## APPROACH FOR THE DETERMINATION OF HEAT TRANSFER COEFFICIENTS FOR FILLING PROCESSES OF PRESSURE VESSELS WITH COMPRESSED GASEOUS MEDIA

Na Ranong Ch.\*, Maus S. and Hapke J. \*Author for correspondence Department of Plant System Design, Technical University Hamburg-Harburg, D-21071 Hamburg, Phone: +49 40 42878 3148, Fax: +49 40 42878 2992, E-mail: c.naranong@tu-harburg.de

## ABSTRACT

For fast and effective simulation of filling processes of pressure vessels with compressed gaseous media the governing equations are derived from a mass balance equation for the gas and from energy balance equations for the gas and the wall of the vessel. For simplicity the gas is considered as a perfectly mixed phase and two heat transfer coefficients are introduced. The first one is the mean heat transfer coefficient between the gas and the inner surface of the pressure vessel and the second one is the heat transfer coefficient between outer surface of the vessel and the surroundings. Although the process is transient, steady-state heat transfer coefficients for free convection are used between outer surface of the vessel and the surroundings. The use of available correlations for steady-state heat transfer coefficients to describe transient processes is common practice, e.g. in the modelling of the transient behaviour of heat exchangers [1]. But no correlations - neither steady-state nor transient - are available for the heat transfer coefficient between inflowing gas and inner surface of the vessel. To solve this problem a CFD tool is used to determine the gas velocities at the vicinity of the inner surface of the vessel for a number of discrete surface elements. The results of a large amount of numerical experiments show that there exists a unique relationship between the tangential fluid velocities at the vicinity of the inner surface of the vessel and the gas velocity at the inlet. Once this unique relationship is known the complete velocity distribution at the vicinity of the inner surface can be easily calculated from the inlet velocity of the gas. The nearwall velocities at the outer limit of the boundary layer are substituted into the heat transfer correlation for external flow over flat plates. The final heat transfer coefficient is the areaweighted mean of all local heat transfer coefficients. The method is applied to the special case of filling a 70 MPa composite vessel for fuel cell vehicles with hydrogen. Because

of the heat capacity of the composite wall consisting of an inner aluminium liner wrapped with carbon fibre, heat transfer from the compressed gas to the vessel wall strongly influences the temperature field of the gas which is predicted by the model and confirmed by experiments.

### INTRODUCTION

During filling of pressure vessels with compressed gaseous media, the pressure of the gas and the temperature of the gas and the vessel walls are transient. The shorter the duration of the filling process the larger is the increase of temperature of the gas during the process. This is especially important for composite vessels of fuel cell vehicles operated with hydrogen [2]. Figure 1 shows such a vessel connected to a filling station of the single buffer bank type. More advanced types of filling stations can be found in [2].



filling station.

The duration of the filling process is in the range of minutes resulting in a steep increase of temperatures, being relevant for safety aspects of design, especially for composite vessels [3] [4]. According to pressure vessel codes and pressure equipment directives the maximum gas temperature is the relevant design temperature [5] [6]. Therefore, it is desirable to predict the transient temperature distribution of high-pressure composite vessels by a simple calculation procedure during the design process.

#### NOMENCLATURE

Α	$m^2$	surface area
а	m <sup>2</sup> /s	temperature diffusivity
$C_p$	J/(kg K)	specific isobaric heat capacity
h	$W/(m^2 K)$	heat transfer coefficient
k	W/(m K)	thermal conductivity
$L_c$	m	characteristic length, i.e. length of the vessel
т	kg	mass
m	kg/s	mass flow rate
Nu	-	Nusselt number, $Nu = (h L_c)/k_F$
n	-	exponent, $n = 1$ for cylindrical vessel walls,
		n = 2 for spherical vessel walls
Pr	-	Prandtl number, $\Pr = v_F/a_F$
р	bar	pressure
Re	-	Revnolds number. Re = $w_W L_v v_F$
r	m	spatial coordinate perpendicular to the vessel wall
T	K	temperature
u	J/kg	specific internal energy
V	m <sup>3</sup>	volume
w	m/s	velocity of the gas
		, , , , , , , , , , , , , , , , , , ,
Greek letters		
1)	$m^2/s$	kinematic viscosity
0	$kg/m^3$	density
ν τ	8	time coordinate
19	°C	temperature
υ	C	temperature
Subscripts		
a		outer surface of vessel wall
е		entrance, inlet
F		fluid
forced		forced convection
free		free convection
i		inner surface of vessel wall
lam		laminar
sur		surroundings
total		total
turb		turbulent
W		vessel wall
0		initial
Abbreviations		
MBWR		modified Benedict-Webb-Rubin

### **GOVERNING EQUATIONS**

Figure 2 shows a sketch of a pressure vessel with the system boundary for the gas.



Figure 2 Sketch of a pressure vessel with the system boundary for the gas. An important property of the considered system is the constant control volume of the gas  $V_F = const$ .

The mass balance of the gas inside the control volume is given by equation 1.

$$\frac{dm_{\rm F}}{d\tau} = \dot{m}_{\rm e} \tag{1}$$

Equation (2) describes the energy balance. Due to high velocities of the gas at the inlet the specific kinetic energy  $w_{*}^{2}/2$  cannot be neglected.

$$\frac{d(m_F u_F)}{d\tau} = \dot{m}_e \left( u_e + \frac{p_e}{\rho_e} + \frac{w_e^2}{2} \right) + \bar{h}_i A_i \left( T_{Wi} - T_F \right)$$
(2)

The focus of this work is the determination of an appropriate mean heat transfer coefficient  $\overline{h_i}$  between gas and the inner surface of the vessel. In general  $\overline{h_i}$  refers to heat transfer by forced and free convection and by radiation, respectively. For the considered hydrogen pressure vessels radiation is negligible because hydrogen is non-radiating and the inner surface of the pressure vessel is nearly isothermal [2]. At the beginning of the filling, heat transfer by forced convection dominates. At the end free convection is determining, equation (3).

$$\overline{h}_{i} = \sqrt[4]{\overline{h}_{i,forced}^{4} + \overline{h}_{i,free}^{4}}$$
(3)

Equations (1) and (2) have to be solved for the initial condition

$$m_{F}(\tau=0) = m_{F0}$$
. (4)

The transient mass flow rate of the gas into the pressure vessel  $\dot{m}_e(\tau)$ , its temperature  $T_e(\tau)$  and pressure  $p_e(\tau)$ , Figure 2, result from the consideration of the coupled system consisting of pressure vessel and filling station, Figure [2].

The energy balance for the composite wall of the vessel is given by equation (5) taking into account heat conduction perpendicular to the vessel wall.

$$\rho_{W}c_{pW}\frac{\partial T_{W}}{\partial \tau} = \frac{1}{r^{n}}\frac{\partial}{\partial r}\left[r^{n}k_{W}\frac{\partial T_{W}}{\partial r}\right]$$
(5)

The boundary conditions at the inner surface of the vessel

$$-k\frac{\partial T_{w}}{\partial r}\Big|_{i} = \overline{h}_{i}(T_{wi} - T_{F})$$
(6)

and at the outer surface of vessel

$$-k \frac{\partial T_{w}}{\partial r}\Big|_{a} = \overline{h}_{a} \left( T_{wa} - T_{sur} \right)$$
<sup>(7)</sup>

have to be fulfilled.

In equation (7) the mean heat transfer coefficient  $h_a$  between the outer surface of the vessel and the surroundings refers to free convection and radiation and is obtained from [7].

Due to high pressures and temperatures during the filling process thermal and caloric equations of state for real gases are required. For compressed hydrogen a MBWR equation is appropriate [8]. For pure gases the specific internal energy not only depends on temperature but also on pressure [8] [9]

$$u = u(T, p). \tag{8}$$

The initial conditions with respect to the specific internal energy to solve equation (2) are given by initial temperature and pressure.

$$T_F(\tau=0) = T_{F0} \tag{9}$$

$$p_{F}(\tau = 0) = p_{F0} \tag{10}$$

## NUMERICAL EXPERIMENTS APPLYING CFD

In contrast to  $\overline{h}_{i,free}$  [7] no correlations can be found in literature for  $\overline{h}_{i,forced}$  of the considered filling process. Therefore, numerical experiments applying a CFD code with high Reynolds number turbulence model and standard wall function [10] are carried out. Figure 3 shows a typical velocity distribution. Compressed hydrogen is filled into a composite pressure vessel [2].



**Figure 3** Velocity profile of the gas during filling. The actual gas velocity at the inlet is 30 m/s.

The tangential fluid velocities in the vicinity of the vessel wall  $w_W$  are decisive for the heat transfer coefficient  $\overline{h}_{i,forced}$ . The numerical experiments reveal that there is a unique relationship between these velocities and the fluid velocity at the inlet. Figure 4 presents this relationship for a typical filling process. Each column of Figure 4 shows the fraction of the total inner surface where the velocity ratio  $w_W/w_e$  lies in a specific interval. This distribution is calculated by dividing the velocity range  $[0, w_e]$  into 400 intervals. The CFD calculations refer to the filling of a 70 MPa composite vessel for fuel cell vehicles with hydrogen. The maximum inlet velocity of hydrogen is 60 m/s. At no point of the surface the tangential velocity at the vicinity of the inner surface exceeds 4 % of the inlet velocity, i.e. the maximum fluid velocity at the outer limit of the boundary layer is 2.4 m/s.



Figure 4 Statistical velocity distribution of the gas at the vicinity of the inner surface of the vessel.

As can be seen in Figure 5 the statistical velocity distribution is nearly independent from the filling time. This relationship could be proved by further investigations taking into account short and long filling periods of vehicle tanks with compressed hydrogen. Figure 6 shows the velocity distribution of a 70 MPa tank supplied with hydrogen from filling stations without and with a booster [2]. There are nearly no differences between the velocity distributions of the various processes. Finally it can be stated that the statistical velocity distribution can be used to determine the complete velocity distribution at the vicinity of the inner surface from the inlet velocity of the gas for arbitrary filling processes. It has to be kept in mind that the statistical velocity distribution is obtained for a specific geometry of the vessel and for a specific gas, i.e. hydrogen. Nevertheless, this method is not restricted to the presented case but can be extended to vessels containing other gases than hydrogen and to vessels of other geometries by CFD calculations of new statistical velocity distributions.



**Figure 5** Statistical velocity distribution of the gas at the vicinity of the inner surface of the vessel.



**Figure 6** Statistical velocity distribution of the gas at the vicinity of the inner surface of the vessel. a) fast filling with constant inlet mass flow rate in 3 minutes, b) slow filling with constant mass flow rate in 8 minutes and c) filling from three different pressure banks and final booster in 3 minutes.

# CALCULATION PROCEDURE OF $\overline{h}_{i,forced}$

For the calculation of  $\overline{h}_{i,forced}$  the statistical velocity distribution and the inlet velocity are required. This leads to the following procedure:

- Calculate the tangential near-wall velocities from the inlet velocity using the statistical velocity distribution, Figure 4, Figure 5 and Figure 6.
- Calculate local Nusselt numbers from the correlation for flat plates by substituting the near-wall velocities  $w_W$  into equations (11) – (13) [7]. The fluid properties are determined with the actual temperature  $T_F$  and pressure  $p_F$ , respectively. The curvature of the vessel can be neglected because the boundary layers of velocity and temperature are small in comparison to the dimensions of the vessel.  $Nu_{forced} = \sqrt{Nu_{lam}^2 + Nu_{nurb}^2}$  (11)

$$Nu_{lam} = 0.664\sqrt{Re}\sqrt[3]{Pr}$$
(12)

$$Nu_{nurb} = \frac{0.037 \,\text{Re}^{0.8} \,\text{Pr}}{1 + 2.443 \,\text{Re}^{-0.1} (\text{Pr}^{\frac{2}{3}} - 1)}$$
(13)

Calculate the area-weighted mean of all Nusselt numbers.

$$\overline{\mathrm{Nu}} = \frac{\int_{A} \mathrm{Nu} \, \mathrm{d}A}{A_{\mathrm{total}}} \tag{14}$$

• Calculate  $\overline{h}_{i,forced}$  from the mean Nusselt number,  $\overline{h}_{i,forced} = \overline{\text{Nu}} k_F / L_c$  (15)

Figure 7 shows the mean heat transfer coefficients as a function of time for the three filling strategies of Figure 6. The contribution of free convection is included according to equation (3). The numerical values of 
$$\overline{h}_i$$
 are in the range between 100 W/(m<sup>2</sup> K) and 350 W/(m<sup>2</sup> K).



Figure 7 Mean heat transfer coefficients between gas and inner surface of the vessel for three different filling strategies of Figure 6.

#### RESULTS

For a fuel cell vehicle with a 70 MPa composite vessel, pressure and temperature of the hydrogen inside the vessel are measured during the filling process and compared with simulated data. Figure 8 shows good agreement between simulation and experiment, confirming the approach by the governing equations and the validity of the determination of the mean heat transfer coefficient between gas and inner surface of the vessel on the basis of the statistical velocity distribution.



**Figure 8** Comparison between simulation and experiment of gas temperature and pressure. a) process at the filling station in Sindelfingen. b) process at a mobile filling facility. Straight lines: measurement; dashed lines: experiment.

#### CONCLUSION

During the design phase it is desirable to predict the transient filling and discharging behaviour of pressure vessels. In particular this is valid for vessels of hydrogen-fuelled road vehicles in individual traffic. The importance will be underlined by the introduction of fuel cell cars with 70 MPa hydrogen vessels. With the described method the filling process of such vessels can be calculated using the introduced statistical velocity distribution for a given vessel geometry. This method is not restricted to the presented case but can be extended to vessels of other geometries and to vessels containing other gases than hydrogen.

### REFERENCES

- [1] Roetzel W., Yimin X., Dynamic Behaviour of Heat Exchangers, WIT Press, Boston, 1999
- [2] Maus S., Modellierung und Simulation der Betankung von Fahrzeugbehältern mit komprimiertem Wasserstoff, Fortschr.-Ber. VDI Reihe 3, Nr. 879, VDI Verlag, Düsseldorf, 2007
- [3] Inada T., Chou I., Eguchi H., Shigegaki Y., Tanaka T., Challenges to the Ultra High Pressure Hydrogen Tank for Fuel Cell Vehicles, *Proceedings of the 15th World Hydrogen Energy Conference*, Yokohama, 2004
- [4] Duncan M., Macfarlane S., Fast Filling of Type 3 Hydrogen Storage Cylinders, Dynetek Industries Ltd., Calgary, *General Hydrogen*, Richmond, 2003
- [5] AD 2000-Regelwerk, Arbeitsgemeinschaft Druckbehälter (AD), Verband der Technischen Überwachungs-Vereine (VdTÜV), Essen, Beuth, Berlin, 2008

- [6] *Directive 97/23/EC* of the European Parliament and of the Council of 29 May 1997 on the approximation of the laws of the Member States concerning pressure equipment
- [7] VDI-Wärmeatlas, Berechnungsunterlagen für Druckverlust, Stoffund Wärmeübergang, 10th edition, Springer, Berlin, 2006
- [8] Younglove B., Thermophysical Properties of Fluids. Argon, Ethylene, Parahydrogen, Nitrogen, Trifluoride and Oxygen, Journal of Physical and Chemical Reference Data 11, 1, 1982
- [9] Baehr H.-D., Thermodynamik, Springer, Berlin, 2005
- [10] Ferziger J. H.; Perić M., Computational methods for fluid dynamics, Springer, Berlin, 2002