

Development and Validation of a Numerical Thermal Simulation Model for Compressed Hydrogen Gas Storage Tanks

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ABSTRACT

The fueling of hydrogen vehicles in three minutes enabling ranges above 500 km offers a significant advantage over other types of electric powertrain vehicles. SAE [J2601](#), published in 2010, offers the first and only worldwide guideline to standardize fueling methodology. Due to the properties of hydrogen and compressed storage, each type and geometry tank heats up differently. Therefore, a hydrogen fueling methodology needs to take into account the range of storage anticipated from all automakers. This paper will describe a simulation tool developed in order to be able to assist in the development of a fueling procedure for GM; SAE [J2601](#) team and the validation thereof.

A reduced numerical simulation model has been developed that simulates the thermal response of a compressed gas storage tank operated under transient conditions. The stored gas is represented as a lumped mass with a spatially uniform temperature and pressure distribution inside the cylinder; a real gas model is employed to calculate the gas properties. The heat transfer through the cylinder wall is modeled by one-dimensional heat conduction in radial direction. The heat transfer coefficient from stored gas to the inner cylinder wall was provided by detailed three-dimensional transient computational fluid dynamics (CFD) simulations. These CFD simulations resolved all solid material layers as well the gas volume utilizing a real gas model. An instrumented tank with thermocouples inside both gas and cylinder walls was built and tested over a wide range of operating conditions to evaluate the quality of the simulation results. The test series included refueling and defueling at hydrogen gas flow rates ranging from 0.5 to 30 g/s at ambient temperatures from -40 to +40°C. The reduced simulation model predicts the average

gas temperature evolution during refueling to an accuracy of approximately 1°C.

INTRODUCTION

On-board compressed hydrogen gas storage is one challenging issue in the development of fuel cell powered electric vehicles. Due to the physical principals related to compression and expansion of gases, the stored hydrogen gas undergoes significant amplitudes in temperature during rapid fueling and extraction of the gas. The main development focus however is on fast and complete fueling, a “customer acceptable” fueling duration is 3 minutes for a 70 MPa rated tank system. In the past years there has been a multi-OEM approach coordinated by SAE to develop a common refueling standard for gaseous hydrogen surface vehicles. The result has been published recently by SAE in March 2010 as TIR [J2601](#) “Fueling Protocols for Light Duty Gaseous Hydrogen Surface Vehicles” [1]. Special attention has been paid to the diversity of refueling initial conditions, variety of fueling stations, and multitude of vehicle storage system designs. The resulting number of conceivable combinations rendered a sole experimental approach infeasible.

Instead, numeric simulation models were validated and employed to cover the variability occurring in real world. The huge number of simulations required demanded a reduced simulation model that was fast enough to produce the required results in an acceptable development time. This requirement excluded comprehensive CFD simulations due to their long computation time.

The reduced simulation model employed by GM and its validation using experimental data is described in the following. This includes the derivation of the mathematical

description, an instrumented cylinder, an experimental test series with hydrogen refueling and defueling, a detailed CFD simulation to provide heat transfer coefficients, and a comparison of simulation results with experimental data.

NUMERIC SIMULATION MODEL

The reduced numeric simulation model that is described in the following was developed to compute the transient temperature and pressure evolution of the stored gas as well as the temperature profile in the container wall within seconds. The two primary domains of a compressed gas cylinder are treated separately: the fluid domain containing the compressed gas and the solid domain which constitutes the cylinder wall. Each transition from gas to solid requires a heat transfer calculation, this comprises the outer cylinder shell to the ambient air as well as the liner's inner surface to the compressed gas inside the cylinder.

FLUID DOMAIN

The compressed gas is assumed to be in a perfectly mixed condition inside the fluid control volume at any given time. Its state is defined by the gas mass m and the internal energy U . The mass balance in [equation \(1\)](#) contains the inflowing and out flowing gas flow rates F_{in} and F_{ex} , respectively. The inflowing gas stream carries a specific enthalpy h_{in} while it is assumed that the out flowing gas has an enthalpy h equal to that of the gas inside the cylinder, $h_{ex} = h$. Any heat flux $\dot{Q}$ into the gas is accounted for by the third term in the energy balance [\(2\)](#). Both mass and energy balance are numerically solved by integration with respect to time, cf. [equations \(3\)](#) and [\(4\)](#). Refer to [figure 1](#) for an illustration of the fluid control volume.

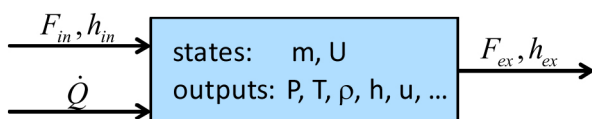


Figure 1. Illustration of fluid control volume

$$\frac{dm}{dt} = F_{in} - F_{ex} \quad (1)$$

$$\frac{dU}{dt} = F_{in}h_{in} - F_{ex}h + \dot{Q} \quad (2)$$

$$m = \int_0^t \frac{dm}{d\tau} d\tau \quad (3)$$

$$U = \int_0^t \frac{dU}{d\tau} d\tau \quad (4)$$

All derived properties of the fluid in the control volume are obtained by computing the density and specific internal energy according to [equations \(5\)](#) and [\(6\)](#), respectively, using the fluid volume V .

$$\rho = \frac{m}{V} \quad (5)$$

$$u = \frac{U}{m} \quad (6)$$

A fluid property database supporting real gas behavior by McCarty [2] is used to compute any fluid state variable such as pressure P , temperature T , and enthalpy h from the given density and specific internal energy, cf. [equation \(7\)](#).

$$P, T, h = f(\rho, u) \quad (7)$$

For the comparison between experiment and simulation, the enthalpy of the inflowing gas h_{in} is calculated according to [equation \(8\)](#) from the known pressure P_{in} and temperature T_{in} as well as the mass flow rate F_{in} at the inlet. The first term is the static contribution while the second term represents the kinetic energy of the flowing gas, it uses the cross sectional area A_{in} of the inlet pipe at the location where P_{in} and T_{in} are measured.

$$h_{in} = h(T_{in}, P_{in}) + \frac{1}{2} \left(\frac{F_{in}}{\rho(T_{in}, P_{in}) \cdot A_{in}} \right)^2 \quad (8)$$

SOLID DOMAIN

The heat transfer through the multi-layered solid cylinder wall is reduced to a one-dimensional problem by taking into account the radial component only. This simplification seems justified by the large cylindrical portion of the cylinder wall where heat transfer in radial direction dominates.

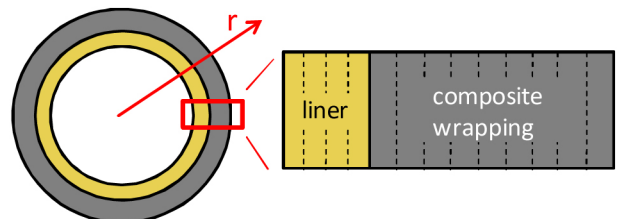


Figure 2. Illustration of solid cylinder wall

The transient heat transfer equation in radial direction considered here is presented in [equation \(9\)](#). The exponent q

depends on the coordinate system: For cylinder coordinates, $q = 1$. For spherical coordinates, $q = 2$.

$$\frac{\partial T}{\partial t} = \frac{1}{c(r,T) \cdot \rho(r,T)} \cdot \frac{1}{r^q} \frac{\partial}{\partial r} \left(r^q \lambda(r,T) \frac{\partial T}{\partial r} \right) \quad (9)$$

Equation (9) can be solved directly by defining a suitable exponent q , this has been done in [3]. A different approach has been pursued here. The heat transfer equation is solved numerically with a finite volume approach. The wall is modeled as composed of n finite volumes stacked in radial direction. They are wrapped around the fluid volume in the layered fashion of an onion skin. Each finite volume is assumed to have a homogeneous temperature distribution. Therefore, each finite volume has a contribution from both the cylindrical section and the two dome sections. The discretized form of the heat transfer equation is a set of n ordinary differential equations (10), (11), (12) for the temperatures T_k of each finite volume. The radial position of the center (node) of each finite volume is r_k . Each finite volume may have individual thermal properties, hence density ρ , specific heat capacity c , and thermal conductivity λ are functions of r_k . The two external heat fluxes $\dot{Q}_a$ and $\dot{Q}_b$ are applied to the set of equations in the form of given Neumann boundary conditions, cf. equations (10) and (12).

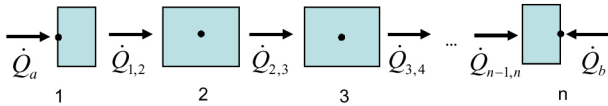


Figure 3. Illustration of wall discretization

First volume V_1 at inner surface boundary a:

$$\frac{dT_1}{dt} = \frac{1}{c(r_1, T_1) \cdot \rho(r_1, T_1) \cdot V_1} \cdot (\dot{Q}_a - \dot{Q}_{1,2}) \quad (10)$$

Intermediate volume V_k :

$$\frac{dT_k}{dt} = \frac{1}{c(r_k, T_k) \cdot \rho(r_k, T_k) \cdot V_k} \cdot (\dot{Q}_{k-1,k} - \dot{Q}_{k,k+1}), 1 < k < n \quad (11)$$

Last volume V_n at outer surface boundary b:

$$\frac{dT_n}{dt} = \frac{1}{c(r_n, T_n) \cdot \rho(r_n, T_n) \cdot V_n} \cdot (\dot{Q}_{n-1,n} + \dot{Q}_b) \quad (12)$$

The internal heat fluxes $\dot{Q}_{k,k+1}$ between the finite volumes are expressed in terms of the temperature difference of two adjacent nodes and a geometry dependent thermal resistance $R_{k,k+1}$:

$$\dot{Q}_{k,k+1} = \frac{1}{R_{k,k+1}} \cdot (T_k - T_{k+1}), 1 \leq k < n \quad (13)$$

The geometry dependent thermal resistance $R_{k,k+1}$ is computed according to [4], cf. equations (14), (15), (16).

Planar geometry with perpendicular heat flux (not used here for the compressed gas cylinder):

$$\frac{1}{R_{k,k+1}} = \frac{A}{r_{k+1} - r_k} \cdot \lambda_{k,k+1} \quad (14)$$

Cylindrical geometry with radial heat flux (used for cylindrical section of cylinder):

$$\frac{1}{R_{k,k+1}} = \frac{2\pi l_{cyl}}{\ln \frac{r_{k+1}}{r_k}} \cdot \lambda_{k,k+1} \quad (15)$$

Spherical geometry with radial heat flux (used for both end domes of cylinder):

$$\frac{1}{R_{k,k+1}} = \frac{4\pi}{\frac{1}{r_k} - \frac{1}{r_{k+1}}} \cdot \lambda_{k,k+1} \quad (16)$$

For the cylinder modeled here a combination of cylindrical and spherical geometry is used according to equation (17). The two hemispherical domes conduct heat parallel to the cylindrical section, hence the inverse thermal resistances are added.

$$\frac{1}{R_{k,k+1}} = \left(\frac{2\pi l_{cyl}}{\ln \frac{r_{k+1}}{r_k}} + \frac{4\pi}{\frac{1}{r_k} - \frac{1}{r_{k+1}}} \right) \cdot \lambda_{k,k+1} \quad (17)$$

The effective thermal conductivity $\lambda_{k,k+1}$ at each interface between two finite volumes is obtained from equation (18).

$$\lambda_{k,k+1} = \lambda \left(\frac{T_k + T_{k+1}}{2} \right) \quad (18)$$

HEAT TRANSFER

At both outer and inner cylinder surface, a simple heat transfer correlation is employed according to equations (19) and (20) to compute the heat flux across the surface. The heat transfer coefficient at the outer surface α_{amb} is held constant for all simulations presented in the following. This assumption is realistic since the instrumented cylinder described in the next section was located inside a climate chamber with constant ambient conditions (i.e. temperatures

and air circulation) throughout the experiment. The heat transfer coefficient α_{amb} will certainly not be constant for a vehicle driving at varying velocities, but this is not considered here. The heat transfer coefficient α in the fluid phase was treated in two ways. First, it was set constant, and secondly, it was set to the time dependent value obtained with a reference CFD simulation.

$$\dot{Q}_{\text{amb}} = -\dot{Q}_b = \alpha_{\text{amb}}(T_b - T_{\text{amb}}) \quad (19)$$

$$\dot{Q} = -\dot{Q}_a = \alpha(T_a - T) \quad (20)$$

INSTRUMENTED CYLINDER

An instrumented type IV pressure cylinder was built for the purpose of validating the numeric simulation model. The rated pressure was 70 MPa, the maximum allowed working pressure was 87.5 MPa. The valid temperature range was -80°C to $+85^{\circ}\text{C}$ for the stored gas and -40°C to $+60^{\circ}\text{C}$ for the environment. The internal volume was 129 liters. The liner was made of a high density polyethylene while the composite wrapping consisted of carbon fiber embedded into an epoxy resin. No components for regular operation (e.g. shut off valve, pressure relief device) were installed into the cylinder except for a mere test plug serving as a feed port for instrumentation sensors and fluid inlet/outlet.

All relevant material properties density, thermal conductivity, and specific heat capacity were measured for both liner and composite wrapping. Thermal conductivity and specific heat capacity were determined as functions of temperature in the range -100°C to +140°C in increments of 10°C. [Table 1](#) summarizes the range of values for each property and material.

Table 1. Solid material properties

Property	Liner	Composite
density, kg/m ³	900 ... 1000	1400 ... 1600
thermal conductivity, W/m/K	0.3 ... 0.8	0.3 ... 0.8 ¹ —
specific heat capacity, J/kg/K	1000 ... 3000	500 ... 1500

¹thermal conductivity in the cylinder's radial direction, i.e. perpendicular to carbon fibers

The cylinder was instrumented with 53 thermocouples (TCs) type K both in the fluid (14 TCs) and in the solid (39 TCs) domain. Additionally, three pressure transducers were installed in the inlet duct and inside the cylinder, cf. [figures 4](#) and [5](#). A horizontal array of five TCs (T7*) was dedicated to recording the axial temperature profile while a vertical array of five TCs (T8*, T73) measured the vertical profile along

the diameter. Three TCs (T6*, T161) were placed in the inlet duct, see figure 4.

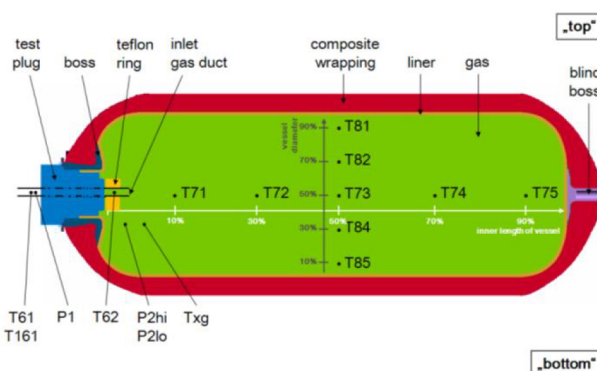


Figure 4. Fluid instrumentation

The main solid instrumentation consisted of two arrays of six TCs each in radial direction, one placed in the upper half of the cylinder (T1-T6) and a corresponding one in the lower half (T101-T106), cf. [figure 5](#). Thermocouples T1 and T2 were placed on the inner and outer liner surface, T6 was located on the outer composite wrapping surface, and T3 through T5 were positioned inside the composite wrapping, at radial increments of 25% of the composite thickness. In order to evaluate axial temperature profiles, reduced radial arrays (T11-T16, T21-T26, T111, T121) were positioned at the fore and rear end of the cylindrical section. Additional sensors were placed in the dome sections (T3*, T4*, T13*, T14*) and inside the test plug (T5*, T15*). The sensor Txo was dedicated to measuring the temperature of the sealing o-ring, it was used by the test bench to control a heating system that prevented the sealing from leaking at cold temperatures.

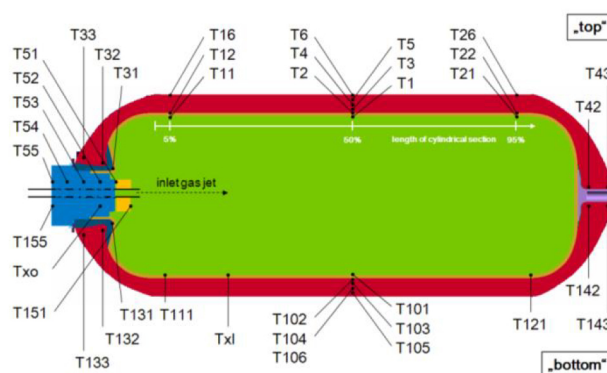


Figure 5. Solid instrumentation

The relevant temperature sensors were grouped by their location to form a reduced set of temperature information: