Final design, fluid dynamic and structural mechanical analysis of a liquid hydrogen Moderator for the European Spallation Source

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Abstract. The European Spallation Source (ESS) is currently in the construction phase and should have first beam on Target in 2019. ESS, located in Sweden, will be the most powerful spallation neutron source worldwide, with the goal to produce neutrons for research. As an in-kind partner the Forschungszentrum Juelich will among others, design and manufacture the four liquid hydrogen Moderators, which are located above and below the Target. Those vessels are confining the cold hydrogen used to reduce the energy level of the fast neutrons, produced by spallation in the Target, in order to make the neutrons usable for neutron scattering instruments. Due to the requirements [1], a fluid dynamic analysis with pressure and temperature depended hydrogen data, taking into account the pseudo critical phenomena and the pulsed neutronic heating (pressure waves) is necessary. With the fluid dynamic results, a structure mechanical analysis including radiation damage investigation (RCC-MRx code [5]), low temperature properties as well as strength reduction by welding can be realized. Finally, the manufacturing and welding completes the design process.

1. Introduction

In addition to the low operating temperature (17-21 K), the cold moderator is permanently subjected to interactions of neutrons with the structural material (AL6061-T6) and the moderator medium (LH₂). These conditions cannot be simulated in experimental tests. On the one hand, this is due to the lack of hydrogen infrastructure (pumps for this operation conditions are not available off the shelf). On the other hand, the enormous volumetric heat input by neutrons, which depends mainly on the proton beam of 5 MW, is almost impossible to be reproduced by an experiment. Therefore, in this case, the fluid dynamic simulations are of particular importance, since before commissioning no further real flow tests can be experimentally carried out. For the subsequent strength analysis according to nuclear code RCC-MRx [5], in addition to the simulation of the temperature- and pressure- field the flow analysis need to answer some basic questions like: whether such large heat load can ever be sufficiently dissipated; how the pulsed heat input affects the pressure (pulses) and local boiling phenomena, etc. Finally, the current stage of manufacturing will be shown.
2. Design of cold Moderator vessel

The shape of the moderators is mainly based on the neutron-optimization calculations (outer envelope geometry) [1]. The inner shape of the vessel needs optimization. These flow guides are necessary, in order to avoid recirculation areas, local bubbling and to increase the stability of the vessel (figure 1, bottom right). The final design is shown in figure 1.

Figure 1: ESS cold moderator design solution: Left: vessel including friction welding adapter. Right: cut view including optimized fluid guides.

One requirement is to use an aluminum alloy for the fabrication of the moderators. Nevertheless, due to the high thermal expansion of the aluminum alloy, the long attached pipework (~ 6 m) should be made out of invar (alloy 36) which has a very low thermal expansion coefficient. The Invar pipework is connected via friction welding to the vessel (see figure 1). Additionally between aluminium and invar, a layer of stainless steel is implemented, because stainless steel has almost half of the thermal expansion of aluminum and reduces significantly the inner, thermal induced stresses in the friction welded area. The vessel itself is welded in a vacuum chamber via electron beam welding, in order to reduce the build-up of a deleterious oxide layer. To avoid heat cracks, which is a special issue of hardened aluminium alloys, an additional weld filler is used, which has 12% silicon content (AlSi12). The silicon content reduces the risk of heat cracks during welding significantly [6].

3. Material properties for structural-mechanical and fluid dynamical analyses

Pure aluminum is almost transparent for cold and thermal neutrons. Due to the high operating pressure of hydrogen (15 bar), it was necessary to use a high-strength aluminum alloy (AL6061-T6) even though because of their alloy constituents more neutrons are absorbed than in pure aluminum. The necessary material data were taken as functions, which have the form of f(T) from [2]. For the hydrogen properties, a range of 10-20 bar and 15-40 K were selected, so that pressure and temperature fluctuations in the pulse can be taken into account. Because of the abrupt changes in the material properties at some points, (phase change) no functions for H₂ could be created. Instead, real gas property (RGP) tables were created, which have the form of f(T, p) and could be taken from [3].
3.1 Fluid parameters

When choosing the operating parameters, the following requirements have to be considered: Temperature range (average inlet temperature 17 K and average outlet temperature 21 K) to avoid changes of neutronic performance, avoidance of phase changes (burnout, instability of the flow), mechanical stresses on the structure material (pressure, pressure pulses) and possibility to remove the heat (liquid).

![Phase Diagram H2](image)

**Figure 2:** Phase diagram of hydrogen including simulation area and pseudo-critical line.

Besides the usual three phases (solid, gaseous and liquid), according to the H\textsubscript{2} phase diagram (fig. 2) there is still an undefined area. This area, a kind of mixed phase, is called supercritical phase, because it exceeds the critical point (defined by \( p_c \), \( T_c \)). We need to distinguish among three areas: subcritical pressures with overcritical temperatures, overcritical pressures with subcritical temperatures and overcritical pressures with overcritical temperatures. Only the last case represents a so-called supercritical fluid, which means that, as the temperature increases, no more phase change phenomena are observed. Operation with overcritical pressures and subcritical temperatures, however, can result in normal phase change phenomena such as blisters and film boiling, which should be avoided. That means, there exists a kind of boiling curve, called pseudo-critical line (PS). This can be interpreted as an extension of the normal boiling curve. Therefore, a pressure-dependent pseudo-critical boiling temperature \( T_{ps}(p) \) also exists. Hydrogen has (whether over- or subcritical pressure) a very small temperature range in the clear liquid phase, which, however, increases with increasing pressure. Thus, a high operating pressure should be sought in order to avoid phase changes. On the other hand, by increasing the pressure, the load on the structural material increases. Due to these requirements, for the ESS Moderator, an operating pressure of 15 bar with an inlet-temperature of 17 K and outlet-temperature of 21 K have been chosen leading to an overcritical pressure with subcritical temperature. Whereby the maximum local temperature in hydrogen is given by the pseudo-critical boiling temperature \( T_{ps}(p) \) according to hydrogen phase diagram: \( T_{max}(p=15 \text{ bar})<T_{ps}(p=15 \text{ bar})<34 \text{ K} \). The mass flow depends on the heat capacity, the total heat input and the allowable temperature rise to a total of:

\[
\dot{m} = \frac{\sum Q_i}{(c_p \rho_m \Delta T)}
\]

and amounts to \( \dot{m} = 1 \text{ kg/s} \)
4. Neutron heat

In order to calculate the stresses in the materials of the cold moderators caused by unsteady pressure and temperature gradients at different operation conditions, the heat generation by neutrons in the moderators was calculated by the Neutronic Group of ESS [1] and provided for fluid dynamic simulations. The calculated data of heat distribution was obtained using a Monte-Carlo-method. Therefore, to include the heat data into the fluid dynamic simulations, approximation functions to the heat data have been developed and are presented in this chapter. The heat input by neutrons in the moderators is an intermittent process with a particular pulse frequency and pulse length and is approximated assuming rectangular shaped pulses for maximum heat input. Then, the relation between the time averaged constant heat \( h_{st} \) and the transient heat \( h_{tr} \) is:

\[
\frac{h_{st}}{h_{tr}} = f_{\text{pulse}} \cdot t_{\text{pulse}}
\]

with the pulse frequency \( f_{\text{pulse}} \) = 14 Hz and the pulse duration \( t_{\text{pulse}} \) = 2.86 ms [1]. The heat generated during one pulse is, therefore, 25 times higher than the time averaged heat input and must be handled. Generally, the heat load generated in a specific body strongly depends on the material density, the cross-section and on the distance to the spallation source. In general with increasing material density, the interaction probability of the neutrons with the material of the body increases, and thus, more heat is deposited compared to a light material. The heat load almost decreases with the square of the distance to the spallation centre. In addition, the heat load depends on the material that acts as barrier between the point of interest and the source. The distribution of the volumetric heat \( h_{st} \) that depend on Cartesian coordinates and material density, as calculated and provided by the Neutronic Group of ESS, is shown in figure. 3.a and figure. 4.a for hydrogen and aluminium, respectively. The spherical decrease in heat intensity with distance to the spallation centre \((x = 0, y = 0, z = 0)\) is clearly visible. Materials and fluids like Hydrogen that are closer to this centre is exposed to a higher heat generation by neutrons. Typical for the neutron flow of the spallation process is the shifted peak of the heat load in forward direction of the protons beam (negative x-direction) impacting onto the target which is well observed in the calculated heat distribution in aluminium (figure. 4.a).

\[h_{[W/cm^3]}\]

\[h_{[W/cm^3]}\]

\[(y^2+z^2)^0.5 [cm]\]

**Figure 3:** Analysis of neutron heat in hydrogen: a) visualization of the heat distribution in hydrogen; b) approximation function of the heat distribution (surface layer) and original data points, assuming an axis-symmetrical distribution for CFD simulation.
Figure 4: Analysis of neutron heat load in aluminium: a) visualization of the heat distribution in aluminium; b) approximation function of the heat distribution (surface layer) and original data points, assuming an axis-symmetrical distribution

The distribution of the time averaged volumetric heat \( h_{st} \) generated in the moderators is characterized by non-linear surface approximation functions fitted from neutron simulation data depending on the distance to the spallation source as well as on the material, where the moderators consist of aluminium and hydrogen. For the functions, an axis-symmetrical distribution of the heat \( h_{st} \) is assumed along the direction of the proton beam (x-direction) in order to use approximation functions of the form:

\[
h_{st} = f(x, r), \quad \text{with: } r = \sqrt{y^2 + z^2}
\]

Two different surface approximation functions are used for aluminium and hydrogen, as their distribution characteristics are different and the relative error should be minimized. Hence, a Lorentz- and a Gauss function are used for H\(_2\) and Al, respectively. The Lorentz function used for hydrogen is:

\[
h_{h}(x, y, z) = h_{0,h} + \frac{a_1}{1 + \left(\frac{x + a_2}{a_3}\right)^2} \left[1 + \left(\frac{\sqrt{y^2 + z^2} + a_4}{a_5}\right)^2\right]
\]

with coefficients \( h_{0,h} = -0.173 \text{ W/cm}^3, a_1 = 101.786 \text{ W/cm}^3, a_2 = -0.423 \text{ cm}, a_3 = 18.204 \text{ cm}, a_4 = 3.566 \text{ cm} \) and \( a_5 = 3.343 \text{ cm} \), and the Gauss function used for aluminium is:

\[
h_{a}(x, y, z) = h_{0,a} + b_1 \exp \left(-\frac{1}{2} \left(\frac{x + b_2}{b_3}\right)^2 - \frac{1}{2} \left(\frac{\sqrt{y^2 + z^2} + b_4}{b_5}\right)^2\right)
\]

with coefficients \( h_{0,a} = 2.287 \text{ W/cm}^3, b_1 = 33.9 \text{ W/cm}^3, b_2 = -5.34 \text{ cm}, b_3 = 13 \text{ cm}, b_4 = 17.24 \text{ cm} \) and \( b_5 = 18.18 \text{ cm} \). The coefficients \( h_{0,h}, h_{0,a}, a_i, b_i \) were calculated iteratively using the Levenberg-Marquardt algorithm. The resulting functions as well as the corresponding heat data are shown in fig. 3.b and 4.b. The non-linearity of the data is well observable and the discrepancy in heat depends on the location. The total heat induced into the moderators as calculated by summarizing the heat load data is:

\[
Q_{t,mod,orig} = \sum h_i V_i
\]
and the approximated heat load $Q_{\text{mod,approx}}$ as calculated by integration over the total volume of the four cold moderators using the approximation functions is 17.64 kW. The efficiency of the heat approximation is shown in figure 5. The heat load in aluminium is overestimated by 14 %, and the heat load in hydrogen is underestimated by 14%, leading to an almost equal heat load for the complete moderators.

$\overline{\Delta h_{er}} = \frac{1}{N} \sum_{i=1}^{N} \frac{h_{\text{approx},i} - h_{\text{calc},i}}{h_{\text{calc},i}}$

and is mainly influenced by the assumption of an axis-symmetry of the heat distribution in proton beam direction. The calculated heat data provided by the Neutronic Group (ESS) is well reproduced by the obtained approximation functions with an average relative error of less than 1 %. Finally, a function was used which includes the location, the material and the proton pulse time structure.

5. Fluid dynamic results

Details of the simulation setups can be found in [4]. The general question whether the heat removal is possible or not, could be answered positively as shown in fig. 6. One indicator of non-sufficient heat removal in this regard would be a steady increase of the temperature, which does not occur here. Between pulses, the time is sufficient to remove the heat totally.
Figure 6: CFD results, a) temperature (aluminium and hydrogen) and b) pressure fluctuation (hydrogen) during five heat pulses.

Even the curve of the maximum temperature of aluminium (figure 6 a, red line) does not exceed the allowable temperature $T_{ps}(p=15 \text{ bar}) = 34 > T_{\text{max}} = 32 \text{ K}$, wherein the temperature is the outside temperature for the aluminium vessel under vacuum and therefore would not be critical. More important is the interface (Al-LH$_2$) temperature $T_{\text{Interface,max}} = 31 \text{ K} < T_{ps}(p=15 \text{ bar}) = 34$ (figure 6 a, yellow line), because both hydrogen and aluminium have the same temperature at this point. In this case, it is also noted that no impermissible temperatures are reached. The maximum hydrogen temperature in the pulse (figure 6 a, blue line) is $T_{\text{LH}_2,\text{max}} = 20 \text{ K}$, the requirement, to stay all the time in the range of 17-21 K, is therefore fulfilled. Whether the pressure peaks (figure 6 b, green and orange line) lead to fatigue of the material is still under investigation.

6. Structural mechanics results

Strength analysis according to RCC-MRx could be started using the results of the fluid dynamic simulations, i.e. temperature and pressure distributions in the moderator. First, the allowable stress should be determined: $S=f(\text{material, radiation damage, manufacturing type})=55 \text{ MPa} \geq \sigma$, which must not be exceeded [5]. Unlike under operational conditions, the allowable stress in the test case (fig. 7b) is higher due to the missing radiation: $S_{\text{Test}}=f(\text{material, manufacturing type})=84 \text{ MPa} \geq \sigma$ [5].

Figure 7: a) Stress 15 bar / 20 K operation case; b) Stress 21.45 bar / 300 K test case $S_{\text{Test}}=84 \text{ MPa}$
It was found that the local stress exceeds allowable values only in small areas (Figure 8a design case). That can be eliminated by small changes in geometry e.g. increasing the radius. Build-up of the ESS cold moderator vessel, strict according to the RCC-MRx code, is unfortunately impossible, because no cryogenic components are implemented in this code. Therefore, in addition to the RCC-MRx calculation, a machining test, a welding test, a leak test and a burst test are in progress to back up the simulation results. The first milled cold moderator vessel for the tests is shown in Figure 8b.

7. Summary
By the numerical simulations in combination with the ongoing manufacturing pre-tests (Figure 7d) it could be shown that the design of the ESS Moderator environment, under mentioned conditions, is possible in principle. However, welding issues and for the operating license, a number of obstacles are still to be addressed.

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