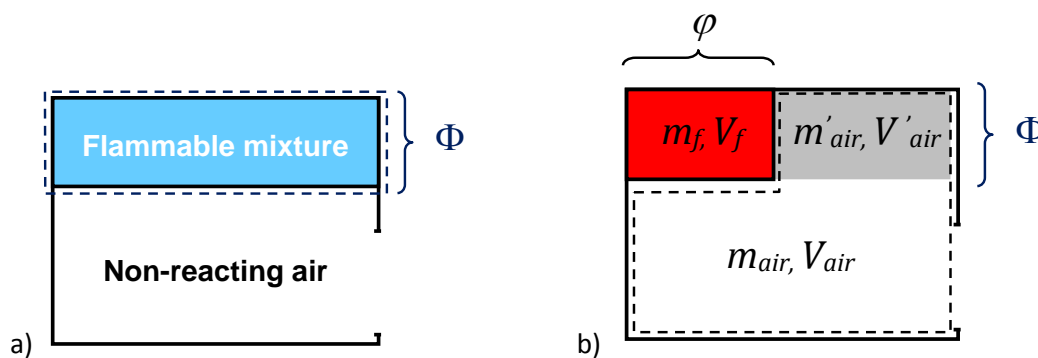
Figure 22. Localised flammable mixture in a vented enclosure: a) layout, b) calculation scheme. (Makarov et al., 2018a)

3.5.13.2 Nomenclature and model constants

Table 12 – Nomenclature and model constants.

Parameter	Symbol	Unit
Enclosure volume	$V = H_E x W_E x L_E$	m³
Enclosure height	H_E	m
Enclosure width	W_E	m
Enclosure length	L_E	m
Maximum absolute pressure	P_{max}	Pa
Vent area	F	m²
Initial absolute pressure	P_i	Pa
RMS fluctuating velocity of initial turbulence	u'	m/s
Dimensionless reduced pressure	$\Delta\pi$	ND
Turbulent Bradley number	Br_t	ND
Factor to account for presence of obstacles in enclosure	Ξ_O	ND

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

Initial burning velocity	S_{ui}	m/s
Expansion coefficient	E_i	ND
Empirical coefficient	ψ	ND
Hydrogen volume fraction	X_{H2}	ND
Air volume fraction	$X_{air}=1-X_{H2}$	ND
Initial temperature	T_{ui}	K
Internal surface area of an enclosure	A_{EW}	m^3
Area of the sphere of the same volume as enclosure	A_S	m^3
Speed of sound	c_{iu}	m/s
Pi number	$\pi_0=3.1415...$	ND
Specific heat ratio	$\gamma_u=1.41$	ND
Universal gas constant	$R_g=8314.5$	J/(kmol K)
Radius of equivalent volume sphere	R	m
Characteristic flame radius	R_0	m
Theoretical maximum of wrinkling factor due to turbulence generated by the flame front itself	Ξ_K^{max}	ND
Wrinkling factor due to turbulence generated by the flame front itself	Ξ_K	ND
Maximum leading point wrinkling factor	Ξ_{LP}^{max}	ND
Leading point flame wrinkling factor	Ξ_{LP}	ND
Internal surface area of an enclosure	A_{EW}	m^2
Aspect ratio wrinkling factor	Ξ_{AR}	ND
Fractal wrinkling factor	Ξ_{FR}	ND
Factor to account for the presence of obstacles in the enclosure	Ξ_O	ND
Temperature index	m_0	ND
Laminar flame velocity	S_u	m/s
SGS wrinked flame burning velocity	S_u^{SGS}	m/s
Turbulent burning velocity	S_t	m/s
Wrinkling factor to account for initial turbulence	$\Xi_{u'}$	ND
Deflagration-outflow interaction number	χ/μ	ND
Speed of sound	c_{ui}	m/s
Molecular mass of mixture	M_{ui}	kg/kmol
H$_2$ molecular mass (fuel)	$M_f=2.016$	kg/kmol
Air molecular mass	$M_{air}=28.97$	kg/kmol
Fractal dimension	$D=2.33$	ND

3.5.13.3 Choice of the option to calculate

When the tool is selected, the screen with the choice should appear prompting to select the option.

Please select the option you would like to calculate and methodology:

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

☐ 1. Vent area required to reduce deflagration pressure to a given level

☐ 2. Estimate an overpressure for a vent of known size

⚪ a) Best fit   ⚪ b) Concervative

3.5.13.4 Option 1: Calculation of vent area to reduce deflagration pressure to a given level

3.5.13.4.1   Input values

Please provide values for calculation and select the methodology.

Table 13 – Input values.

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Maximum absolute pressure	P_{max}	139828.5	Pa	101325 - 209225	
Initial absolute pressure in enclosure	P_i	101325	Pa	33700 - 107900	101325
Hydrogen volume fraction in localised mixture	X_{H2}	0.123	ND	0.04 - 0.34	
Localised mixture volume fraction in enclosure	Φ	0.22	ND	0.01-1	
RMS fluctuating velocity of initial turbulence	u'	1	m/s	≥0	0
Factor to account for presence of obstacles in enclosure	Ξ_O	1	ND	≥1	1
Initial temperature	T_{ui}	298	K	233 - 313	
Enclosure height	H_E	2.5	m		
Enclosure width	W_E	2.5	m		
Enclosure length	L_E	5	m		

Note:

- When the option is selected, the screen with input values as in Table 3 should appear prompting to input values for calculation.
- If the input maximum absolute pressure is above the limits a warning message should appear that the model was not validated above specified value but allowing to calculate with higher values.
- The default value of factor to account for presence of obstacles in enclosure is 1 means absence of obstacles. The model was validated against experiments without obstacles. User may choose any value above 1.

3.5.13.4.2   Output values

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

Table 14 – Model outputs (Best fit).

Parameter	Value	Symbol	Unit
Maximum absolute pressure	104192.49	P_{max}	Pa
Localised hydrogen volume fraction in an enclosure	0.123	X_{H2}	ND
Volume of enclosure	31.25	V	m^3
Vent area required not to exceed maximum pressure	**0.448**	**F**	**m^2**

3.5.13.5 Option 2: Calculation of an overpressure for a vent of known size

3.5.13.5.1   Input values

Please provide values for calculation and select the methodology.

Table 15 – Input values.

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Initial absolute pressure	P_i	101325	Pa	33700 - 107900	
Hydrogen volume fraction	X_{H2}	0.123	ND	0.04 - 0.75	
Initial temperature	T_{ui}	298	K	233 - 313	
Initial turbulence	u'	1	m/s	≥0	
Factor to account for presence of obstacles in enclosure	Ξ_O	1	ND	>1	
Enclosure height	H_E	2.5	m		
Enclosure width	W_E	2.5	m		
Enclosure length	L_E	5	m		
Vent area	F	0.448	m^2		

When the option is selected, the screen with input values as in Table 3 should appear prompting to input values for calculation.

3.5.13.5.2   Output values

Table 16 – Model outputs.

Parameter	Value	Symbol	Unit
Vent area	0.448	F	m^2
Hydrogen volume fraction in an enclosure	0.123	X_{H2}	ND
Volume of enclosure	31.25	V	m^3
Maximum absolute pressure	104192.49	P_{max}	Pa

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3.5.13.6 Calculation procedure

Follow procedure as per Table below.

Table 17 – Calculation procedure.

	General calculations for Option 1 and Option 2		
1	Specific heat ratio	$\gamma=1.4$	ND
2	Speed of sound	$c_{ui} = \sqrt{\dfrac{\gamma R_g T_{u0}}{M_{u0}}}$	m/s
3	Enclosure volume, *V*	$V = W_E \cdot H_E \cdot L_E$ (W_E, H_E L_E – User inputs)	m³
	Calculation of deflagration-outflow interaction number		
4		$Sui = 997.96 \cdot X_{H_2}^5 - 1677.3 \cdot X_{H_2}^4 + 774.7 \cdot X_{H_2}^3 - 102.51 \cdot X_{H_2}^2 + 6.0408 \cdot X_{H_2}^1 - 0.0906$	m/s
5	Expansion coefficient, E_i	$Ei = 8775.5185528 \cdot X_{H_2}^6 - 12712.180895 \cdot X_{H_2}^5 + 6167.6542811 \cdot X_{H_2}^4 - 1364.5614133 \cdot X_{H_2}^3 + 124.27324034 \cdot X_{H_2}^2 + 19.766929968 \cdot X_{H_2}^1 + 1.147791802$	
6	Empirical coefficient, ψ	**If 4% ≤ X_{H_2} < 20%** $\psi = 1$ **If 20% ≤ X_{H_2} < 30%** $\psi = -5X_{H_2} - 2$ **If 30% ≤ X_{H_2} ≤ 75%** $\psi = 0.5$	ND
7	Radius of equivalent volume sphere , *R*	$R = \sqrt[3]{3V/4\pi}$	m
8	Characteristic flame radius, R_0	**If 4% < X_{H_2} <20%** $R_0 = 6.7515 X_{H_2} - 0.1215$ **If 29.5% ≤ X_{H_2} < 75%** $R_0 = 1.2$	m
9	Theoretical maximum of wrinkling factor due to turbulence generated by the flame front itself,	$\Xi_K^{max} = (E_i - 1)/\sqrt{3}$	

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10	Wrinkling factor due to turbulence generated by the flame front itself, Ξ_K	$$\Xi_K = 1 + \left(\psi \cdot \Xi_K^{max} - 1\right) \cdot \left[1 - \exp\left(- R/R_0\right)\right]$$	ND
11	Maximum leading point wrinkling factor, Ξ_{LP}^{max}	**If 6% ≤ X_{H_2} < 17.42%** $$\Xi_{LP}^{max} = -14359602.023 \cdot X_{H_2}^6 + 10123867.773 \cdot X_{H_2}^5$$ $$- 2916887.3772 \cdot X_{H_2}^4 + 440588.70586 \cdot X_{H_2}^3$$ $$- 36817.553635 \cdot X_{H_2}^2 + 1602.0558168 \cdot X_{H_2}^1$$ $$- 25.461905777$$ **If 17.42% ≤ X_{H_2} < 29.66%** $$\Xi_{LP}^{max} = -51.456479236 \cdot X_{H_2}^2 + 17.427219398 \cdot X_{H_2}^1$$ $$+ 0.63502119987$$ **If 29.66% ≤ X_{H_2} < 71.27%** $$\Xi_{LP}^{max} = -143.23023003 \cdot X_{H_2}^5 + 425.62891627 \cdot X_{H_2}^4$$ $$- 496.19245746 \cdot X_{H_2}^3 + 286.05307157 \cdot X_{H_2}^2$$ $$- 82.455320688 \cdot X_{H_2}^1 + 10.550603906$$ **If 71.27% ≤ X_{H_2} ≤ 75%** $$\Xi_{LP}^{max} = 0.9333$$	ND
12	Leading point flame wrinkling factor	IF R ≤ R_0/2 $$\Xi_{LP} = 1 + \frac{\left(\Xi_{LP}^{max} - 1\right) \cdot 2R}{R_0}$$ ELSE $$\Xi_{LP} = \Xi_{LP}^{max}$$	ND
13	Internal surface area of an enclosure, A_{EW}	$$A_{EW} = 2 \cdot \left(E_W \cdot E_L + E_H \cdot E_L + E_H \cdot E_W\right)$$	m²
14	Area of the equivalent volume, A_S	$$A_S = 4\pi \cdot R^2$$	m²
15	Aspect ratio wrinkling factor	$$\Xi_{AR} = \frac{A_{EW}}{A_S}$$	ND
16	Fractal wrinkling factor	**If $R > R_0$** $$\Xi_{FR} = \left(\frac{R}{R_0}\right)^{D-2}$$ **If $R < R_0$** $$\Xi_{FR} = 1$$	ND
17	Factor to account for the presence of	$$\Xi_O = 1$$	ND

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	obstacles in the enclosure		
18	Temperature index	$m_0 = -25.945589631 \cdot X_{H_2}^5 + 67.152094773 \cdot X_{H_2}^4$ $- 66.699205247 \cdot X_{H_2}^3 + 44.328192289 \cdot X_{H_2}^2$ $- 18.547832349 \cdot X_{H_2}^1 + 4.5752821336$	ND
19	Laminar flame velocity	$S_u = S_{ui} \cdot \left(\dfrac{T_{ui}}{298}\right)^{m_0}$	m/s
20	SGS wrinked flame burning velocity	$S_u^{SGS} = S_u \cdot \Xi_K \cdot \Xi_{LP} \cdot \Xi_{FR} \cdot \Xi_{AR} \cdot \Xi_O$	m/s
21	Turbulent burning velocity	**Solve transcendental equation to find S_t using procedure in section 3.5.7.7** $S_t = S_w^{SGS} \cdot \exp(u'/S_t)^2$	m/s
22	Wrinkling factor to account for initial turbulence	$\Xi_{u'} = S_t / S_w^{SGS}$	ND
23	Deflagration-outflow interaction number	$\chi/\mu = \Xi_K \cdot \Xi_{LP} \cdot \Xi_{FR} \cdot \Xi_{u'} \cdot \Xi_{AR} \cdot \Xi_O$	ND
	IF Option 1 (Vent area for given pressure)		
24	Dimensionless pressure, $\Delta\pi$	$\Delta\pi = (P_{max} - P_i)/P_i$	ND
25	Based on methodology selected in section 3.5.7.4.1 calculate overpressure	**IF BEST FIT** A=0.018 B=0.94 **IF CONCERVATIVE** A=0.089 B=0.94 $Br_t = \dfrac{\left[A\left(\sqrt{\dfrac{E_i}{2}} \cdot MIN\left\{ 1.0;\ \left[E_i^{2/3} \dfrac{1+\left(\dfrac{1}{\varphi}-1\right)\dfrac{M_{air}}{M_f}}{1+\left(\dfrac{1}{\Phi\varphi}-1\right)\dfrac{M_{air}}{M_f}} \right]^{2/3} \right\} \right)^2 \right]^{1/B}}{\Delta\pi}$	ND

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26	**Vent area**	$$F = \dfrac{Br_t \cdot V^{2/3}}{\dfrac{\sqrt{E_i/\gamma}}{(36\pi_0)^{1/3}} \dfrac{1}{(\chi/\mu)} \dfrac{C_{ui}}{S_u} \dfrac{1}{(E_i-1)}}$$	m²
	IF Option 2 (overpressure for a given vent)		
27	Vent area	F-user input	m²
28	Calculate turbulent Bradley number, Br_t	$$Br_t = \dfrac{\sqrt{E_i/\gamma}}{(36\pi_0)^{1/3}} \dfrac{1}{(\chi/\mu)} \dfrac{F}{V^{2/3}} \dfrac{C_{ui}}{S_u} \dfrac{1}{(E_i-1)}$$	ND
29	Based on methodology selected in section 3.5.7.4.1 calculate dimensionless pressure	**IF BEST FIT** A=0.018 B=0.94 **IF CONCERVATIVE** A=0.089 B=0.94 $$\Delta\pi = A\,Br_t^{-B}\left(\sqrt{\dfrac{E_i}{2}} \cdot MIN\left\{1.0;\left[E_i^{2/3}\left(\dfrac{1+\left(\dfrac{1}{\varphi}-1\right)\dfrac{M_{air}}{M_f}}{1+\left(\dfrac{1}{\Phi\varphi}-1\right)\dfrac{M_{air}}{M_f}}\right)^{2/3}\right]\right\}\right)^2$$	ND
30	**Maximum absolute pressure, P_{max}**	$$P_{max} = \Delta\pi \cdot P_i + P_i$$	Pa

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

3.5.13.6.1   Procedure to calculate S_t: Newton-Raphson Method

```
START
```

St_iter=0

Initialisation

S_t=Sui+0.5u'

WHILE St_iter < 100 **AND** f_xn ≥ 1.e-6

St_iter++

$$f\_xn = S_t - S_w^{SGS} \cdot \exp\left[(u'/S_t)^2\right]$$

$$df\_xn = 1 + 2*(S_w^{SGS} \cdot \exp\left[(u'/S_t)^2\right] * \frac{u'^2}{S_t^3})$$

$$S_t = S_t - \frac{f\_xn}{df\_xn}$$

IF St_iter = 100

Show message: S_t error St_iter=100

EXIT
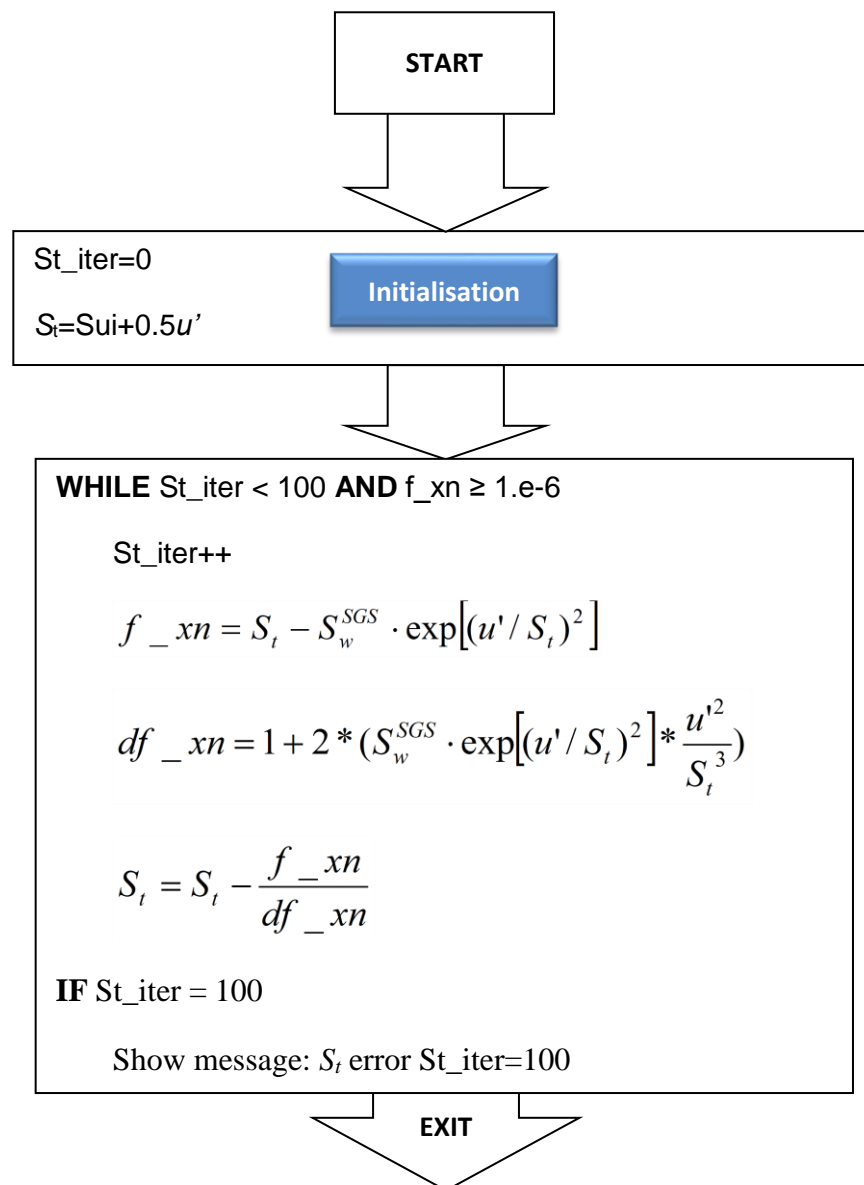
3.5.14 Effect of buoyancy on hazard distances for jet fires (UU)

3.5.14.1 Introduction

This tool shows effect of the hazard distance decrease due to buoyancy in an ignited releases. It is narrow range of applicability for the jet flames which are in buoyancy controlled regime. The tool allows to calculate the distance from the release nozzle to the flame tip where flame start to be affected by buoyancy, as well as the hazard distances to "No harm", "Pain limit", "Third degree burns".

It extends expanded buoyancy controlled part in Figure 9 up to similarity group $(\rho_N/\rho_S) \cdot (U_N/C_N)^3$) <0.0001. This tool allows to calculate more precisely the distance flame tip where the buoyancy changes the direction of the flame from horizontal to vertical.
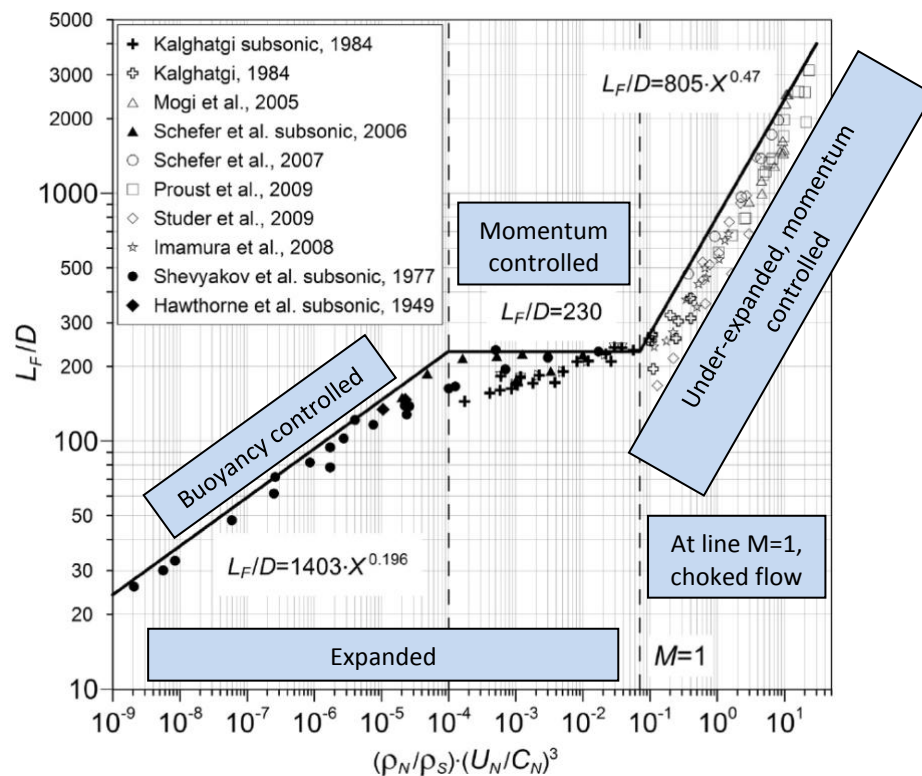
[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

Figure 23– Dimensionless (conservative) correlation for hydrogen jet flames (in formulas shown in figure "X" denotes the similarity group $(\rho_N/\rho_S) \cdot (U_N/C_N)^3$) (V. Molkov and Saffers, 2013)

For hydrogen safety engineering it is important to know when transition from the horizontal to vertical flow direction takes place. The engineering tool presented here is only applicable to the fully buoyancy-controlled expanded jets and is based on the (Saffers, 2010).

Figure 24 shows in logarithmic coordinates the dependence of the distance to nozzle diameter ratio x/D (ordinate) for particular concentration of hydrogen in air on the Froude number (abscissa) in its classical form $Fr = \frac{U^2}{gD}$, where U is the velocity at the nozzle exit (notional nozzle exit for under-expanded jets) in m/s, g is the gravitational acceleration (standard acceleration of gravity on Earth is 9.80665 m/s2), and D is the nozzle diameter (notional nozzle exit diameter for under-expanded jet) in meters. Expanded jets obey the same functional dependence with accuracy 20% acceptable for engineering applications.

Application of the HySAFER model to jet fires – black solid lines: theoretical curves by Shevyakov – black dashed line: separation between sonic and subsonic releases – blue, green and red lines are location of respectively hydrogen concentration of 8%, 11 % and 16 % by volume.

The best fit equation is close to the axial concentration decay of 11% by volume, however 8% (blue line) were chosen as a conservative to determine the flame tip. The black dashed line is a tentative to show the discrepancy between the original theoretical reverse curve, and the actual position of sonic and subsonic data on the graph.

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]
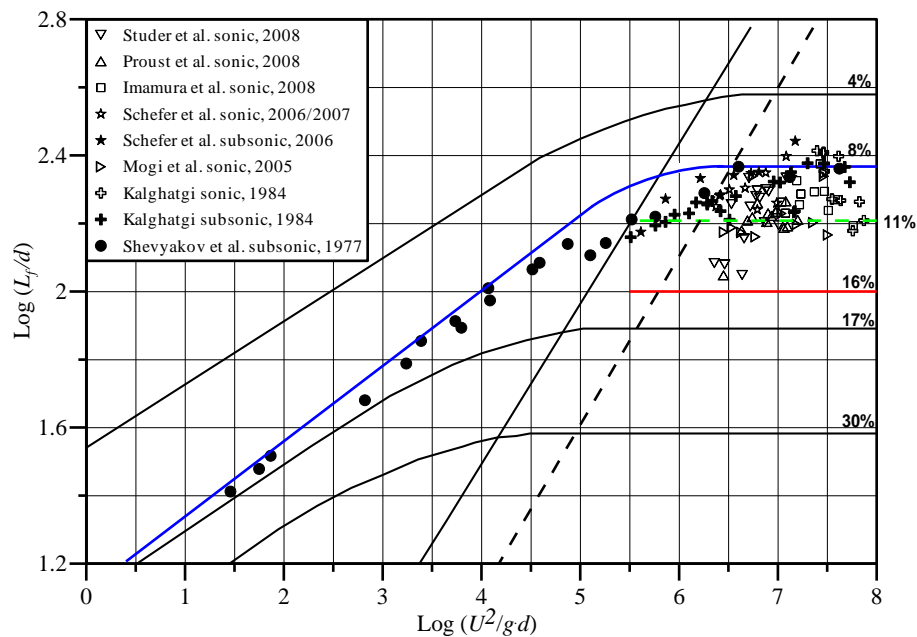
Figure 24 – Application of the HySAFER model to jet fires – black solid lines: theoretical curves by Shevyakov – black dashed line: separation between sonic and subsonic releases – blue, green and red lines are location of respectively hydrogen concentration of 8%, 11 % and 16 % by volume.

3.5.14.2 Nomenclature

Parameter	Symbol	Unit
Hydrogen pressure in reservoir	p_1	Pa
Ambient pressure	p_{atm}	Pa
Critical pressure ratio	p^*=1.89595	-
Hydrogen temperature in reservoir	T_1	K
Orifice diameter	D	m
Froude number	$Fr = \dfrac{V_3^2}{gD_3}$	ND
Velocity at the notional nozzle	V_3	m/s
Gravity acceleration	g=9.80665	m^2/s^2
H$_2$ co-volume constant	b=0.00769	m^3/kg
Hydrogen specific gas constant	R_{H_2}=4124.24107	J/(kg K)
Notional nozzle diameter	D_3	m
Logarithm of Froude number	Log_{Fr}	ND
Axial distance to nozzle ratio	X_over_D	-
Logarithm of axial distance to nozzle ratio	$Log_{X/D}$	-
Axial distance to flame tip where it turns to vertical	X	m

3.5.14.3 Input values

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Hydrogen pressure in reservoir	p_1	20500000	Pa	190000-100000000	20500000

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

Hydrogen temperature in reservoir	T_1	288	K	230-330	288
Orifice diameter	D	0.0095	m	0.0001-0.1	0.0095
Ambient pressure	p_4	101325	Pa	33700-107900	101325

3.5.14.4 Calculation procedure

Step 1. Check critical pressure ratio

$$\text{IF} \quad \frac{p_1}{p_{atm}} < p^*$$

YES

Expanded jet

Proceed to **Step 2.**

NO

Show message:
"This is under-expanded jet and it is always momentum, please use Flame length correlation tool"
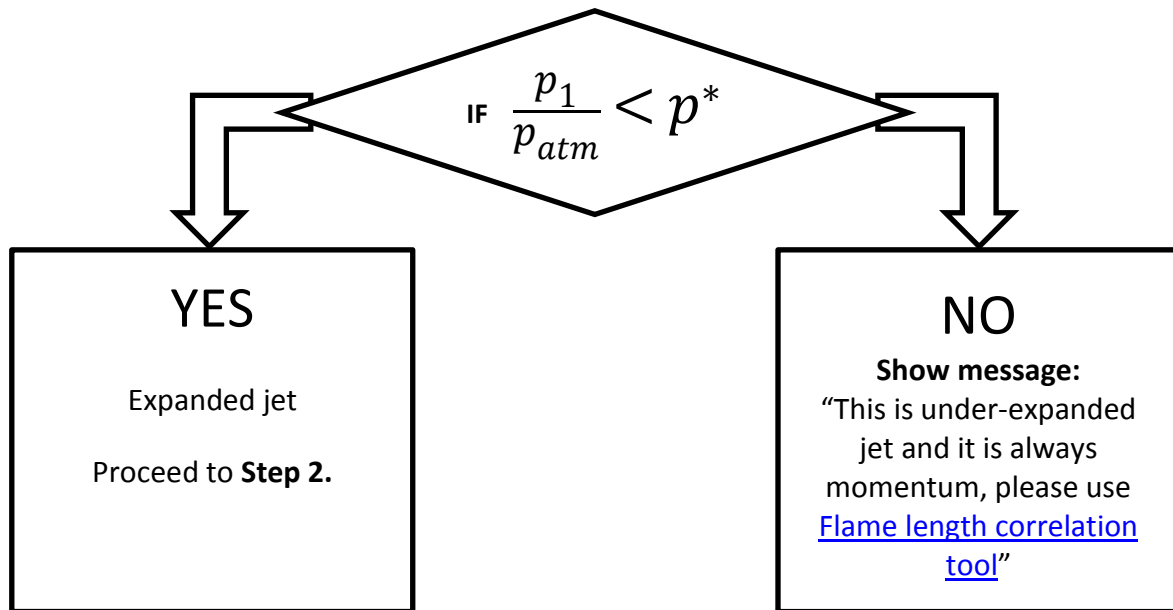
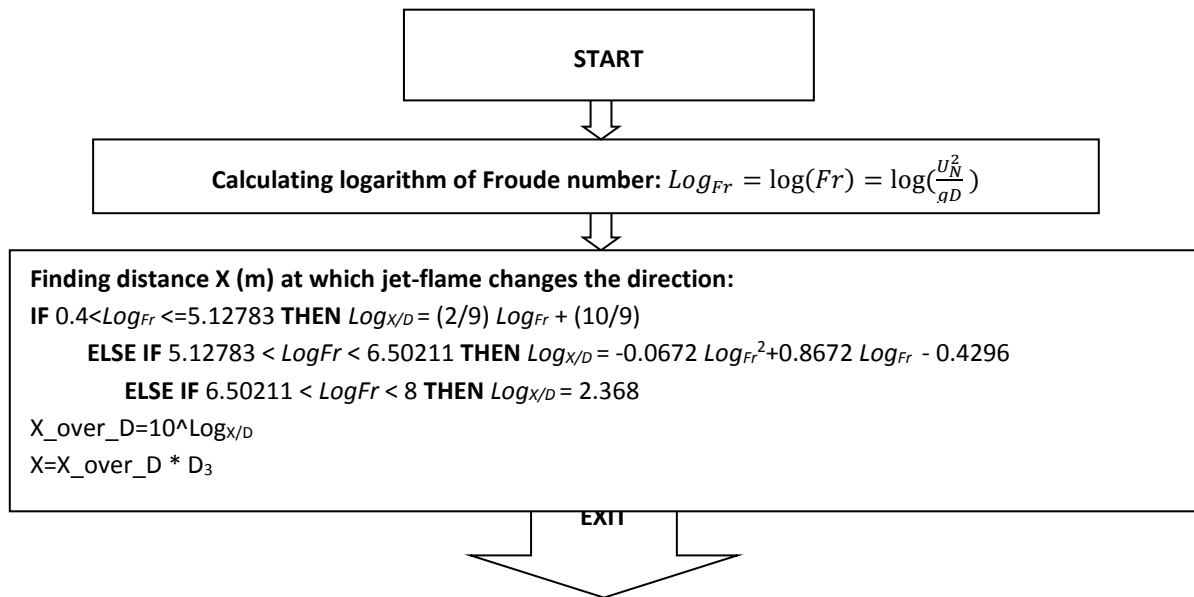**Step 2. Check whether expanded jet-flame buoyancy or momentum controlled (dimensionless group calculation)**

Initial conditions		
1	Hydrogen pressure in reservoir	p_1 - user input	Pa
2	Hydrogen temperature in reservoir	T_1 - user input	K
3	Orifice diameter	D - user input	m
4	Ambient temperature	T_{atm} - user input	K
Calculation		
5	Density in the reservoir	$\rho_1 = \dfrac{p_1}{[(p_1 \cdot b) + (R_{H_2} \cdot T_1)]}$	kg/m³l
6	Density at the nozzle	$\rho_N = \rho_1 \cdot \left(\dfrac{p_{atm}}{p_1}\right)^{1/\gamma}$	kg/m³
7	Mach number at the nozzle	$M_N = \sqrt{\dfrac{2\left[\left(\dfrac{p_1}{p_{atm}}\right)^{\frac{\gamma-1}{\gamma}} - 1\right]}{(\gamma - 1)}}$	-

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

8	Temperature at the nozzle	$$T_N = T_1 \cdot \left(\frac{p_{atm}}{p_1}\right)^{(\gamma-1)/\gamma}$$	K
9	Nozzle speed of sound	$$C_N = \sqrt{\frac{\gamma \cdot R \cdot T_N}{M_{H_2}}}$$	m/s
10	Velocity at the nozzle	$$U_N = M_N \times C_N$$	m/s
11	Ambient density	$$\rho_{atm} = \frac{p_{atm} \cdot M_{air}}{R \cdot T_{atm}}$$	kg/m^3
12	Dimensionless group	$$Dimensionless\ group = \left(\frac{\rho_N}{\rho_{atm}}\right) \cdot \left[\left(\frac{U_N}{C_N}\right)^3\right]$$	-
13	IF statement	**IF** $\left(\frac{\rho_N}{\rho_{atm}}\right) \cdot \left[\left(\frac{U_N}{C_N}\right)^3\right] < 0.0001$ **THEN** proceed to **Step 3** **ELSE** STOP Show message: "Expanded jet-flame is momentum controlled please use [Flame length correlation tool]"	-

Step 3. Calculation of distance to flame tip where the buoyancy changes the direction of the flame from horizontal to vertical

START

Calculating logarithm of Froude number: $Log_{Fr} = \log(Fr) = \log(\frac{U_N^2}{gD})$

Finding distance X (m) at which jet-flame changes the direction:
IF 0.4<Log_{Fr} <=5.12783 **THEN** $Log_{X/D}$ = (2/9) Log_{Fr} + (10/9)
    ELSE IF 5.12783 < $LogFr$ < 6.50211 **THEN** $Log_{X/D}$ = -0.0672 $LogFr^2$+0.8672 $LogFr$ - 0.4296
        ELSE IF 6.50211 < $LogFr$ < 8 **THEN** $Log_{X/D}$ = 2.368
X_over_D=10^$Log_{X/D}$
X=X_over_D * D$_3$

EXIT

Step 4. Calculations of hazard distances

"No harm" (70°C) hazard distance $X_{70°C} = 3.5 \times X$

"Pain limit" (5 mins, 115°C) hazard distance $X_{115°C} = 3.0 \times X$

"Third degree burns" (20 s, 309°C) hazard distance $X_{309°C} = 2.0 \times X$

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

3.5.14.5 Output values

Parameter name	Symbol	Output value	Unit
Axial distance from nozzle to the turning point where the flame becomes buoyant	X		m
"No harm" (70 °C) hazard distance	X_{70^oC}		m
"Pain limit" (5 mins, 115 °C) hazard distance	X_{115^oC}		m
"Third degree burns" (20 sec, 309 °C) hazard distance	X_{309^oC}		m

3.5.15 Calculation of fireball diameter for rupture in a fire of a stand-alone and an under-vehicle hydrogen storage tanks (UU)

3.5.15.1 Introduction

Note: Model description should appear upon pressing the appropriate button on the home screen of the tool.

This model allows to calculate fireball size for the stand-alone and under-vehicle (onboard) tank location.

The methodology is based on the work by Dadashzadeh et. al 2017 (Dadashzadeh, Kashkarov, Makarov, & Molkov, 2017). Calculation of a fireball size after a stand-alone tank rupture is a part of the methodology for the calculation of the blast wave decay after compressed gas vessel rupture (V. Molkov & Kashkarov, 2015) and hazard distances attributed to the blast parameters. According to the technique, the fireball size is calculated as a hemisphere occupied by combustion products resulting from complete combustion of released hydrogen in air (non-premixed turbulent combustion at contact surface occurs at stoichiometric concentration of reactants). The estimated fireball size for stand-alone tank is then scaled for onboard tank ("under-vehicle" tank in terminology (V. Molkov & Kashkarov, 2015)) based on the experimental data (Weyandt, 2006, 2005).

3.5.15.2 Nomenclature

Parameter	Symbol	Unit
Pressure in reservoir	p_1	Pa
Temperature in reservoir	T_1	K
Volume of reservoir	V	m^3
Hydrogen mass in reservoir	m_{H2}	kg
Molecular mass	$M=2.016$	kg/kmol
Amount of hydrogen in reservoir	$H2\_mol$	kmol
Volume of hydrogen in reservoir	V_{H2}	m^3
Amount of air to burn hydrogen	Air_mol	kmol
Volume of air to burn hydrogen	V_{air}	m^3
Volume of combustion products	V_{burned}	m^3
Fireball diameter stand-alone	D_{SA}	m
Fireball diameter onboard	D_{OB}	m

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

3.5.15.3 Input values

Parameter name	Symbol	Input value	Unit for calculation	Limits (min-max)	Defaults
Hydrogen pressure in reservoir	p_1	35000000	Pa	101325-100000000	20500000
Hydrogen temperature in reservoir	T_1	312	K	230-330	288
Volume of reservoir	V	0.0724	m^3	0.0001-10	0.0724

3.5.15.4 Calculation procedure

	Initial conditions		
1	Hydrogen pressure in reservoir	p_1 - user input	Pa
2	Hydrogen temperature in reservoir	T_1 - user input	K
3	Volume of reservoir	V - user input	m
	Calculation		
4	Hydrogen mass in reservoir	Calculate m_{H2} using The Abel-Noble EOS tool based on user input of p_1, T_1 and V	kg
5	Amount of hydrogen in reservoir	H2_mol= m_{H2}/M	kmol
6	Volume of hydrogen in reservoir	V_{H2}=H2_mol*22.4/1000	m^3
7	Amount of air to burn hydrogen	Air_mol=H2_mol*2.38	kmol
8	Volume of air to burn hydrogen	V_{air}=Air_mol*22.4/1000	m^3
9	Volume of combustion products	V_{burned}=(V_{air}+V_{H2})*6.85	m^3
10	Fireball diameter stand-alone	$$D_{SA} = 2 \times \left(\frac{3V_{burned}}{2\pi}\right)^{1/3}$$	m
11	Fireball diameter onboard	$$D_{OB} = 5.2 \times \left(\frac{3V_{burned}}{2\pi}\right)^{1/3}$$	m

3.5.15.5 Output values

Parameter name	Symbol	Output value	Unit
Fireball diameter stand-alone	D_{SA}	11.697	m
Fireball diameter onboard	D_{OB}	30.412	m

3.5.16 H2 properties and Tank Blowdown (NCSRD)

Due in D3.3

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

4   Conversion units

This section describes the conversion units to be implemented into e-Laboratory.

4.1   Standard units for calculation and storage in database (all values would be stored and processed in these units)

Parameter name	Standard unit name	Symbol	Unit
Pressure	Pascal	P	Pa
Temperature	Kelvin	T	K
Length	Meter	L	m
Volume	Cubic meter	V	m^3

4.2   Alternative units for user inputs and outputs

Parameter name	Unit name	Symbol	Unit	Conversion from standard unit	Conversion to standard unit
Pressure	Bar	P	Bar	$\dfrac{P_{(Pa)}}{100000}$	$P_{(bar)} \times 100000$
	Atmosphere	P	Atm	$\dfrac{P_{(Pa)}}{101325}$	$P_{(atm)} \times 101325$
	Pounds per square inch	P	Psi	$\dfrac{P_{(Pa)}}{6894.76}$	$P_{(psi)} \times 6894.76$
	Mega Pascal	P	MPa	$\dfrac{P_{(Pa)}}{1000000}$	$P_{(MPa)} \times 1000000$
	Kilo Pascal	P	kPa	$\dfrac{P_{(Pa)}}{1000}$	$P_{(kPa)} \times 1000$
Temperature	Degree Celsius	T	C	$T_{(K)} - 273.15$	$T_{(C)} + 273.15$
	Degree Fahrenheit	T	F	$T_{(K)} * \dfrac{9}{5} - 459.67$	$(T_{(F)} + 459.67) * \dfrac{5}{9}$
Length	Foot	L	ft	$\dfrac{L_{(m)}}{0.3048}$	$L_{(ft)} \times 0.3048$
	Inch	L	in	$\dfrac{L_{(m)}}{0.0254}$	$L_{(inch)} \times 0.0254$
	Centimeter	L	cm	$\dfrac{L_{(m)}}{0.01}$	$L_{(cm)} \times 0.01$
	Millimeter	L	mm	$\dfrac{L_{(m)}}{0.001}$	$L_{(cm)} \times 0.001$
Volume	Liter	V	Liter	V(m^3)*1000	L(Liter)/1000
	Cubic foot	V	ft^3	V(m^3)*35.3146667	V(ft^3)/35.3146667
	Cubic inch	V	in^3	V(m^3)*61023.7441	V(in^3)/61023.7441

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

5   Structure and planning of e-Laboratory delivery

			Tools	Description	Programming	Verification	Interface	Final verificat
e-Laboratory	e-Engineering	Renewable energy system (RES) tools	1. Design & Optimisation of hybrid RES – Hydrogen autonomous power systems for isolated communities and sites.	NCSRD M18	NCSRD M18	NCSRD M19	M20	NCSRD M20
		Fuel cells (FC) tools	1. Simulation of SOFC based on natural gas as fuel	DTU M23(12,7)	M24	M14	M15	M25
			2. Energy balances and hydrogen costs for various electrolysis techniques	DTU M25(11,6)	M26	M13	M14	M27
			3. Cell and stack models for both fuel cells and electrolysis	DTU M15(10,5)	M16	M12	M13	M17
			4. Thermo-mechanical models to predict lifetime of high temperature FCs and electrolysis	DTU M19(9,4)	M20	M11	M12	M21
		Storage/Separation tools	1. Storage material properties estimation and performance assessment based on a "materials-by-design" multi-scale approach; a. Hydrogen Storage in Carbon-based Materials, b. Hydrate equilibrium pressure of H2 mixtures, c. Hydrate-based separation of the binary mixture H2+CO2	NCSRD M12	NCSRD M16(12)	NCSRD M17(13)	M17(14)	M18(14)
		FC integrated into CHP tools	1. Simulation of FC system integrated into mCHP application, including electrolyser operation	UNIPG M2	M4	M8	M10	M10
		Safety engineering tools	1. Jet parameters model	UU M2	M7	M8	M10	M10
			2. Adiabatic and isothermal model of blowdown of storage tank dynamics	UU M2	M8	M9	M10	M10
			3. Flame length correlation and three hazard distances for jet fires	UU M3	M8	M9	M10	M10
			4. Similarity law for concentration decay in hydrogen expanded and under-expanded jets and unignited jet hazard distances	UU M4	M9	M10	M11	M11
			5. Pressure peaking phenomenon for unignited releases	UU M3	M9	M10	M11	M11
			6. Passive ventilation in an enclosure with one vent: uniform hydrogen concentration	UU M1	M4	M6	M10	M10
			7. Mitigation of uniform mixture deflagration by venting technique	UU M4	M14	M15	M16	M15
			8. Forced ventilation system parameters	UU M5	M15	M16	M16	M17
			9. Blast wave from high-pressure rupture without and with combustion	UU M14(12,10)	M15	M16	M16	M17
			10. Effect of buoyancy on decrease of hazard distance for unignited releases	UU M6	M10	M11	M12	M12
			11. Pressure peaking phenomenon for ignited releases	UU M6	M17	M18	M18	M18
			12. Upper limit of hydrogen inventory in closed space	UU M7	M8	M9	M10	M10
			13. Mitigation of localised non-uniform deflagration by venting	UU M8	M16	M14	M15	M15
			14. Effect of buoyancy on hazard distances for jet fires	UU M14(12,8)	M15	M16	M17	M17
			15. Calculation of fireball diameter for rupture in a fire of a stand-alone and an under-vehicle hydrogen storage tanks	UU M9	M14	M15	M16	M16
			16. H2 properties and Tank Blowdown	NCSRD M24	NCSRD M24	NCSRD M25	M26	NCSRD M26
	e-Science	Property tools	1. Normal Hydrogen thermo-physical properties using the NIST-EoS, (Helmholtz free energy based)	NCSRD M17	NCSRD M17	NCSRD M18	M19	NCSRD M19
			2. The Abel-Noble EOS to calculate CGH2 mass in a volume at particular pressure and density	UU M9	M16	M17	M18	M18
		Electrochemistry tools	1. Fundamental electrochemistry equations, design PEM, optimal porosity of gas diffusion electrodes, ionic conductivity: a. Electrochemical potential; b. Nernst equation; c. Faraday laws of electrolysis; d. Butler-Volmer equation; e. Tafel equation; f. Ionic conductivity g. Levich equation	IEES M4	M17	M18	M19	M19
		Storage tools	1. Comsol Multiphysics for simulation of hydrogen production and FCH technologies; a. Methane steam reformer; b. Solid Oxide Fuel Cell (SOFC)	NCSRD M12	NCSRD M12	NCSRD M13	M14	NCSRD M14
		FC tools	1. Modelling of transport processes in electrodes and electrolytes:	DTU M21(12,4)	M22	M18	M19	M23
		HyFOAM	1. Release and dispersion of horizontal under-expanded hydrogen jet (HSL)	UU M13	M17	M18	M18	M18
			2. Large scale deflagration in the open atmosphere (Fraunhofer ICT)	UU M16	M16	M18	M18	M18
			3. Blast wave and fireball from high-pressure tank rupture in a fire (Weyandt)	UU M25	M25	M27	M27	M27
			4. Hydrogen/helium dispersion in vented enclosures (CEA)	NCSRD M17	M17	M19	M19	M19
			5. Vented deflagration (FM Global)	NCSRD M26	M26	M27	M27	M27

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The structure of e-Laboratory is outlined in a table above with detailed planning on the delivery of each tool including provision of tool description by the responsible partner, programming, verification of the back-end code, programming of user interface and final verification by the tool developer.

Colour code for the table is as follows:

Green – Delivered

Red – Delayed

Yellow – Approaching deadline

Grey – No programming required (manual as a document to be delivered and published in HyFOAM section as pdf)

[D3.1 Report on technical and digital concepts and structure of e-Laboratory_v1.6.docx]

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