

# Thermal Simulation for Cryogenic Storage Systems

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## Abstract

The scope of this paper is the thermal simulation of a hydrogen supply system for future aircraft applications. The thermal model treats a whole cryogenic tank system with its main focus on influences and interactions of respective system components getting a better understanding of operational conditions and possible failure modes.

The thermal simulation model platform is based on a MATLAB/Simulink program, which results in fast, stable simulation runs and makes additional software redundant.

Supporting system's and components design in early concept phases is the overall goal, however in later development phases the thereby derived knowledge can be implemented into the control electronics of future aircraft applications.

## 1. Introduction

Reducing greenhouse gases is an important factor for future aircraft concepts. For this reason leading aircraft manufacturers are working on alternative energy supply concepts replacing the existing auxiliary power unit with fuel cell systems. Here, Solid Oxide Fuel Cells (SOFC) and Proton Exchange Membrane Fuel Cells (PEMFC) are the promising fuel cell concepts, which can be operated by hydrocarbons or hydrogen. As an environmental friendly energy form, hydrogen offers in its liquid state the highest energy density and the best mass to volume ratio [1] for this kind of systems.

The thermodynamic behaviour of a cryogenic liquid with the key aspects of pressurization and maximum storage time can be idealized by different mathematical approaches [4]. These models only describe the steady state behaviour of pressurization time, which sometimes is insufficient for a comprehensive system's understanding. By using CFD methods this problem could be partially solved, however from a budgetary point of view it is not suitable for early development phases.

The herein explained thermal simulation model is a zero-dimensional transient calculation tool based on a MATLAB/Simulink program, a code well suited for performing parametric studies as well as handling large volumes of data (e.g. fluid properties). It treats a whole cryogenic tank system with components for heating, feeding and safety devices as well as its environmental and operational conditions. The system's key requirements like control valve specifications, required heat input for feeding, dimensioning of safety devices and consideration of ambient conditions are also represented by this model.

Out of the above mentioned facts the simulation model can be seen as a comprehensive tool for early cryogenic tank system concept and design phases providing maximum flexibility with a minimum of analysis effort. Furthermore gained results, for example valve set pressure or response times, can be implemented into system's design respectively control electronics.

The National Institute for Standards and Technology [3] provides fluid properties in tabular form which are used in the thermal simulation model. Hydrogen can exist in two different energetic states, ortho-hydrogen (o-H<sub>2</sub>) and para-hydrogen (p-H<sub>2</sub>), showing differences in fluid properties such as specific heat and thermal conductivity. Below 50 K p-H<sub>2</sub> occurs to almost 100 %, at ambient conditions the distribution is 25 % p-H<sub>2</sub> and 75 % o-H<sub>2</sub>, this state is also specified as normal-hydrogen (n-H<sub>2</sub>). Due to the relatively slow para-ortho conversion in comparison to the heating process, the p-H<sub>2</sub> state is even valid for ambient conditions, therefore it has been selected for all simulation conditions.

A part of the work on the simulation model arose from an Austrian funded project in cooperation with a leading aircraft manufacturer and MAGNA STEYR participation in the SAE Working Group 80 "Hydrogen Fuel Cells". The model itself is a "living" model which is continuously refined and improved. The simulation results are constantly compared and validated with experimental data.

## 2. Thermodynamics

There are several ways and approaches existing to describe the thermodynamics of a fluid in the two-phase region. S. Gursu et al [4] analysed different models for the prediction of pressurization time: Homogeneous model, surface-evaporation model, thermal stratification model.

It is necessary to consider thermal stratification if no motion of the tank occurs and long boil-off times are expected. However, for aircraft operated hydrogen storage systems continuous extraction and a persistent motion of the fluid can be assumed, therefore the homogeneous model is a correct mathematical approach which provides sufficient accurate results. Note, that the motion of the fluid is not necessarily resulting from a motion of the complete tank system but rather convection effects induced by heat input from the inner tank heat exchanger. A short equation description is given in the following sub paragraph – for detailed explanation see [1].

### 2.1 Pressurization

In the thermal model we only consider non-isobaric change of state, expressing the first law of thermodynamics for an open system. In our case, we can neglect kinetic and potential energy as well as mechanical work:

$$\frac{dQ}{dt} = \frac{dU}{dt} - h \frac{dm}{dt} \quad (1)$$

The internal energy is a function of mass and pressure inside the tank:

$$\frac{dQ}{dt} = \frac{\partial U}{\partial m} \frac{dm}{dt} + \frac{\partial U}{\partial p} \frac{dp}{dt} - h_2 \frac{dm}{dt} \quad (2)$$

The change of specific internal energy according to the mass is defined by

$$\frac{\partial U}{\partial m} = u' - \frac{v'}{v'' - v'} (u'' - u') \quad (3)$$

and according to the pressure

$$\frac{\partial U}{\partial p} \approx \frac{U(p + \Delta p) - U(p - \Delta p)}{2\Delta p} \quad (4)$$

With the definition

$$\frac{dm}{dt} = -\dot{m} \quad (5)$$

and conversion to the pressure gradient we obtain

$$\frac{dp}{dt} = \frac{Q - \frac{dU}{dm} \dot{m} - h_2 \dot{m}}{\frac{dU}{dp}} \quad (6)$$

Equation (6) is the basis for calculating the pressurization gradient from one to another time step. All outside thermal influences are described and included by the heat into the system (Q). Mass change due to boil-off or feeding depends on the mass flow ( $\dot{m}$ ). The model is based on thermodynamic equilibrium, which means, that within the same time step the temperature and pressure inside the tank is uniform.

## 2.2 Heat Input

In general we distinguish between two types of heat input, the parasitic heat transfer through the insulation, pipes and suspension as well as the heat input by a heat exchanger. The omnipresent parasitic heat input has to be considered always and results in a moderate rise of pressure for a proper designed cryostat. Whereas the additional heat, induced by the heat exchanger, has to be considered only during its operation and provides a relatively high pressure gradient during feeding.

Depending on the cryogenic fluid, several insulation methods are applied on cryogenic storage systems. In case of foam insulation solid and convective heat transfer are the major heat transfer mechanisms, for superinsulated tank systems radiation and solid heat transfer are the significant parameters. Solid heat transfer is considered through Fourier's law, convective heat transfer with Newton's formulation and radiation by Stefan-Boltzmann law.

If we extract a cryogenic fluid from its vessel, an additional heat input is often required. The amount of required heat depends strongly on insulation performance, fluid thermodynamic properties (enthalpy, specific heat, specific volume, etc.), extraction mass flow, kind of extraction (gaseous/liquid) and mission of the cryogenic system.

## 3. Cryogenic Tank System

The simulation model is based on a tank system, which consists of a double walled, superinsulated liquid hydrogen ( $LH_2$ ) tank and an auxiliary systems box (ASB) with predefined components for a certain layout:

- $LH_2$  mass 25 kg
- Boil-off pressure 5 bar
- Boil-off valve
- 2 safety valves
- ASB heat exchanger for external coolant
- Inner tank heat exchanger (evaporator)
- Three way valve (TWV) to control  $H_2$  flow to evaporator
- Sensors
- Typical extraction 1 – 4 g/s

The modification of the tank system layout is user-defined and can be adapted to various configurations. Figure 1 shows a simplified scheme of the assumed system.

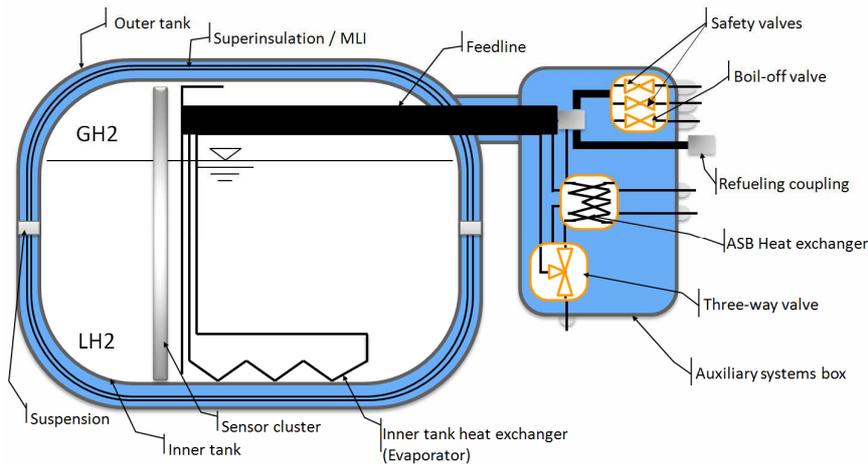


Figure 1: Simplified cryogenic tank system

The ASB heat exchanger has the function to heat up hydrogen to ambient conditions. The TWV controls the extracted mass flow. In position "open" a part of the extracted  $H_2$  mass flows through the inner tank heat exchanger and provides an additional heat input to evaporate hydrogen inside the tank and, at a minimum, maintains the inner tank pressure. Boil-off and safety valves protect the vessels against excessive overpressure.

## 4. Modeling in Matlab/Simulink

The challenge in the creation of the simulation model was to have a good overview of all input parameters and to get the main output parameters clearly and logically presented. Hence the idea was to prepare and initialize all data for Simulink in a m-File. During simulation, Simulink saves all necessary information in workspace variables which can be plotted afterwards in Matlab.

During development of the simulation model, the number of input parameters rose rapidly, so a good structuring of the m-File into different sections was necessary. For a good overview of the various input parameters, they are printed out to the command window during initialisation.

### 4.1 Boundary and Initial Conditions

All initial parameters and boundary conditions are predefined in a m-File. In general these conditions are

- Fluid type
- Initial pressure
- Boil-off pressure
- Tank geometry
- Initial filling level
- Boil-off and safety valve parameter (open/close characteristics)
- Heat exchanger parameter
- Extraction scenario (mission profile)
- Abort condition
- Failure scenarios

The component parameters can be adapted to user defined specifications. Figure 2 shows a generic opening and closing characteristic for a safety valve. The cross section of the valve determines the maximum mass flow at nominal pressure.

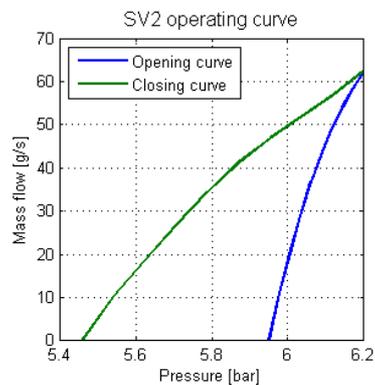


Figure 2: Generic valve characteristic

The ASB heat exchanger model is very detailed. Thus adjustments like the type of heat exchanger, heat exchanger geometry, flow direction (counter/parallel flow) and coolant (mass flow/temperature) can be defined by the user. The three-way-valve is the major component to control the bypass mass flow through the evaporator. The main settings are the opening position in % of the main H<sub>2</sub> stream and the pressure operating range.

An extraction scenario allows to specify a mission profile which includes the consideration of mass flow demand of consumer and environmental conditions (basic setting: International Standard Atmosphere). The next diagram (figure 3) shows a generic example for a flight mission with a certain mass flow at different flight phases from taxi over takeoff, climb, cruise and descend to landing.

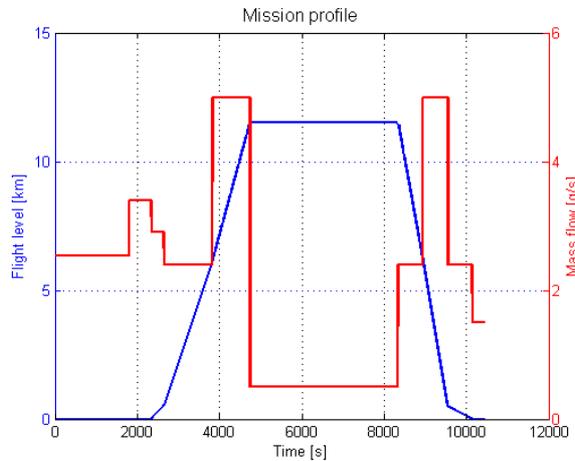


Figure 3: Generic mission profile

Stop criteria are defined by user specified time limits, residual fuel mass or system pressure. Also other stop criteria (e.g. boil-off, touchdown) can be easily implemented. Failure scenarios (e.g. insulation defects, heat exchanger failure, valve failure) enable the definition of operating limits and dimensioning of safety devices under given failure modes. The simulation model shows the behaviour of the cryogenic fluid if there is an exceptional situation, thereby unforeseen situations can be prevented by predefined measures.

The flow chart describes the sequence of initialisation and simulation steps:

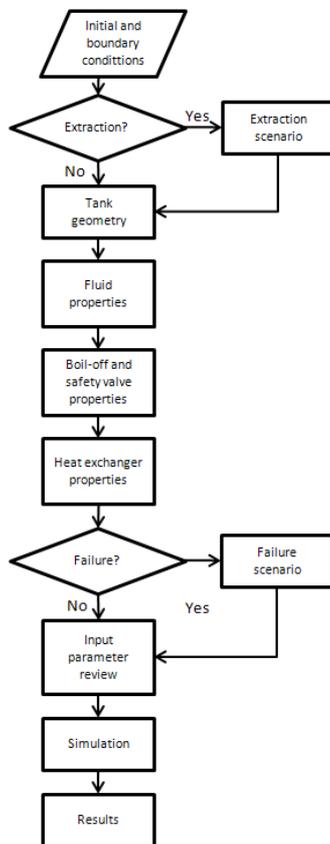


Figure 4: Simulation flow chart

For every time step the model calculates the new thermodynamic state with respect to the mass fraction of liquid and vapour. The simulation time depends mainly on the extraction scenario and failure simulation. The following table shows two examples of parameters:

Table 1: Simulation examples

	<b>Case 1</b>	<b>Case 2</b>
	<b>Pressurization</b>	<b>Extraction</b>
Fluid	H <sub>2</sub>	H <sub>2</sub>
Start condition [bar]	3	3
Tank volume [litre]	400	400
Filling [%]	80	80
Extraction [g/s]	0	3.4
Failure	no	no
Time step [s]	0.01	0.01
Abort (simulated) time [s]	60000	8240
Simulation time [s]	286	56

## 4.2 Output Parameters

The simulation model shows a number of parameters which can be defined by the user. The most important output information of the assumed system are listed below.

- Pressurization during operation and non-operation
- Boil-off rates at normal conditions and failure conditions
- System limitations due to environmental boundaries
- Operation conditions of Three-way-valve
  - Ideal valve flow rate
  - Ideal valve operating range
  - Switching cycles (Lifetime determination)
  - Operational characteristics for different mass flows and temperatures
- Residual mass (Range determination)
- Estimation of refueling cycles

### 4.3 Model Validation

To validate the simulation results, existing measured data from an automotive liquid hydrogen tank system (volume of 160 litre for 8 kg of LH<sub>2</sub>) have been compared to the calculated data.

Figure 5 demonstrates the comparison of measured and simulation data for maximum extraction mass flow (~6.7 g/s). At maximum extraction, stratification or temperature gradients inside the tank system do not matter, because the heat input through the evaporator is about 3000 W and the convective behaviour is comparable to that of an immersion heater in boiling water. The switch points of the TWV are set to 3.6 and 4.1 bar.

The pressure shows a similar behaviour at full tank as well as nearly empty tank fill levels for both, test and simulation results. The shorter time period between the switch points can be attributed to the descending fill level.

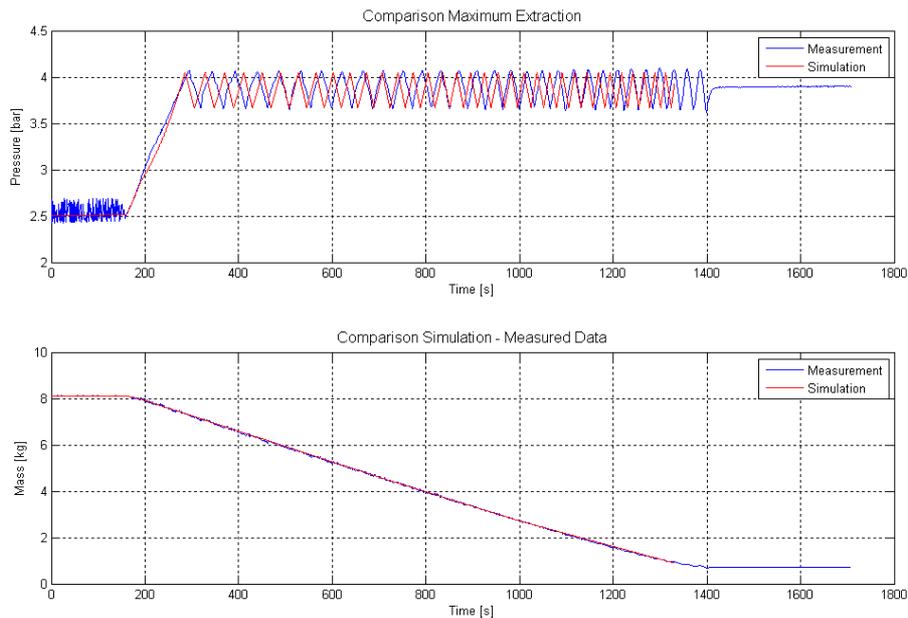


Figure 5: Simulation validation maximum extraction

Figure 6 shows the comparison of minimum extraction (~0.5 g/s). In that case no additional heat input is necessary, because of the low pressure drop. The simulated data shows a good compliance with the measured data.

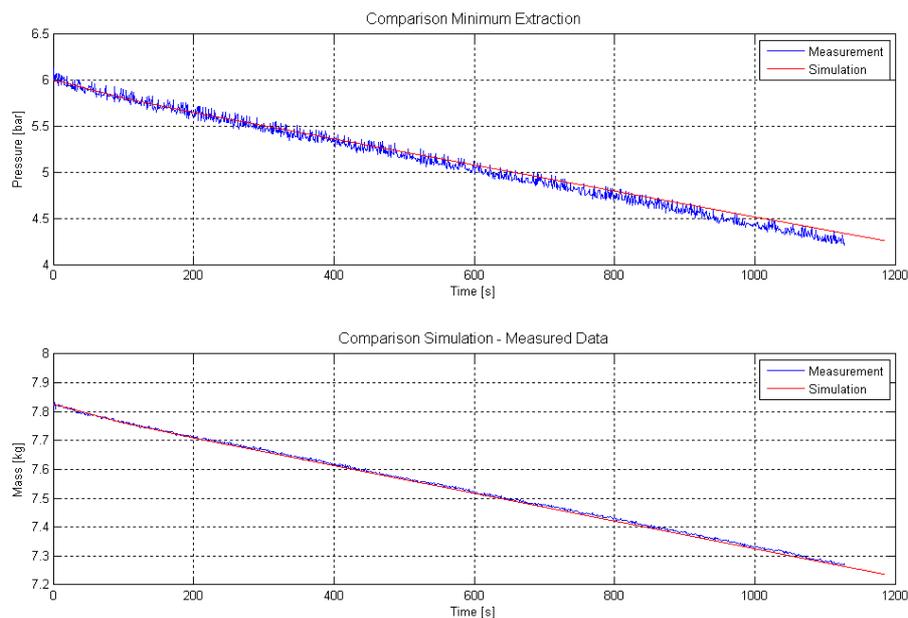


Figure 6: Simulation validation for minimum extraction

## 5. Results

### 5.1 Heat Input

The following plots give an overview of the simulation output possibilities. Figure 7 shows different H<sub>2</sub> mass flows at constant pressure and varying coolant temperatures. The four horizontal lines represent the minimum required heat input into the tank for a certain feeding mass flow to keep the pressure level constant. The graphs indicate that a TWV opening position for 10 to 20% flow rate of the total H<sub>2</sub> mass flow is adequate. A further aspect is the varying coolant temperature which has nearly the same influence over the whole control range.

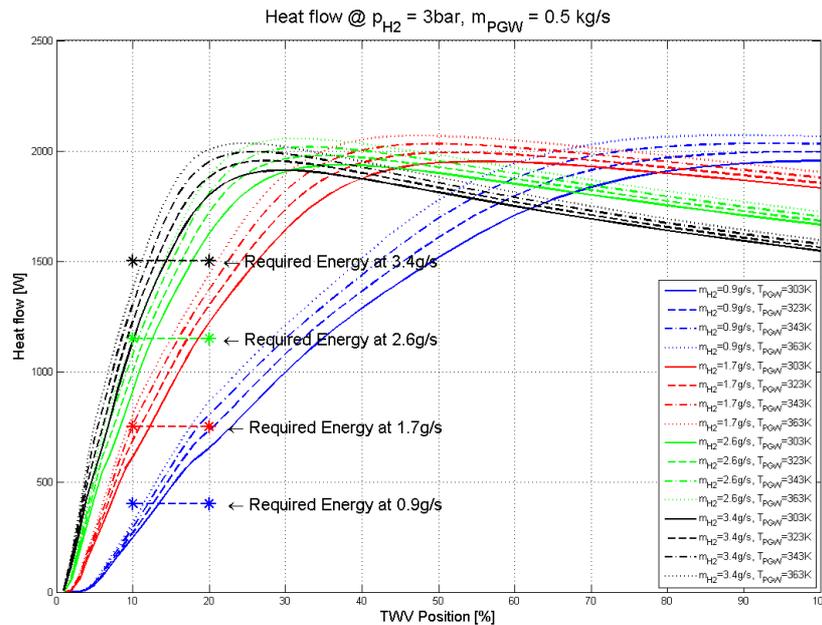


Figure 7: Heat input at changing coolant temperatures

Figure 8 shows a similar plot with the influence of changing H<sub>2</sub> pressures at constant coolant conditions. The graphs show that H<sub>2</sub> pressure has no considerable influence in the range of 10 – 20 % mass flow. At higher mass flows, the influence of H<sub>2</sub> pressure rises significantly.

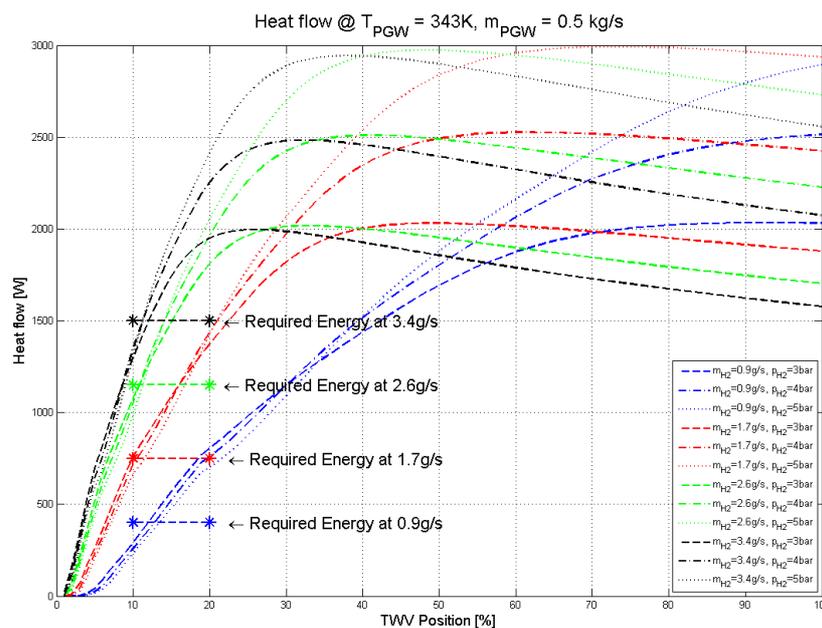


Figure 8: Heat input at changing H<sub>2</sub> pressures

### 5.1 H<sub>2</sub> Conditioning

Hydrogen consumers like fuel cells have minimum temperature (~278 K) and pressure requirements (~2.5 bar). The graphs in figure 9 give information about maximum hydrogen mass flow respectively minimum coolant temperature. In the control range of 10 to 20 %, the flowing H<sub>2</sub> mass can be heated up to the required conditions, even at low coolant temperatures. In the control range of about 70 to 80 % H<sub>2</sub> mass flow through the inner tank heat exchanger, the coolant temperature of 303 K would be too low.

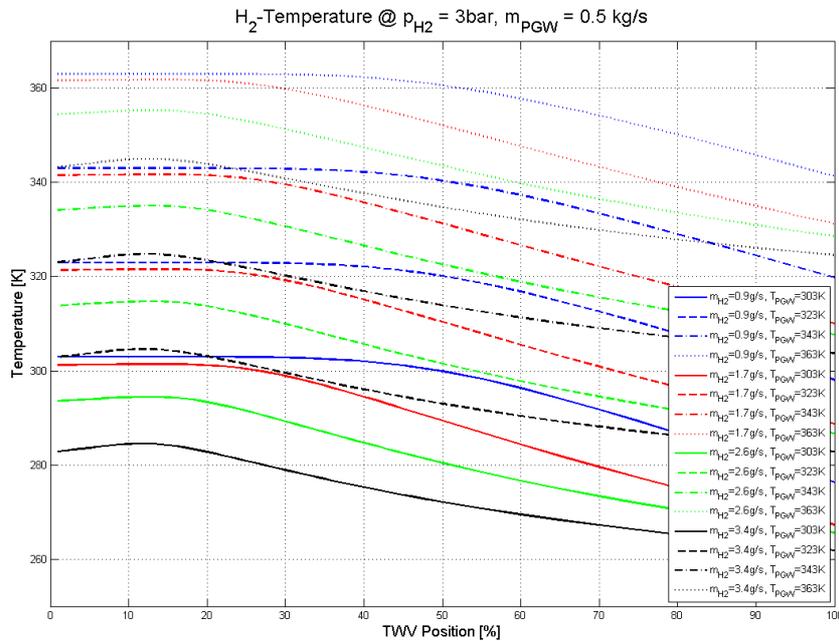


Figure 9: H<sub>2</sub> temperature at tank interface

Figure 10 illustrates pressure behaviour inside the tank and opening signal of the TWV over time at constant extraction. The number of TWV operation cycles are not constant over time and can be monitored with this diagram. In that case the red graph shows 68 switches in 1050 sec. (17.5 min). The extraction signal informs about extraction duration.

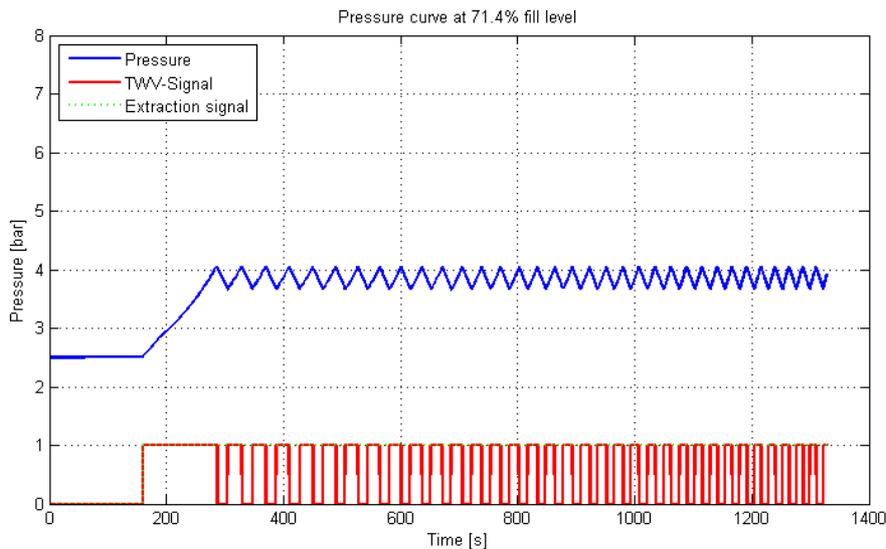


Figure 10: Constant extraction

## 6. Application Field

The thermal model offers a wide range of simulation possibilities where the user can map various cryogenic storage systems. The modular design allows a number of simulation options, different modules can be upgraded or replaced in a flexible way. The simulation model's main focus lies on mobile cryogenic storage systems and thus its applicability comprises a large extend of typical aerospace applications, such as:

- Primary or secondary energy source onboard commercial airplanes
- LH<sub>2</sub> storage for UAV propulsion
- LH<sub>2</sub>, LHe, LO<sub>x</sub> storage for space propulsion
- LHe storage for scientific space instrumentation (coolant)
- LNG storage for aerospace applications

Additionally, the storage of liquid natural gas (LNG) represents another but relatively new energy source for aerospace applications. The importance as mobile energy source grows fast and not only long haul heavy duty road transportation is the main application possibility of LNG. Although thermodynamic properties are totally different compared to LH<sub>2</sub>, the present simulation approach allows LNG modelling with only minor changes in input parameters.

Effects of microgravity or zero-gravity have not been included yet, however respective means of idealisation are possible and can be implemented.

## 7. Conclusion

The thermal simulation model for cryogenic storage systems predicts system behaviour of liquid hydrogen as well as other cryogenic storage systems. Assumption of thermodynamic equilibrium for mobile tanks gives sufficient accurate results under certain conditions to predict fluid behaviour inside the tank which is validated with measurement data.

Illustration of results shows different operation parameters and represents interaction of system components. Especially lightweight tank systems benefit from perfectly harmonized components and thus avoiding the installation of unnecessary weight (e.g. optimization of tank insulation, heat exchanger, etc.).

Implementation of failure scenarios indicate system application limits and give the possibility to implement measures for aircraft safety. The simulation model is also suitable for dimensioning the safety devices.

The main goal is supporting system's and components design in the early concept phase, however the derived knowledge can be implemented into control electronics in later development phases.

Next steps are validation tests with different tank geometries and other cryogenic fluids. Here boil-off tests are planned with different filling levels as well as different extraction scenarios. If there are further differences between measurement and simulation, they will be integrated into the simulation model.

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