A Numerical Simulation of the Filling Process in the Pressure Bottle

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***Abstract*— A filling process of the pressure bottle used for the air storage was investigated by numerical simulations. During the filling process, the temperature was rising up to maximal value and after that started to decline. The good match was found between experimental and numerical results. In order to reproduce the experimental conditions, the process of the filling bottle was controlled by the pressure which varied in time. This filling strategy influenced furthermore the mass flow rate and the air flow velocity. Because of the geometrical symmetry, the simulation was calculated as an axisymmetric problem.**

***Index Terms*— filling process, pressure bottle, temperature peak, turbulent flows**

I. Introduction

There is a possible to find many applications where the topic of the gas storage is attractive for many reasons. The vessel can store the gas under the high pressure; however, the capacity of the pressured gas is not as high as the usage of the liquefied gas. On the other hand, the filling process is less technical demanding. Nevertheless the filling process in a short time is required which has to be properly controlled to insure safety. Due to compression effects during the gas fast filling of a cylinder a temperature rise was induced whose intensity depends on filling rate, thermal properties of the walls and also geometric characteristics of the cylinder. The most attractive application of the filling gas process is to use in the vehicles for the hydrogen storage. The hydrogen as an alternative fuel seems to be promising in the future, however, the safety filling process must be ensured. The filling process and the study of the parameters having an effect on the safety process will be investigated in [1], [2], [3] and [11]. The raised temperature inside of the pressure bottle during the filling process is influenced by e.g. the heat transfer intensity in the bottle, time of the filling, inlet temperature, pressure at the begging and by the end of the filling etc. The size of the filling time controlled significantly the maximal temperatures, for instance, the slower filling process means lower temperature peaks [2]. Besides hydrogen, the liquid propane gas is usually store in the similar pressure bottles as well. The filling process and safety storage under extreme conditions were investigated by experiments and by numerical simulations in [13], [14] and [15]. For the filling of the breathing-gas bottles, air is used instead of the hydrogen, however, the similar effect of the raising temperature during the filling process could be observed as well [4]. Moreover, numerical study can predict the behavior of the gas inside of the pressure bottle if the pressure is exposed by extreme conditions, for instance, raising surrounding temperature [12]. In order to calculate the temperature increase, the heat coefficients for heat transfer from the gas to the surrounding of the pressure bottle is needed to be determine and furthermore used for heat calculations [5].

The objective of the paper is to calculate the temperature progress in time during the filling process of the breathing gas into the pressure bottle. Numerically obtained results are compared with experimental results [4]. Experiments were carried out on the measurement equipment which is presenting the real application at the Berlin fire brigade. During the filling process, measurements involved the temperature value saving inside of the breathing air bottle in order to identify the maximum occurring temperature and the corresponding specific location. Some comprehensive information about the numerical settings and testing of the numerical approaches can be found in [10].

II. Problem Formulation

A. Previous Studies

The complete 3D model of the pressure bottle was considered for numerical studies. The tetrahedral element type was used for meshing (see Fig. 1). Because of the higher demands on computational time due to huge amount of the mesh elements, only the first 10 second of the filling process was numerically examined. However during the first 10 seconds, it was possible to observe the significant variations of temperature and pressure at all. Founded results were in a good match with experiments and results obtained by the 2D axi-symmetrical flow simulation. This fact confirmed an assumption that 2D axi-symmetrical calculation can provided qualitatively

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adequate results and moreover the small mesh can save time required for a calculation process.

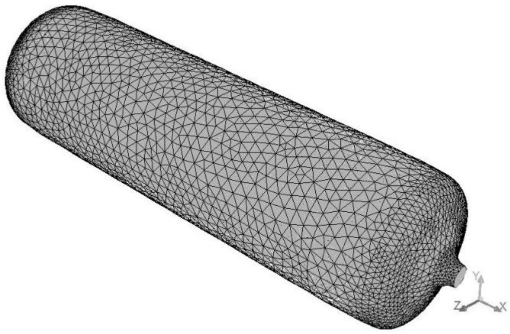

Figure 1. The 3D mesh of the pressure bottle

The assumption that the flow formed during the filling process should be seen as a transient process was confirmed by the steady state calculation study. Obtained results provided by the steady state calculation was completely different to real measured results. Even, if the steady state calculation was used only for the initialization, numerical results such as temperature values and the trend of the progress were completely wrong. Fig. 2 shows described this founded phenomena.

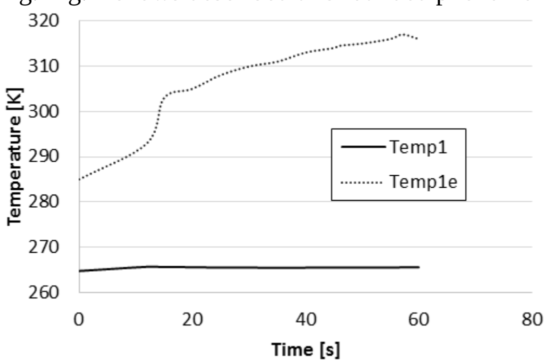

Figure 2. Progress of the temperature measured (point lines) and calculated (solid line)

So that the time depended calculation was further applied for a numerical study. This conclusion affected the pressure condition at the inlet of the vessel. According to the pressure measurement in the pipe line system of the gas filling equipment, the pressure in time was setting at the inlet into the calculation using UDF (User Defined Function). Several mathematical formulations were adopted in order to find appropriate flow and pressure results. Two different turbulence models the k-ε Standard and the SST k-ω respectively were tested and it was found, that the k-ω SST model provided generally more accurate results regarding the experimental data. In fact, the k-ω SST model combines advantageous of two turbulent approaches: k-ε and k-ω turbulent models [8]. One turbulence approach is used for the flow resolution in the area nearby walls (k- ω model), another one for free steam flow areas (k-ε model). Because the formed flow inside of the pressure vessel demonstrated different flow features combining the free stream flow and wall effects in time, the k-ω SST model is able to predict this complex flow effects more accurately.

B. Geometry and Filling Conditions

The pressure bottle and parameters of the gas filling are described as follows in Tab. 1.

TABLE I. BOTTLE PARAMETERS

Final bottle pressure	287 bar
Temperature of the inlet gas	-8 ℃ / 265 K
Diameter of the bottle	13.5 cm
Length of the bottle	49 cm
Thickness of the wall bottle	3 mm
Material	aluminum
Filling time	600 s

C. Experiments

For the experiment, two bottles were getting filled simultaneously, which is different from the case at the fire brigade that they fill up to 6 bottles simultaneously. There were six temperature sensors positioned inside the breathing air bottle and a temperature sensor in the Aluminum liner and two other self-adhesive surface thermocouples directly on the outer surface of the breathing air bottle.

For the temperature sensors for measuring the temperature inside the breathing air cylinder and in the inlet tube, type K thermocouples were used with a diameter
of 2 mm and a sheath. These temperature sensors were selected to the speeds of the filling process and a pressure to withstand 300 bar. The diameter of the drill holes were chosen to be 2.2 mm. This is to give the glue the possibility that to wet complete borehole. The temperature sensor in the aluminum liner was also Type K, but with a diameter of 0.5 mm. In the self-adhesive surface thermocouples are resistance thermometers PT100 probe for sticking.

In order to estimate a inaccuracy during the experiments, the two bottles being filled simultaneously, would be expected to have the exact readings yet there was minor differences. Other details about measurement can be found, for, example, in [4].

D. Numerical Models

The numerical study was performed using Ansys 17.2. The coupling between pressure and inlet is linear function, so that the difference between pressure at inlet and pressure inside the bottle is low enough to use the pressure-solver. The geometry of the pressure bottle is symmetrical so the 2D symmetrical model was considered for calculation. The 4 processes were used in a parallel solver, solver is pressure based in a 2D axisymmetric simulation. Because of the compress of the air, the compressibility must be solved. Because of the fact, that air contains mainly nitrogen, Soave-Redlich-Kwong gas model [6] was used. To capture a turbulence effect on the flow, the SST k-ω turbulence model [7] was adopted. Equation (1) is needed to calculate the turbulent kinetic energy.

$$\frac{\partial k}{\partial t} + U_j \frac{\partial k}{\partial x_j} = P_k - \beta^* k\omega + \frac{\partial}{\partial x_j}\left[(\upsilon + \sigma_k \upsilon_T)\frac{\partial k}{\partial x_j}\right] \quad (1)$$

The second equation used for the turbulence calculation is defined as in Eq. (2).

$$\frac{\partial\omega}{\partial t}+U_j\frac{\partial\omega}{\partial x_j}=\alpha S^2-\beta\omega^2+\frac{\partial}{\partial x_j}\left[(\upsilon+\sigma_\omega\upsilon_T)\frac{\partial\omega}{\partial x_j}\right]+2(1-F_1)\sigma_{\omega 2}\frac{1}{\omega}\frac{\partial k}{\partial x_i}\frac{\partial\omega}{\partial x_i} \quad (2)$$

For the turbulent boundary conditions at the inlet of bottle, the turbulent intensity used was 5% and the turbulent viscosity ratio was 10. To close the calculation procedures of the Eq. (1) and (2), auxiliary coefficients and relations are needed. Details about values and relations can be found in [7]. Several coefficients were suggested by Wilcox for original k- ω turbulence model [8].

For the boundary conditions an axis was defined in order to use the axisymmetric model, with a pressure inlet at the bottle nozzle, in which the UDF function was defined in the field of the Gauge total pressure. The steam total temperature was – 8 ℃. The room temperature was assumed to be 27 ℃, with a wall thickness of 3 mm made of Aluminum.

For the solution method a coupled scheme was used, standard initialization was used with values computed from a steady state simulation first. The other parameters used for the calculation were: gauge pressure 2.5 bar, axial initial velocity -1.5 m/s, turbulent kinetic energy 329.5255 m^2/s^2, specific dissipation rate: 2254961 s^{-1} and gauge temperature 265 K (-8 ℃).

For the heat transfer calculation, the outside wall heat transfer coefficient was of 50 W/m^2K, the heat transfer coefficient for heat conduction throughout the wall was given by aluminum and inside heat transfer coefficient was calculated by the numerical models. Details about basic heat transfer phenomena used in the theory of the numerical calculation can be found, for instance, in [9].

Most of the leading equations were discretized using second order upwind schemes. The transient formulation was based on the first order implicit.

E. Mesh and Boundary Conditions

The computational hexahedral mesh contains 4100 elements with maximum aspect ratio of 15.1. The 2D mesh and geometry is sketched on Fig. 1. ANSYS Mesh tools were sufficient for meshing as quadrilateral elements were used, and using an axisymmetric mesh shape (see Fig. 3) decreased the time of simulation by almost half. Several element layers were made close to the walls of the bottle as it was observed in earlier simulations that the flow is more complex as we get closer to the wall, other than that the geometry of the bottle can be considered simple and the filling process of the bottle yielded acceptable results.

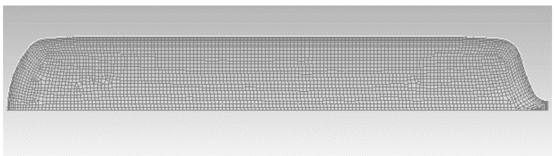

Figure 3. Geometry and mesh of the pressure bottle.

III. Results

A. Filling Process

The intensity of the filling process is controlled by the varying filling pressure, which was measured and inserted in to the computational code in order to reproduce the real experimental conditions.

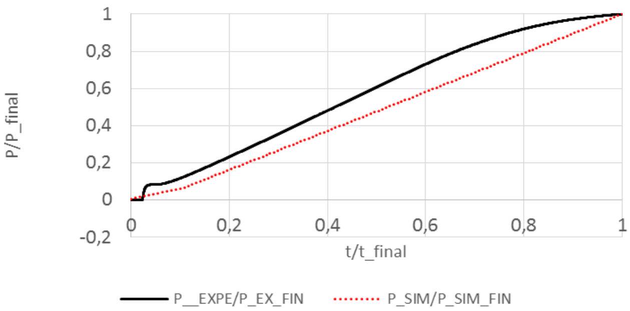

Figure 4. Change of the filling pressure in time.

Fig. 4 shows the pressure distribution in time for experimental and numerical investigation. The time was scaled by the final time and pressure by the final pressure when the bottle will be filled completely. The same non-dimensional expression was applied later for velocity, temperature variables etc.

The pressure in the experiment was obtained by means of a sensor drilled inside the cylinder. In order to decrease error during the measurement there were two pressure bottles measured under the same conditions, and the two sensors had a minor difference in the reading. So after obtaining the increase curvature of the pressure inside the bottle, it was required to write a UDF code into the CFD Software to simulate the pressure increase inside the air bottle as accurate as possible. For that reason a UDF function was written as a linearly increasing function. This function was prescribed at the bottle inlet condition.

Minor observed differences between these two curves can be identified in Fig. 4, especially that it in case of leaking bottle. It would be hard to get a linear pressure increase as it was used in the simulation, but even though that was the case, the error was within the acceptable range of 10%.

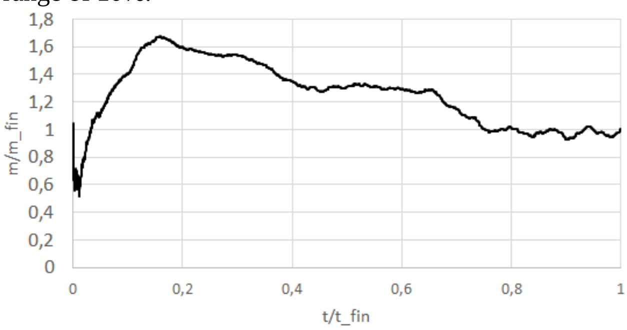

Figure 5. Change of the calculated mass flow rate at the inlet of the bottle.

The filling pressure influenced the mass flow rate in the time so that the total time of the filling as well. Fig. 5 describes the change of the mas flow rate in time at the inlet of the pressure bottle. The maximal gas filling intensity was found to be around non-dimensional time of 0.2.

B. Velocities in the Pressure Bottle

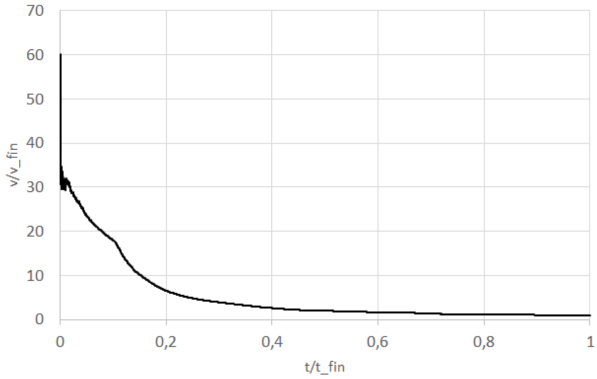

Figure 6. Nondimensional inlet velocity.

Fig. 6 shows the inlet velocity, scaled by the inlet velocity at the end time of the filling process, in time which was again scaled by the total time. The maximal inlet velocity intensity was detected at the beginning of the filling process where the pressure different between filling pressure and pressure in the empty bottle was the highest. During time, the inlet velocity intensity was gradually declining. The maximal velocity magnitude reached the level of 60 times higher than the velocity magnitude at the roughly full pressure bottle. Later the inlet velocity magnitude declined to the level of 30 times higher than the final inlet velocity. During this time period of the higher inlet velocity, the maximal temperature was identified (see Fig. 7).

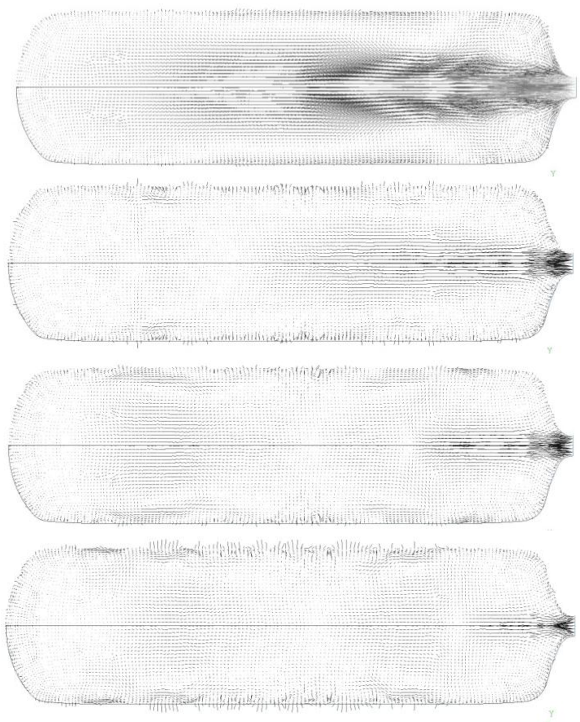

Figure 7. Velocity vectors for different non-dimensional time steps: t*=0.0083, 0.2, 0.5 and 1.

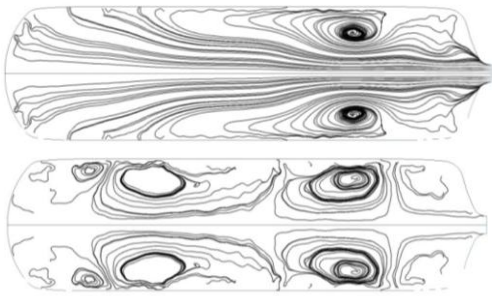

Figure 8. Velocity iso-lines in time t*=0.0083 and 1.

Fig. 7 shows the velocity vector fields for different time steps. For the non-dimensional time 0.0083, the jet of the air was created and the maximal velocity intensity was detected at the inlet of the bottle. This air jet slowly weakened during the time of the filling progress. Fig. 8 illustrates isolines of the instantaneous velocity for time 0.0083 (at the beginning of the filling phase) and 1 (the end of the gas bottle filling). At the time of 0.0083, the strong air jet was visible in simulations and two vortices were simultaneously formed in inside space of the bottle. At the time of 1, the more vortices with different intensity and orientation were found. The heat transfer phenomena influenced the final air temperature inside of the pressure bottle and this effect was involved by the calculation of the heat coefficient at the inner part of the bottle wall.

C. Temperatures in the Pressure Bottle

Temperatures of the air inside of the bottle calculated numerically were compared by the experimental results at the three different positions: behind the inlet (T1), middle (T2) and close to the bottom (T3) of the bottle. For the position T1, the temperature deviation between numerical results and experiments was varying between 3.8% and 14.8% and even for the maximum deviation the results could be considered in a good match in respect to the accuracy of the numerical approaches.

At the position T2, the calculated inlet temperature stayed the same until the air flow reached second sensor, which is somewhere in the middle of the bottle while the experiment showed that even at the start of the filling process the sensor indicated some higher temperature (280 K). It could be due to the fact that in the simulation the air bottle was assumed to be empty, while that could not have been the case in the real experiment. It was also observed that the two readings catch up as time went by reaching a zero deviation somewhere around t = 0.05 and then the difference was maintained till the end of simulation with a maximum deviation of about 6% (see Fig. 9).

Figure 9. Temperature in time - experiments versus numerics.

At the position T3, there was a higher deviation about 9%. The temperature deviation seemed to be varying violently all through the first 60 seconds (up to 0.1), even reaching zero twice, which could be due to several factors include inaccurate results in the experiment itself. At the beginning there was an assumption that might be causing this deviation, which was the initial pressure difference between the inlet and the pressure inside the bottle. The deviation seemed to stabilize as the simulation carried out with a maximum of 6% which could be considered as a good match between experimental and numerical results.

IV. Conclusion

Numerical simulations were adopted to identify a change of gas temperature during the filling of the pressure bottle. The particular bottle and filling conditions were considered for the flow study. To obtain an appropriate temperature development the heat transfer coefficients must be setting up or calculating. The filling process was control by the pressure change which furthermore influences a mass flow rate and in other words the intensity of the filling process.

The found numerical results were in a good match to the experimental results. The maximal temperature deviation was found close to the inlet of the bottle, however, during the filling process, this temperature deviation reached temporally maximal 14.8 %. Because of the turbulence flow, the k-ω SST model was successfully adopted. The numerical study was calculated effectively if the axi-symmetrical conditions were considered which furthermore led to the axi-symmetrical swirl flow calculations. In the perspective, effect such as the filling time or heat transfer coefficients at the outside of the pressure bottle should be involved for parameter studies.

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