Deliverable D3.1

Report on the characteristics of the cases to be studied in the preliminary simulations

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REPORT

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ACRONYMS AND ABBREVIATIONS

APRR	Average Pressure Ramp Rate
CHSS	Compressed Hydrogen Storage System
FCEV	Fuel Cell Electric Vehicle
FC	Fuel Cell
GHG	Greenhouse Gas
GT	Gas Turbine
H_2	Hydrogen
HDV	Heavy Duty Vehicle
LDV	Light Duty Vehicle
NWP	Nominal Working Pressure
MOP	Maximum Operating Pressure
SoC	State of Charge
WP	Work Package

1 INTRODUCTION

This document introduces the efforts in PRHYDE Work Package 3 (WP3) to develop concept(s) for heavy duty vehicle (HDV) fuelling protocol(s) that addresses the specifications from WP2 (state-of-the-art of existing fuelling protocols and gap analysis). This requires diligent considerations, development efforts and weighing of multiple aspects, that in some cases may be conflicting:

- The HDV performance requirements (tank size, fuelling pressures and times) may vary greatly across the different vehicle and market segments. It may therefore be necessary to develop multiple protocols to sufficiently address the specific requirements for each segment.
- Fuelling has to avoid overheating and overfilling in any instance based upon vehicle and station conditions. The protocol(s) to be developed will in parallel undergo safety and risk assessment.
- The WP2 analysis of current state-of-the-art-nozzle, receptacle and communication hardware on both station and vehicle side shows a significant capability gap with regards to meeting the HDV performance requirements. It may be required to define new components different from what is on the market today, to achieve sufficiently fast fuelling to meet the target.

The objective of this document is to define characteristics for WP4 efforts on preliminary computations on single tank refuelling in order to give an order of magnitude of temperature increase during refuelling of large tank for different case considered as representative. The results of these simulations are anticipated to be published during a later stage of the project by the PRHYDE consortium as deliverable D4.1.

It should be noted that the selected scenarios and cases do not reflect the future refuelling protocol approach. Instead, they will help to support the future work of the project such as protocol development and experimental campaign in WP5.

2 METHODOLOGY

2.1 Workflow

The development efforts in WP3 are based on deliverables from WP2.

Work packages WP3, WP4, and WP5 will enter an iterative collaboration process, where:

- WP3 will discuss and formulate the simulation task list based on input from other work packages. The simulation task list is handed to WP4.
- WP4 will perform simulations and quantify simulation results. Simulation results relevant to field testing are handed to WP5. Technical feedback relevant to design of experiments are handed to WP3.
- WP5 will perform field tests and obtain field test results for comparison with simulation results. Results are shared with WP3 for further optimization of fuelling protocol.

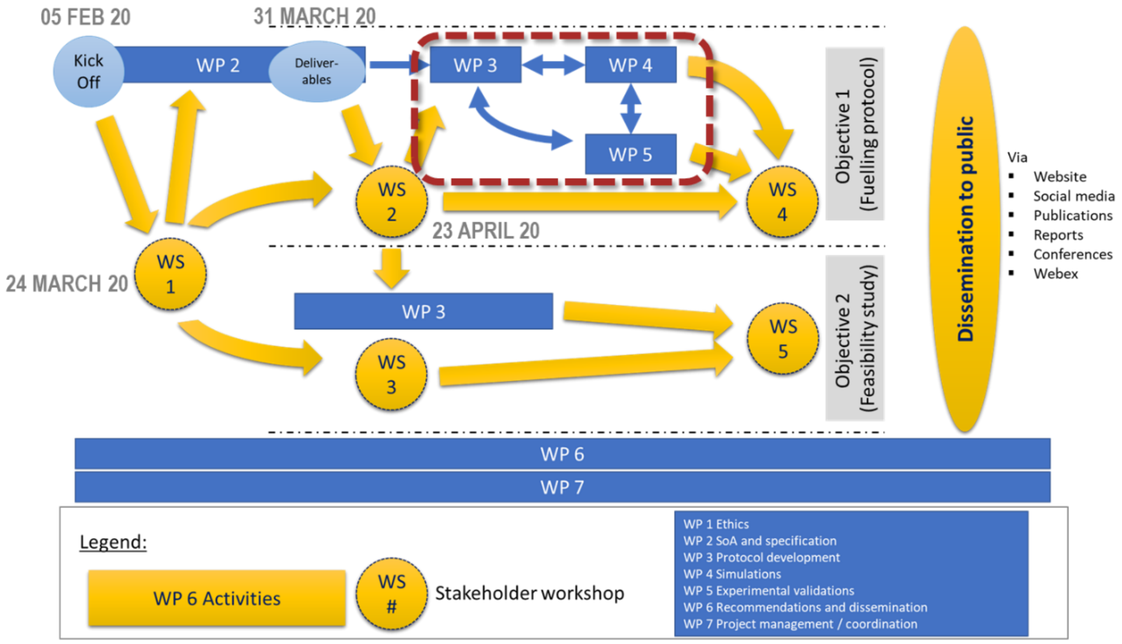

Figure 1: PRHYDE work plan – focus on collaboration between WP3, WP4, and WP5 (Source: PRHYDE)

The collaboration between the work packages are broken into five phases:

Phase 1 – Preliminary study

In the first phase, a sensitivity study is made to determine the impact on pressure and temperature characteristics by identified relevant input variables (see Section 3). The number of simulations increases multiplicatively with the number of cases of each variable.

The simulation specification is handed to WP4 for carrying out the simulations.

Phase 2 – Development of initial protocol

The feedback from WP2 will be used as performance targets of the final protocol, while the feedback from WP4 preliminary simulations will be used to assess the gap between the average pressure ramp rate (APRR) approach and the performance targets.

During protocol development, there will be risk assessment sessions for viable initial protocol approach, to study how to safeguard and mitigate risk of using the initial protocol in field tests.

A viable initial protocol (including risk assessment) is proposed to WP4 and WP5.

Phase 3 – Support field testing

When WP4 and WP5 have accepted the viable initial protocol, a new specification for simulations are created from WP5 input on test equipment to be used for field testing.

The specification for simulations is then handed to WP4.

Phase 4 – Iterate and optimize control protocol

The feedback from WP5 field testing will be used as input to adjust the initial protocol. In this phase multiple handovers between WP3, WP4, and WP5 may occur before field testing confirms the performance targets has been reached.

Phase 5 – Final protocol

When the performance targets have been reached in field testing, the specification of the final protocol can be created.

The specification of the final protocol is handed to WP6 for dissemination.

2.2 Model

The development efforts depend on a model which can estimate the dynamics of the compressed hydrogen storage system (CHSS) during refuelling under various conditions.

In present simulation model, a black-box dispenser will deliver hydrogen to CHSS with defined geometries and material properties (see Figure 2).

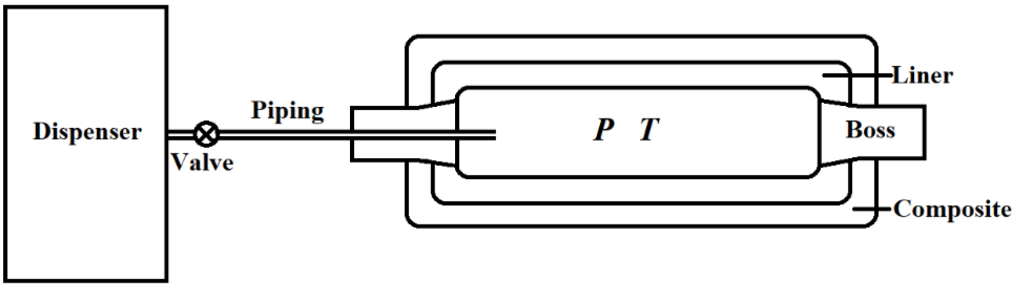

Figure 2: Sketch of simulation model (Source: Air Liquide)

2.3 Variables

In previous protocol development efforts and standards such as [SAE J2601 DEC2016], suitable units are chosen such that multiple variables can be presented in the same graph.

Table 1: Overview of variables and corresponding suitable units

Variables	Unit
Flow Coefficient	Normal cubic meters per hour [Nm^3 hr^{-1}]
Pressure	Megapascals [MPa]
Temperature	Celsius [°C]
Volume	Liters [L]
Time	Seconds [s] Minutes [min] Hours [hrs]
State of Charge	Percentage [%]
Pressure Ramp Rate	Megapascals per minute [MPa min^{-1}]

2.4 CHSS Limits

The definition of the variables for fueling events will affect pressure and temperature inside the CHSS. The following limits apply to ensure no damage occur to the tank:

- CHSS Pressure: Gas pressure shall not exceed 125% NWP.
- CHSS Temperature: Gas temperature shall not exceed 85°C.

3 INPUT

Until a complete specification has been constructed from PRHYDE WP2, the following variables are considered for preliminary simulations

3.1 CHSS Pressure Class

The scope of PRHYDE is to find a fuelling approach for HDVs with following nominal working pressure NWPs:

- H35 – 35 MPa at 15°C.
- H50 – 50 MPa at 15°C.
- H70 – 70 MPa at 15°C.

For preliminary simulations, one of each CHSS pressure class is considered.

3.2 CHSS Tank Type

For this study (focus: road applications) the following tank types for CHSS are considered:

- Type III – Tanks made from composite material with metal liner.
- Type IV – Tanks made from composite material with polymer liner.

For the preliminary simulations, both CHSS tank types are studied for each pressure class.

3.3 CHSS Volume

3.3.1 Total volume

The volume of HDVs considered in PRHYDE vary from 250 L[1] and up to 2500 L, but ideally the outcome of this project will result in fuelling approaches viable for 2500+ L hydrogen systems as well (trains, ferries, etc.)

For preliminary simulations, a fixed 1400 L total CHSS volume is considered, in two configurations:

a) 4x 350 L vessels
b) 28x 50 L vessels

The 1400 L is considered a suitable CHSS volume to all three pressure classes, resulting in a maximum hydrogen capacity of:

- 33.6 kg for H35,
- 44.3 kg for H50, and
- 56.3 kg for H70.

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[1] A volume of 250 L is used as upper threshold for the SAE J2601 fuelling protocols for light duty vehicles (LDVs), with the on-board hydrogen storage fuelled at flow rates up to 60 g/s [SAE J2601 DEC2016].

3.3.2 Single Vessels

The total volume is composed of one or multiple single hydrogen pressure vessels, with following properties to consider:

- Hydrogen volume geometry,
- liner layer thickness and properties, and
- composite wrapping layer thickness and properties.

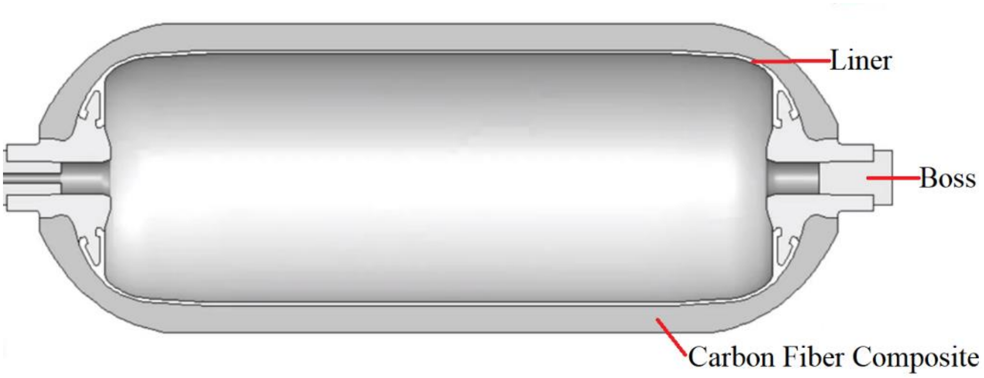

Figure 3 Composition of Type IV Hydrogen Pressure Vessel (Source: Air Liquide)

Note: Type III vessels are assumed to have no bosses.

Table 2: Single Vessel Characteristics – Type III Single Vessel (Small)

Description	H35	H50	H70	Unit
Internal volume	0.050	0.050	0.050	[m^3]
Internal length	0.710	0.710	0.710	[m]
Internal radius	0.150	0.150	0.150	[m]
Liner thickness	0.005	0.005	0.005	[m]
Composite layer thickness	0.010	0.017	0.027	[m]
Liner material density	2700	2700	2700	[kg m^{-3}]
Liner material specific heat capacity	1106	1106	1106	[J kg^{-1} K^{-1}]
Liner material thermal conductivity	164	164	164	[W m^{-1} K^{-1}]
Composite wrapping material density	1494	1494	1494	[kg m^{-3}]
Composite wrapping material specific heat capacity	1120	1120	1120	[J kg^{-1} K^{-1}]
Composite wrapping material conductivity	0.740	0.740	0.740	[W m^{-1} K^{-1}]
Boss material density	-	-	-	[kg m^{-3}]
Boss material specific heat capacity	-	-	-	[J kg^{-1} K^{-1}]
Boss volume	-	-	-	[m^3]
Boss contact surface with hydrogen	-	-	-	[m^2]
Boss contact surface with ambient air	-	-	-	[m^2]

Table 3: Single Vessel Characteristics – Type III Single Vessel (Large)

Description	H35	H50	H70	Unit
Internal volume	0.350	0.350	0.350	[m^3]
Internal length	1.240	1.240	1.240	[m]
Internal radius	0.300	0.300	0.300	[m]
Liner thickness	0.005	0.005	0.005	[m]
Composite layer thickness	0.010	0.017	0.027	[m]
Liner material density	2700	2700	2700	[kg m^{-3}]
Liner material specific heat capacity	1106	1106	1106	[J kg^{-1} K^{-1}]
Liner material thermal conductivity	164	164	164	[W m^{-1} K^{-1}]
Composite wrapping material density	1494	1494	1494	[kg m^{-3}]
Composite wrapping material specific heat capacity	1120	1120	1120	[J kg^{-1} K^{-1}]
Composite wrapping material conductivity	0.740	0.740	0.740	[W m^{-1} K^{-1}]
Boss material density	-	-	-	[kg m^{-3}]
Boss material specific heat capacity	-	-	-	[J kg^{-1} K^{-1}]
Boss volume	-	-	-	[m^3]
Boss contact surface with hydrogen	-	-	-	[m^2]
Boss contact surface with ambient air	-	-	-	[m^2]

Note: Type IV vessels are assumed to have steel bosses.

Table 4: **Single Vessel Characteristics – Type IV Single Vessel (Small)**

Description	H35	H50	H70	Unit
Internal volume	0.050	0.050	0.050	[m^3]
Internal length	0.710	0.710	0.710	[m]
Internal radius	0.150	0.150	0.150	[m]
Liner thickness	0.005	0.005	0.005	[m]
Composite layer thickness	0.015	0.022	0.032	[m]
Liner material density	945	945	945	[kg m^{-3}]
Liner material specific heat capacity	2100	2100	2100	[J kg^{-1} K^{-1}]
Liner material thermal conductivity	0.500	0.500	0.500	[W m^{-1} K^{-1}]
Composite wrapping material density	1494	1494	1494	[kg m^{-3}]
Composite wrapping material specific heat capacity	1120	1120	1120	[J kg^{-1} K^{-1}]
Composite wrapping material conductivity	0.740	0.740	0.740	[W m^{-1} K^{-1}]
Boss material density	7900	7900	7900	[kg m^{-3}]
Boss material specific heat capacity	500	500	500	[J kg^{-1} K^{-1}]
Boss volume	0.002	0.002	0.002	[m^3]
Boss contact surface with hydrogen	0.045	0.045	0.045	[m^2]
Boss contact surface with ambient air	0.047	0.047	0.047	[m^2]

Table 5: **Single Vessel Characteristics - Type IV Single Vessel (Large)**

Description	H35	H50	H70	Unit
Internal volume	0.350	0.350	0.350	[m^3]
Internal length	1.240	1.240	1.240	[m]
Internal radius	0.300	0.300	0.300	[m]
Liner thickness	0.005	0.005	0.005	[m]
Composite layer thickness	0.015	0.022	0.032	[m]
Liner material density	945	945	945	[kg m^{-3}]
Liner material specific heat capacity	2100	2100	2100	[J kg^{-1} K^{-1}]
Liner material thermal conductivity	0.500	0.500	0.500	[W m^{-1} K^{-1}]
Composite wrapping material density	1494	1494	1494	[kg m^{-3}]
Composite wrapping material specific heat capacity	1120	1120	1120	[J kg^{-1} K^{-1}]
Composite wrapping material conductivity	0.740	0.740	0.740	[W m^{-1} K^{-1}]
Boss material density	7900	7900	7900	[kg m^{-3}]
Boss material specific heat capacity	500	500	500	[J kg^{-1} K^{-1}]
Boss volume	0.002	0.002	0.002	[m^3]
Boss contact surface with hydrogen	0.045	0.045	0.045	[m^2]
Boss contact surface with ambient air	0.047	0.047	0.047	[m^2]

3.4 Ambient Temperature

The range of ambient temperature for which hydrogen refuelling is allowed spans from -40°C to 50°C.

For preliminary simulations, the reference ambient temperature is assumed to be 15°C.

3.5 Initial Pressure

The initial pressure of a vehicle allowed to refuel can be between 5 bar (minimum) and NWP (maximum), except for fuelling at sufficiently cold ambient temperatures (less than 15°C) that the maximum pressure for refuelling is lower than NWP to avoid overfilling.

For preliminary simulations, the reference initial pressure shall be adjusted such that the fill transfers 80% of the total mass capacity (starts at 20% mass capacity, fuels to 100% mass capacity)

3.6 Initial CHSS Temperature

For preliminary simulations, the reference initial CHSS temperature shall be equal to ambient temperature.

3.7 Reference Pressure Drop

The flow restrictions in the CHSS may impact the fuelling parameters on an overall level and definitely at the particular fuelling event. In [SAE J2601 DEC2016] is defined a range of characteristic pressure drop from 17 MPa to 35 MPa.

For preliminary simulations, the reference pressure drop is 20 MPa, as expected by vehicles using nozzle-receptacle connections according to [SAE J2600 OCT2015].

3.8 Fuel Delivery Temperature

The pre-cooling of delivered hydrogen has a profound effect on the fuelling time of Light Duty Vehicles (LDVs) but is also a big cost driver. For HDVs, the need for pre-cooling is expected to be less due to the larger CHSS volume and surface area, and compression heat is lower with lower pressure ramp rates.

For preliminary simulations, there will be both non-precooled and -20°C precooled hydrogen.

3.9 Fuelling Approach

The outcome of the PRHYDE project is to determine the optimal fuelling approach for HDV applications.

For preliminary simulations, it is assumed to use an APRR which can go from initial pressure to maximum operating pressure (MOP) in 10 minutes and 15 minutes, respectively. Other methods for further protocol development will be evaluated at a later stage.

3.10 Fuelling Stop Criterium

Present means to stop refuelling are examples of tables with target pressure, state of charge (SoC) and equivalent methods.

For preliminary simulations, the fuelling event shall stop when state of charge reaches 100%.

3.11 Communication

Means of communicating information from FCEVs to hydrogen refuelling station exists, most prominently exemplified by the infra-red communication described in [SAE J2799 APR2014] and used in [SAE J2601 DEC2016].

It is assumed that information provided by the vehicle includes as a minimum what is currently being communicated by existing means of communication between FCEVs and stations. These are

- ID: Protocol identifier
- VN: Vehicle number
- TV: Tank volume
- RT: Receptacle type
- FC: Fuelling command
- MP: Measured pressure
- MT: Measured temperature
- OD: Optional data

For the preliminary simulations, the communication is assumed active to enable SoC calculation on station side, because it is too early to determine non-com and fallback procedures during fuelling in a sensitivity study.

4 CHARACTERISTIC CASES FOR PRELIMINARY SIMULATIONS

In the preliminary simulations, the following variables are studied using the APPR approach.

Table 6: Selected characteristic cases for preliminary simulations

Description		H35	H50	H70	Unit
CHSS Tank Type		III IV	III IV	III IV	
CHSS Volume		1400.0	1400.0	1400.0	[L]
Single Vessel Unit	(28 vessels) (4 vessels)	50.0 350.0	50.0 350.0	50.0 350.0	[L]
Ambient Temperature		15.0	15.0	15.0	[°C]
Initial Pressure		6.0	8.0	10.0	[MPa]
Ref. Pressure Drop		20.0	20.0	20.0	[MPa]
Fuel Delivery Temperature		+15.0 - 20.0	+15.0 - 20.0	+15.0 - 20.0	[°C]
APRR	(10 min. fuelling time) (15 min. fuelling time)	3.78 2.52	5.45 3.63	7.75 5.17	[MPa min^{-1}]
Stop criteria		100.0	100.0	100.0	[%]

As a further assumption, thermal effects on inlet piping are not considered in the preliminary simulations. This totals up 48 simulations for WP4 to run. It is expected that a number of these simulations will exceed the CHSS Limits (see Section 2.4).

The results will answer following questions:

- How does vessel configuration impact end-pressure/temperature (few large vessels vs. many small vessels)?
- Which configurations does not need pre-cooling to achieve 100% fill without overheating at fuelling times of 10 and 15 minutes, respectively?
- Which configurations do need pre-cooling to achieve 100% fill without overheating at fuelling times of 10 and 15 minutes, respectively?
- Which configurations can be optimized by applying other approach than APRR?

5 LITERATURE

[SAE J2600 OCT2015]	Compressed Hydrogen Surface Vehicle Fueling Connection Devices, Revised 2015-10
[SAE J2601-1 DEC2016]	Fueling Protocols for Light Duty Gaseous Hydrogen Surface Vehicles, Revised 2016-12
[SAE J2601-2 SEP2014]	Fueling Protocols for Gaseous Hydrogen Powered Heavy Duty Vehicles, Revised 2016-12
[SAE J2799 APR2014]	Hydrogen Surface Vehicle to Station Communications Hardware and Software, Revised 2014-04

What is PRHYDE?

With funding from the Fuel Cells and Hydrogen 2 Joint Undertaking (FCH 2 JU), the PRHYDE project is aiming to develop recommendations for a non-proprietary heavy duty refuelling protocol used for future standardization activities for trucks and other heavy duty transport systems applying hydrogen technologies.

Based on existing fuelling protocols and current state of the art for compressed (gaseous) hydrogen fuelling, different hydrogen fuelling protocols are to be developed for large tank systems with 35, 50, and 70 MPa nominal working pressures using simulations as well as experimental verification. A broad industry perspective is captured via an intense stakeholder participation process throughout the project.

The work will enable the widespread deployment of hydrogen for heavy duty applications in road, train, and maritime transport. The results will be a valuable guidance for station design but also the prerequisite for the deployment of a standardized, cost-effective hydrogen infrastructure.

Further information can be found under https://www.prhyde.eu. For feedback on the PRHYDE project or the published deliverables, please contact info@prhyde.eu.

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