FLAGSHIPS

Clean waterborne transport in Europe

Deliverable D5.2 - Common safety analysis e-tools

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With the contribution of the University of Ulster

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Contents

1 Introduction

This report resumes the achievements made under the scope of task 5.3, dedicated to the software development cycle of two common safety analysis e-tools.

The first stage of development was to identify the scope of the web-based tools. Interviews were conducted to identify the gaps in RCS knowledge. A panel of maritime shipping stakeholders was asked for input and feedback, including the advisory board of MARANDA project in which Persee is still involved. Initially, FLAGSHIPS project included both gaseous (Lyon) and liquid (Stavanger) hydrogen, so it was decided to cover both states in the tools. The results of the investigations allowed the identification of two main topics:

- the fireball diameter from gaseous or liquid hydrogen storage,
- the bunkering of gaseous hydrogen.

The second stage consisted in acquiring proven models and scientific descriptions. University of Ulster, EU leader and well-established in hydrogen safety, was selected as their work on the two topics (partly financed by the FCH JU as well) had been validated, peer-reviewed and published.

The Persee team was able to perform the programming of the two e-tools, which once ready was tested by safety experts and general users to achieve a comprehensive validation.

Both tools are deployed on the e-laboratory of hydrogen safety developed by Persee in the framework of FCH JU funded Hyresponder. The e-laboratory is open and accessible through self sign up allowing a broad dissemination of the corresponding knowledge.
Persee development team will provide updates, support, and maintenance during the whole agreed duration.

E-laboratory

e-laboratory is a virtual laboratory enabling to apprehend the behaviour of hydrogen and fuel cells (HFC) from a physical, an economic or a safety perspective. Today the platform includes more than 30 learning and training e-tools. It can be accessed through the following url: https://elab.hysafer.ulster.ac.uk/
The platform is free to use.

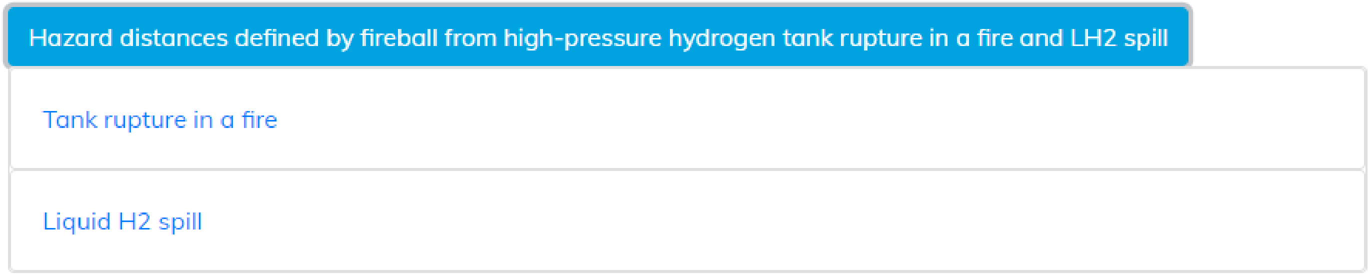
2 The first e-tool: fireball diameter from gaseous or liquid hydrogen storage

The first tool has been designed to support the safety analysis of gaseous and liquid pure hydrogen storage. It is available on the Ulster platform under: Category: Hazard distance -> Hazard distances defined by fireball from high-pressure hydrogen tank rupture in a fire and LH2 spill.

The model consists of two options to allow for the calculation of hazard distances defined by:
1. The size of fireball after high-pressure gaseous hydrogen tank rupture in a fire
2. The size of fireball after liquid hydrogen spill

The output is an estimation of the fireball diameter in case of rupture, with both best fit and conservative fit. A detailed description is available for both options.

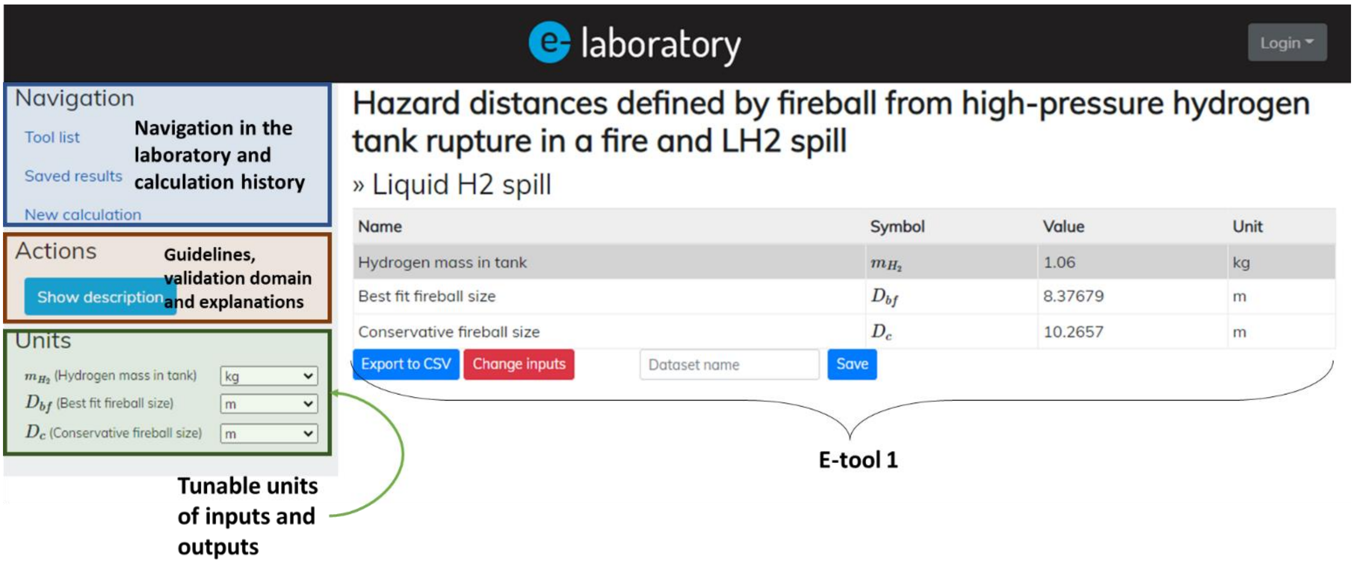
Choice of the model
When the tool is selected, the choice appears prompting to select the option.



Hazard distances defined by fireball from high-pressure hydrogen tank rupture in a fire and LH2 spill

Tank rupture in a fire

Liquid H2 spill



Hazard distances defined by fireball from high-pressure hydrogen tank rupture in a fire and LH2 spill

» Liquid H2 spill

Name	Symbol	Value	Unit
Hydrogen mass in tank	m_{H_2}	1.06	kg
Best fit fireball size	D_{bf}	8.37679	m
Conservative fireball size	D_c	10.2657	m

Units

m_{H_2} (Hydrogen mass in tank): kg

D_{bf} (Best fit fireball size): m

D_c (Conservative fireball size): m

Figure 1. Interface of the tools

2.1 Option 1: The size of fireball after high-pressure hydrogen tank rupture in a fire

This tool uses the engineering correlations [1] to assess hazard distances defined by a size of fireball after high-pressure hydrogen tank rupture in a fire in the open atmosphere (both for stand-alone and under-vehicle tanks).
The term “fireball size” is used for the maximum horizontal size of a fireball that is different from the term “fireball diameter” applied to spherical or semi-spherical shape fireballs. There are different reasons for a fireball to deviate from a spherical shape, e.g., in case of tank rupture under a vehicle, the noninstantaneous opening of tank walls, etc. Two conservative correlations are implemented using theoretical analysis, numerical simulations, and experimental data available in the literature. The theoretical model for hydrogen fireball size assumes complete isobaric combustion

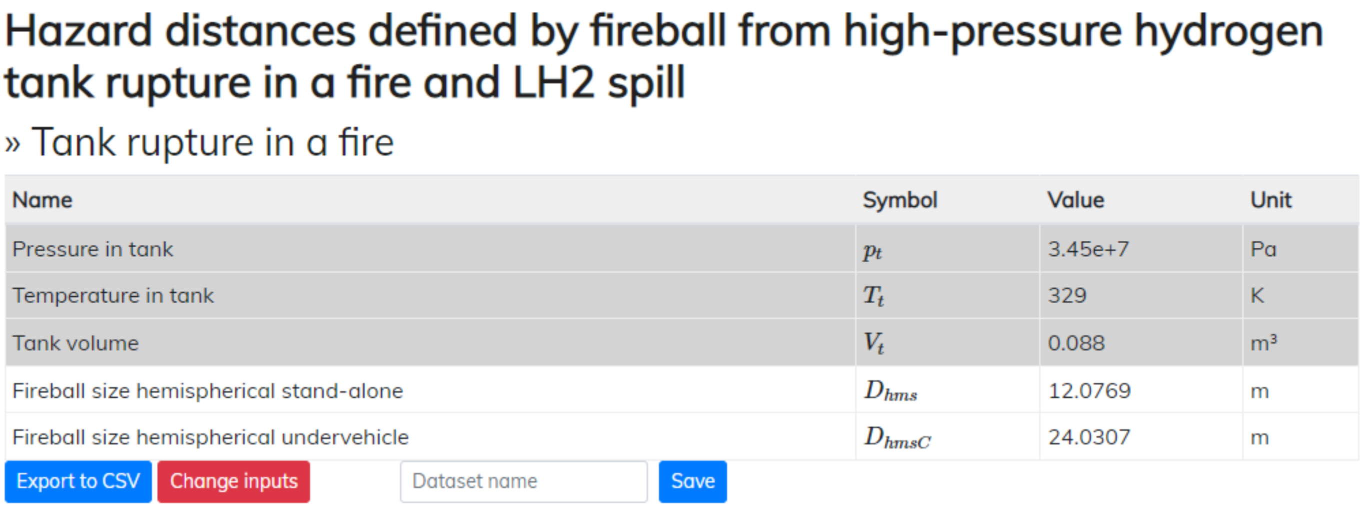
of hydrogen in air and presumes its hemispherical shape as observed in the experiments and the simulations for tank rupturing at the ground level. The correlations are applied as engineering tools to access hazard distances for scenarios of gaseous hydrogen storage tank rupture in a fire in the open atmosphere.

Table 1 Input values

Parameter name	**Symbol**	**Unit for calculation**	**Limits (min-max)**	**Defaults**
Hydrogen pressure in reservoir	p_1	Pa	101325-100000000	34500000
Hydrogen temperature in reservoir	T_1	K	20-1000	329
Volume of reservoir	V	m^3	0.0001-10	0.088

Table 2. Calculation procedure

Calculation		
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
Fireball size hemispherical (stand-alone)	$D_{hms} = 9.8 * m_{H2}^{1/3}$	m
Fireball size hemispherical undervehicle (conservative)	$D_{hmsC} = 19.5 * m_{H2}^{1/3}$	m



Hazard distances defined by fireball from high-pressure hydrogen tank rupture in a fire and LH2 spill

» Tank rupture in a fire

Name	Symbol	Value	Unit
Pressure in tank	p_t	3.45e+7	Pa
Temperature in tank	T_t	329	K
Tank volume	V_t	0.088	m^3
Fireball size hemispherical stand-alone	D_{hms}	12.0769	m
Fireball size hemispherical undervehicle	D_{hmsC}	24.0307	m

Figure 2. Output screen: results can be exported to CSV

2.2 Option 2: The size of fireball after liquid hydrogen spill (Model description)

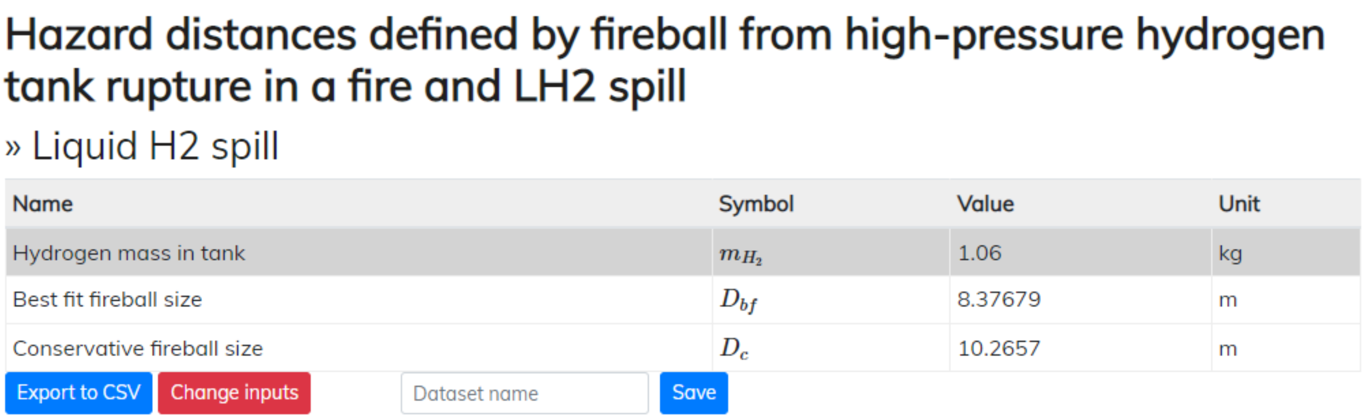
This tool uses the engineering correlations [1] to assess hazard distances defined by a size of fireball after liquid hydrogen spill in the open atmosphere (both for conservative and best-fit) and available
The term “fireball size” is used for the maximum horizontal size of a fireball that is different from the term “fireball diameter” applied to spherical or semi-spherical shape fireballs. Two conservative correlations are implemented using theoretical analysis and experimental data available in the literature. The correlation for liquid hydrogen release fireball is based on the experiments by Zabetakis [2]. The correlations are applied as engineering tools to access hazard distances for scenarios of liquid hydrogen spill in an open atmosphere.

Table 3. Input values

Parameter name	**Symbol**	**Unit for calculation**	**Limits (min-max)**	**Defaults**
LH2 mass in reservoir	m_{H2}	Kg	0.0001-1000000	1.06

Table 4. Calculation procedure

Calculation		
Fireball size (best fit)	$D_{bf} = 8.16\, m_{H2}^{0.45}$	m
Fireball size (conservative)	$D_{C} = 10 * m_{H2}^{0.45}$	m



Hazard distances defined by fireball from high-pressure hydrogen tank rupture in a fire and LH2 spill

» Liquid H2 spill

Name	Symbol	Value	Unit
Hydrogen mass in tank	m_{H_2}	1.06	kg
Best fit fireball size	D_{bf}	8.37679	m
Conservative fireball size	D_c	10.2657	m

Figure 3. Output screen: results can be exported to CSV

2.3 Limitation and boundary conditions in the case of FLAGSHIPS

Regarding limitation and boundary conditions, the validation of the tools is based on light FCV storage (~1-6kg, lack of experimental data for higher capacity). According to the University of Ulster, the range of validity can be extended to approx 15kg and so is relevant for a single bottle in the case of FLAGSHIPS. Beyond, additional phenomena occur (increased time duration, longer buoyancy, radiation increased, initial configuration and chain reaction in the case of multiple bottles...) and their cross-influences are beyond the scope of the paper. Although the conservative fit can be used anyway, the results would not be very useful as the whole ship would be engulfed in the fireball with an explosion of 350kg H2.

The range of use presented in the previous sections has been extended to higher values for educational purposes.

3 The second e-tool: Physical model of fueling of Type IV hydrogen storage tank

This second tool aims to facilitate the development of fueling/bunkering protocols for compressed hydrogen storage systems (CHSS). The calculations are based on the physical model of thermal behavior of hydrogen storage tank [3]. The model and tool account for all main underlying physical phenomena during hydrogen fueling of a composite high-pressure cylinder. The model has been validated against fueling experiments with Type III [5] and Type IV [5] tanks typical for onboard storage. The experimental hydrogen temperature dynamics inside a tank are reproduced by the model within the experimentally measured temperature non-uniformity of 5°C. The scheme of the hydrogen storage tank during the fueling and the phenomena at its boundaries are shown in Figure 6.

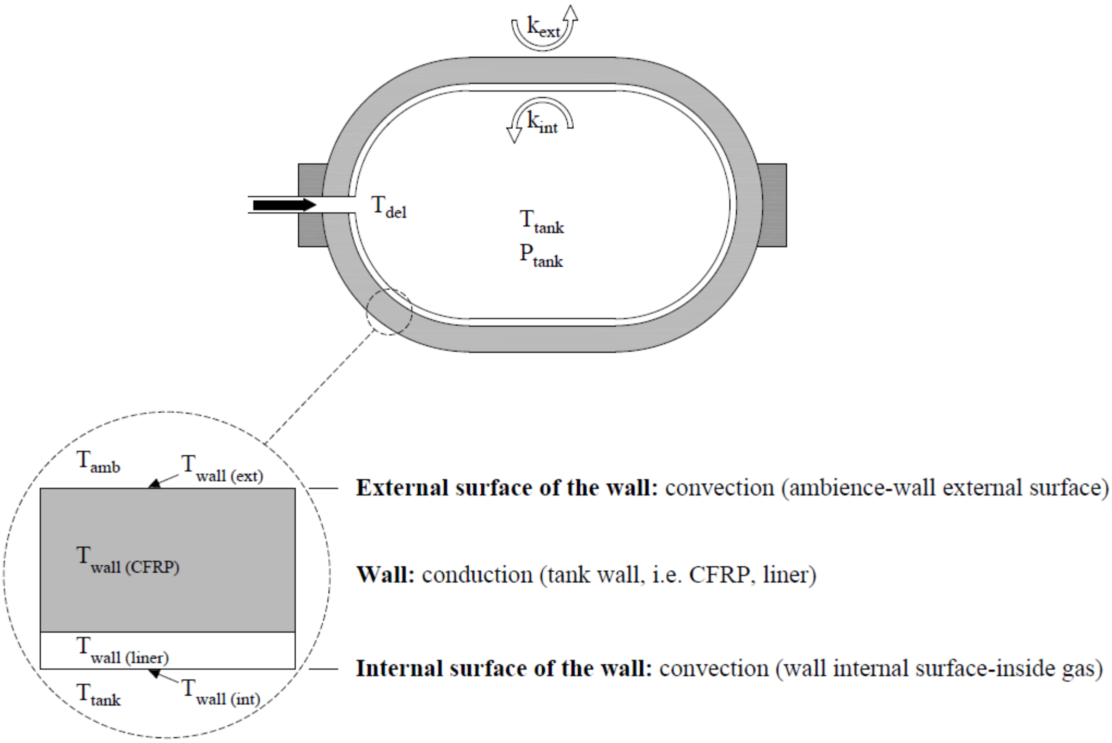


Figure 4. Scheme of a hydrogen storage tank and related phenomena during fuelling [3].

3.1 Tool scope

The model allows to control of the thermal behaviour the tank during the fuelling, including but not limited to hydrogen bulk temperature, pressure, the state of charge (SOC), temperature distribution in the wall, etc. It must be underlined that the control of bulk temperature provided by this tool does not exclude the need of the fuelling protocol designer to provide evidence of temperature uniformity (or acceptable level of its non-uniformity) within the tank to demonstrate the inherent safety of the fuelling/bunkering protocol.

The energy conservation equation, Abel-Noble real gas equation of state, and the entrainment theory are used to calculate the dynamics of hydrogen temperature and pressure inside the tank and distribution of temperature through the wall to control the requirements of the regulation and safety provision. Convective heat transfers between hydrogen and liner, tank wall overwrap and the atmosphere are modelled using Nusselt number correlations. Conductive heat transfer through the tank wall, composed of a load-bearing carbon fibre reinforced polymer and a liner, is modelled by employing a one-dimensional unsteady heat transfer equation. The user is encouraged to read the reference paper for more details on the implemented equations.

The user will be able to design a fuelling protocol for a particular tank by changing the pressure ramp as a design parameter. The tool allows calculating parameters of fuelling, including control of temperature limit (temperature < 85$_o$C), pressure limit (pressure<1.25xNWP) and the SOC limit (100%) during fuelling by using the pressure ramp. The linear pressure ramp is defined as a ratio of pressure change in the tank to the time that this pressure growth will take.

The tool allows to design fuelling protocol for not constant pressure ramp. In this case calculation of fuelling at the next stage (with different pressure ramps) starts with initial parameters which are equal to the parameters at the end of the previous stage of fuelling (with the previous pressure ramp).

The tool is based on an iterative process based on the geometry and the properties of the tank, the initial steady state and the fuelling protocol provided by the user (table 9). The calculation procedure is summed up below (figure 7).

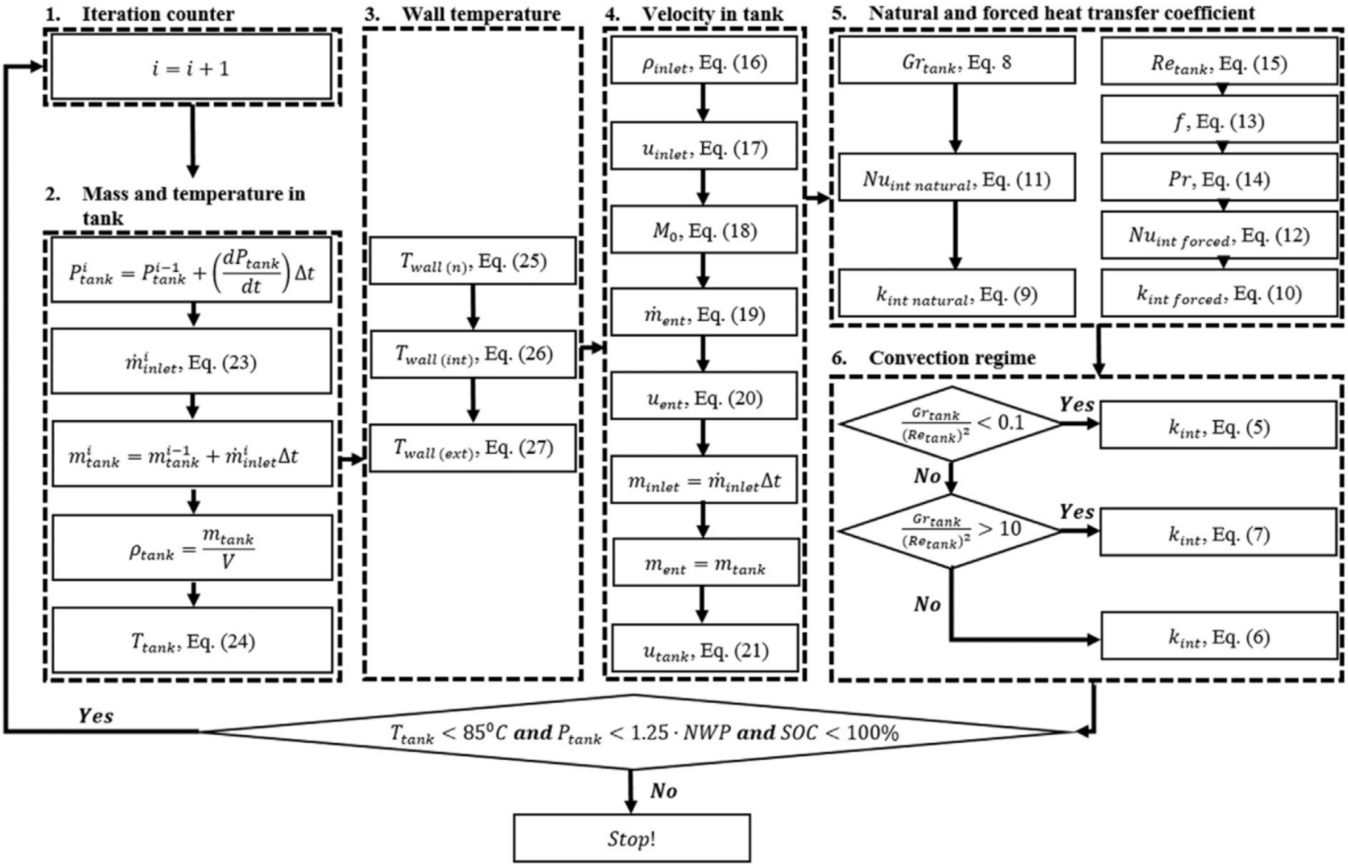


Figure 5. Calculation procedure [3].

Table 5. Input parameters and values

Parameter name	Symbol	Unit for calculation	Limits (min-max)	Defaults
Initial pressure in the tank	$Ptank0$	Pa	0 - 140000000	2000000
Target pressure in the tank*				
If “Continuous pressure ramp” selected, then overall target pressure is specified	$Ptank\ targ.$	Pa	1000000 - 140000000	77000000
If “Stepwise pressure ramp” selected and number of phases specified, then target pressures for each phase is specified	$Ptank\ phase1$, $Ptank\ phase2$, etc	Pa	1000000 - 140000000	
Initial temperature in the tank	$Ttank0$	K	0-700	293.15
Volume of the tank	V	m3	0.01-100	0.029
Tank NWP	NWP	Pa	10000000-100000000	70000000
Internal tank diameter	$Dint$	m	0.001-10	0.23
Liner thickness	$xliner$	m	0.0001-0.1	0.0027
Composite overwrap thickness	$xCFRP$	m	0.0001-0.1	0.0218
Internal tank area	$Aint$	m2	0.0001-200	0.55
Inlet orifice diameter	$Dinlet$	m	0.00001 - 0.5	0.003
Hydrogen inlet/delivery temperature	$Tdel$	K	0-400	298.15
Ambient temperature	$Tamb$	K	0-400	293.15
Fuelling duration				
If “Continuous pressure ramp” selected, then overall fuelling duration is specified	$tfuel$	s	0-7200	250
If “Stepwise pressure ramp” selected and number of phases specified, then the time for each phase change is specified	$tphase1$, $tphase2$, etc	s	0-7200	
Time step	Δt	s	0.000001-10	0.5

Output values

The tool provides the evolution of the mass, the pressure, and the temperature inside the tank at each time step. The results are available and can be saved under excel files or plotted graphs.

3.2 Validation domain

This tool was validated against the experiments with the fuelling of Type III [4] and Type IV [5] with aluminium and high-density polyethylene (HDPE) liners, respectively. Three available experiments on hydrogen tank fuelling were used for the model validation: the volume of tanks in experiments was either 29 L, 40 L or 74 L, and the nominal working pressure was NWP=70 MPa (but fuelled up to 77 MPa, 77 MPa and 70 MPa respectively). Length to diameter ratio of the experimental tanks used in the validation study was in the range LxD=2.4-3.0.

The tool can be used within the validation domain as described above. Beyond that, the use of the tool remains at the user's discretion. Users are encouraged to publish results of comparison of calculated fuelling dynamics with their own of described in the literature fuelling experiments with reference to the model applied. The tool allows to develop the pressure ramp during fuelling that would prevent exceeding hydrogen temperature of 85°C as per regulation (and stop fuelling at the SOC of 100%). The tool allows to calculate fuelling of Type IV tanks. The initial input of the material properties of the tank liner and composite wall are pre-determined and are taken from [5].

4 References:

[1] D. Makarov, V. Shentsov, M. Kuznetsov, and V. Molkov, 'Hydrogen Tank Rupture in Fire in the Open Atmosphere: Hazard Distance Defined by Fireball', Hydrogen, vol. 2, no. 1, pp. 134–146, Feb. 2021, doi: 10.3390/hydrogen2010008.

[2] M. G. Zabetakis, 'Flammability characteristics of combustible gases and vapors', BM--BULL-627, 7328370, May 1964. doi: 10.2172/7328370.

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[5] J. Zheng *et al.*, (2013) Experimental and numerical study on temperature rise within a 70 MPa type III cylinder during fast refueling, *International Journal of Hydrogen Energy*, vol. 38, no. 25, pp. 10956–10962, doi: 10.1016/j.ijhydene.2013.02.053.

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