CRS4 Target for ESS

Simulations with Armando 1.0

Calculation report

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Abstract

The aim of the report is to gather some information on the transient Smoothed Particle Hydrodynamics simulations of the CRS4 spallation target for ESS, run with the CRS4 in-house SPH code Armando.

The problem is briefly described in terms of model, material and loading conditions. Some details on the simulation methods are given and the results are discussed, with focus on the splashing phenomenon.

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1 Introduction

In the framework of the international collaboration on the future European Spallation Source (ESS), in a preliminary conceptual phase during 2010, a Target Station Concept Selection (TSCS) working group has been formed with the aim of making an evaluation of the different target concepts already developed to see which ones are more suited and easily adapted to the ESS objectives.

The main critical component of the Target Station is the Spallation Target. This target must dissipate about 2..8 MW from a 2 mA, 2.5 GeV spallation beam (with a conservative 56% thermal efficiency) within a relatively short space.

In the PDS-XADS FP5 project, a windowless channel like target has already been dimensioned and simulated for a relatively similar proton beam: 2.4 MWth, 5 mA and 600 MeV. In the framework of this project, the spallation target was conceived by Ansaldo and developed mainly by CRS4 and ENEA. We investigate in this report the possibility to adapt the PDS-XADS concept (adopted as is with a simple scaling for the EUROTRANS (FP6 project) EFIT 16 MWe target) to the ESS constraints.

In the framework of the THINS FP7 project we have to operate free-surface simulations with liquid metals and improve their range of application in the nuclear context both gaining know-how on existing models and also improving these models or creating new (better) ones. One of our objective in THINS is to demonstrate the applicability of mesh-less particle techniques to the simulation of fast transient induced by proton beam impact on liquid targets. The application of the algorithm for a free-surface spallation target is ideally in line with the THINS central objective.

The simulations are performed using the serial version of the Armando v1.0 . It is a smoothed particle hydrodynamic code, developed in collaboration with CERN for the study of transients in liquids, with particular care for fast transients in liquid targets due to proton beam. The code is based on a lagrangian description of the liquid. The liquid domain is divided in a set of particles of given mass and occupied volume. The Navier Stokes equations are solved for the computational domain by calculating the interactions between the particles. The model is prepared manually with a dedicated fortran routine, due to the simple geometry analysed, and the graphical postprocessing is made with the meshless extension of ParaView.

The document is organized as follows: first the problem is presented, with a brief description of the target to be analysed, of the boundary conditions and the materials used. Several models have been prepared and analysed for the problem, and are presented afterwards, investigating several aspects of the phenomenon.

2 LBE loop

The target concept that is here analysed may in principle be used with any liquid metal, and the first analysis and proposals were made using mercury as the reference material. The works of the TSCS group of ESS have put in evidence that the use of Hg as spallation material would be faced with huge accreditation issues related to safety, and mainly decommissioning.

It seemed therefore reasonable to switch from mercury to the more promising lead-bismuth eutectic.

2.1 LBE vs Hg

Mercury was the first choice in the ESS design mainly due to its high specific weight. The lower temperature range in which it is liquid is not a great advantage, since higher temperature are positive for the containing structures exposed to radiation damage.
In the following table the properties of interest for mercury, lead and LBE are compared [1].

Property @ atmospheric pressure and melting temperature	Hg	Pb	LBE
Density [kg/m3]	13534	10673	10551
Standard weight [g/mol]	200.6	207.2	208.18
Melting point [K]	234.3	600.6	397.7
Boiling point [K]	630	2022	1943
Heat capacity [J/molK]	28	30.7	30.8
Vapor pressure [Pa]	10 @ 350K	1 E-4 @ 700K	1 E-4 @ 700K
Sound speed [m/s]	1451.4	1791	1774
Thermal exp. coeff [10^{-6}/K]	60.4	120	123

As appears from the table the density of the LBE is not that different form Hg but this material has several interesting properties, like the high value of the boiling temperature and the extremely low value of the vapour pressure. This allows to have higher temperature increase in the liquid with a large free surface tanks to the low value of the vapour pressure.

2.2 Target geometry

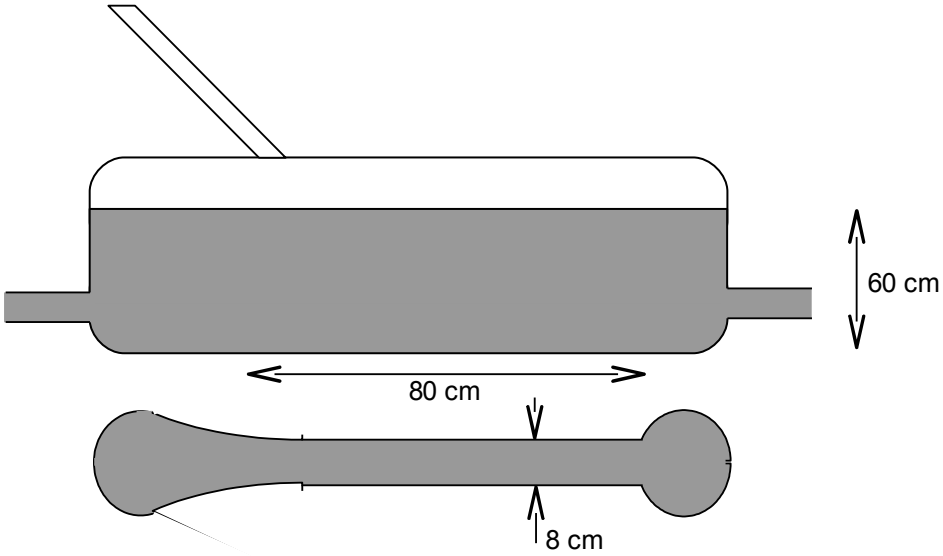


Figure 1: Sketch of the target

The target is basically formed by a channel, containing the liquid LBE under vacuum, with a free surface and exposed to the proton beam coming from the ESS accelerator, see Figure 1.

In the sketch the the LM movement is from left to right, with low velocities and a flow rate of approximately 30 l/s. The active area of the target where the energy is deposited is enclosed in a brick volume 80cm long, 60cm high and 8cm wide.

This is the volume that will be modelled, the details of the rest of the target will be neglected.

2.3 Loading conditions

The ESS beam has an energy of 2.5 GeV, and mean current intensity of 2mA. The beam power is deposited with long pulses, each pulse is 1ms long and the pulse frequency is 20Hz. This means that the peak current and power is 50 times higher than the average.

The spatial distribution of the power inside the target depends on the properties of the material and on the focusing of the beam. The energy distribution per proton inside the material may be approximated with the following function [2].

$$e_p(x_{1,}x_{2,}x_3)=f(x_{1,}x_2)g(x_3)$$

$$f(x_{1,}x_2)=\exp\left(-\frac{1}{2}\left(\left(\frac{x_1}{\sigma_1}\right)^2+\left(\frac{x_2}{\sigma_2}\right)^2\right)\right)$$

$$g(x_3)=\alpha\exp\left(\frac{-x_3}{\beta}\right)\left(1-\exp\left(-\gamma-\frac{x_3}{\delta}\right)\right)$$

This distribution is valid for an impact perpendicular to the target surface, the 3rd axis is oriented along the beam direction and the 1st and 2nd axis form the orthonormal triad. The parameters of this function are: α = 0.00130948, β = 15.5814 , γ = 0.654066, δ = 6.72606 with the measures on the three axis expressed in cm.

The beam direction in the target is oblique on the target and hits the free-surface with an angle of 45 deg. The coordinate transformation is the following.

$$x_1=y+z$$

$$x_2=x$$

$$x_3=-\sqrt{2}\,y$$

It is necessary to apply a coordinate transformation and some minor modification to preserve the total beam power deposited in the target, the parameter α and β are modified as follows:

$$\alpha=\sqrt{(2)}\,\alpha$$

$$\beta=1.4\,\beta$$

The total average power deposited on the target is 2.3MW.

The beam impact position on the free surface of the computational domain is located not on the centre but toward one side, 20cm from the end of this, so that the energy release is approximately centred on the domain.

3 SPH models

Two SPH models have been prepared, a so called large model, that is 80cm long, 60cm high and 8cm wide, and a small model that covers the volume more close to the the energy deposition and is 60cm long, 40cm high and 8cm wide.

The domain is modelled with a set of particles, the inter-particle distance is set to 3.3mm for the large model and to 2.5mm for the small model. The number of particles in both cases is approximately 1.2 millions.

Since we are interested in the fast transients due to the sudden beam power deposition on the liquid metal target we totally neglect the slow movements due to fluid flow and of its free surface in time scales of the order of seconds. The length of our simulations will be of the order of milliseconds, with the most important phenomena that take place in the first microseconds of the simulation.

The fluid will be initially at rest and the gravity is neglected, the side of the box shape are considered rigid. This is not correct for the sides of the box in which the fluid enters and leaves the

channel but it is a conservative approximation to keep all the fluid energy in the computational domain.

The top surface of the domain is free. In SPH no particular boundary condition is required to impose the free surface.

3.1 Lead-bismuth eutectic Equation Of State

The equation of state may be expressed as follows:

$$p = f(\rho, e)$$

that relates the pressure in the liquid to its density and the specific internal energy.

The liquid is assumed initially at rest, the variation of pressure is:

$$dp = \left(\frac{\partial p}{\partial \rho}\right)_e d\rho + \left(\frac{\partial p}{\partial e}\right)_\rho de$$

we can derive a linear relation for pressure as follows:

$$p = p_0 + \int \left(\frac{\partial p}{\partial \rho}\right)_e d\rho + \int \left(\frac{\partial p}{\partial e}\right)_\rho de$$

then we introduce the Gruneisen parameter Γ and we assume that if no energy variation is present the material obeys to a linear relation with acoustic waves.

$$\int \left(\frac{\partial p}{\partial e}\right)_\rho de = \rho\Gamma(e - e_0)$$

$$\int \left(\frac{\partial p}{\partial \rho}\right)_e d\rho = K_s \frac{\rho - \rho_0}{\rho_0} = K_s \mu$$

we also have that:

$$\rho\Gamma = \rho_0\Gamma_0 = \frac{\alpha K_s}{c_p}$$

$$K_s = \rho c^2$$

Ks is the bulk modulus, c is the speed of sound and α is the volumetric thermal expansion coefficient.

The Equation Of State can then be expressed as:

$$p = p_0 + K_s\mu + \Gamma_0\rho_0(e - e_0)$$

It is assumed a reference temperature of 573K, for which the density value is 10338kg/m^3, the sound velocity is 1740m/s, the volumetric expansion coefficient is 127.4E-6 K^{-1} and the specific heat c_p is 146J/kgK, the parameters K_s and Γ_0 are 31.3GPa and 2.66.

It is also important to specify the value of the cavitation pressure. Cavitation is a process in which a bubble of vapour is formed inside the liquid or at the contact with a surface and expands under negative pressure breaking the continuity of the fluid. A liquid can be subject to almost any value of positive pressure. It may cavitate if the pressure is negative and lower than the vapour pressure at that temperature.

The maximum value of the negative pressure a liquid can sustain without cavitation is very difficult to measure and depends strongly not only on the temperature but also on the purity level of the material, on the presence of gases dispersed, on the time history of the load.

The literature reports lots of value for cavitation pressure for mercury, with a huge variations in the datum, of several orders of magnitude. No data was found for LBE.

In the following we assume that the limit is 150kPa a value that we used as reference in previous simulations for mercury. The results for this datum will be compared to those obtained with a very high value that prevents cavitation.

4 Results

4.1 Small model, short run, tensile limit

In the first simulation a detail model is examined with a very short simulation to look at the details of pressure wave propagation inside the solid. The material strength is included in the modelling and the pressure in the material is not allowed to fall below the limit of -150kPa. If this value is reached the density may increase without changing the pressure of the particles, and the material is thus free to expand without any further resistance by the liquid. If the particles movements causes the density value to increase again the pressure can vary again and become positive.

The energy, velocity magnitude and pressure value at times from 0 to 0.1ms are shown in the following Table 1, one half of the model is shown and the cross section used is tangent to the beam axis and flow direction.

In the first column the specific energy is shown, due to the constant in time power deposition the energy grows almost linearly in time. The second column shows the pressure value in the liquid, the specific energy increases causes a rise of the pressure in the liquid, and a pressure wave departs from the beam axis involving the rest of the material. The free surface is subject to a null value of the pressure, and generates a pressure wave that propagates vertically inside the material. At the entrance of the beam in the liquid free surface, negative values of pressure are generated due to the reflection of a positive pressure wave on the free surface and the cavitation conditions are met as can be seen from the blue “bubble” growing at the beam entrance in the liquid. Finally, the third column shows the velocity magnitude field inside the liquid. The acoustic wave propagation is again evident as well as the vertical movement of the portion of the liquid were the continuity is broken that has a maximum vertical velocity reaching 0.375m/s.

In Figure 2, the vertical velocity and the pressure value for a particle located approximately 4 mm below the free surface at the point of entrance of the beam are shown. The pressure is subject to high oscillations, and the velocity of particle grow gradually until it reaches a first plateau after approximately 0.06ms, equivalent to 6% of the pulse length.

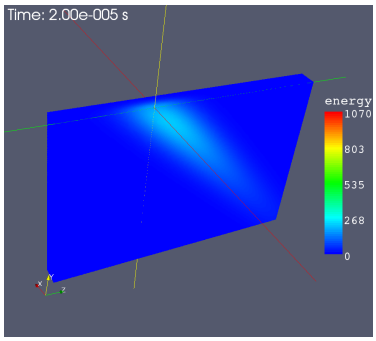
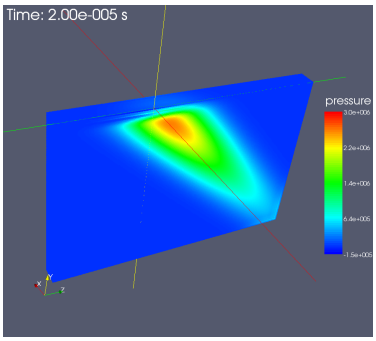
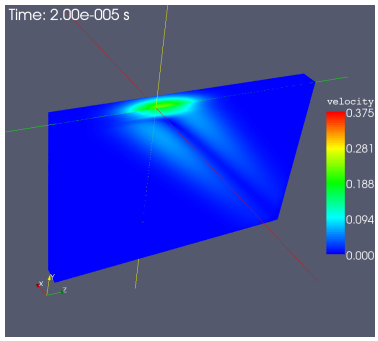
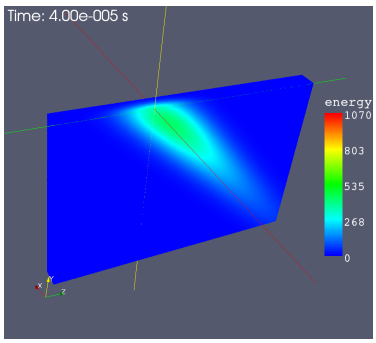
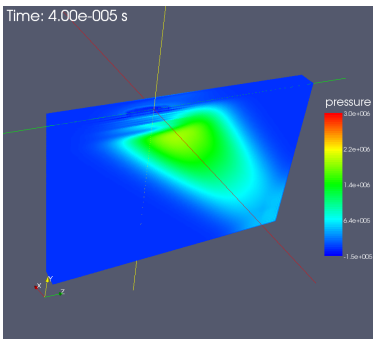
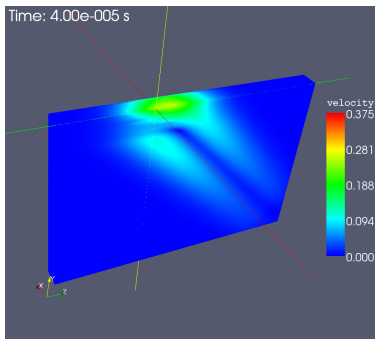
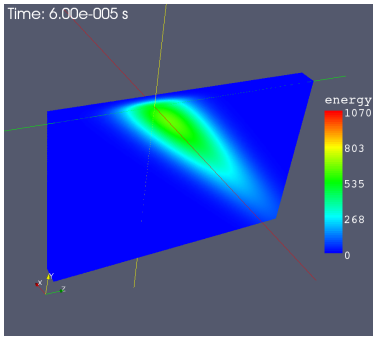
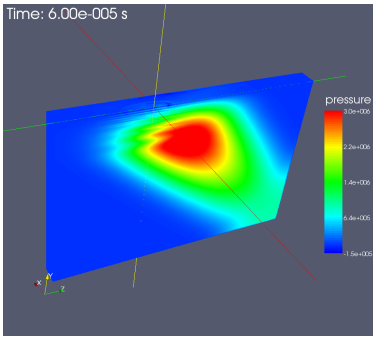
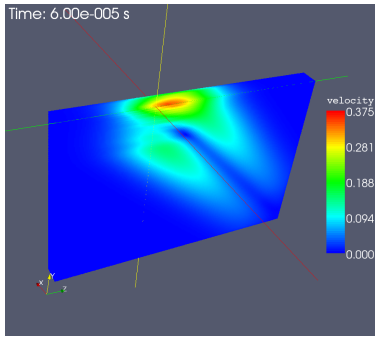
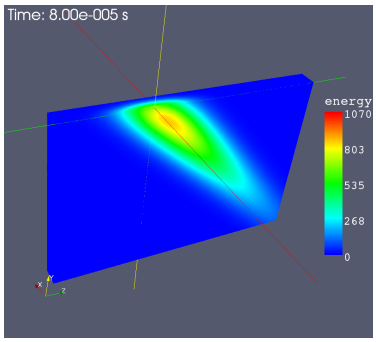
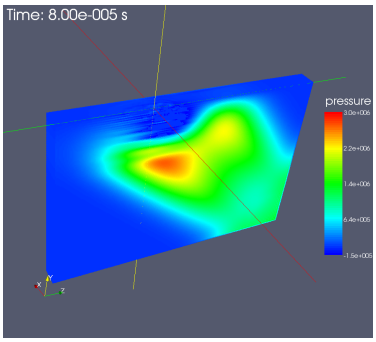
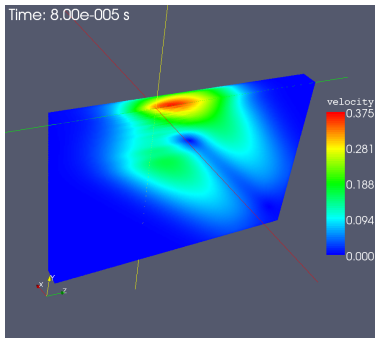
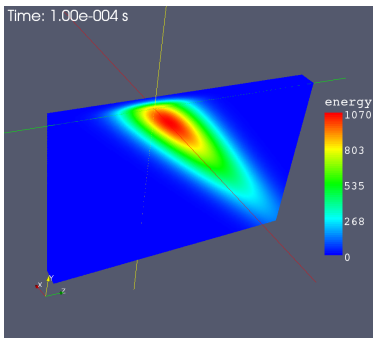
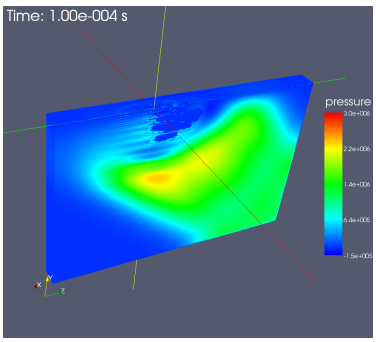
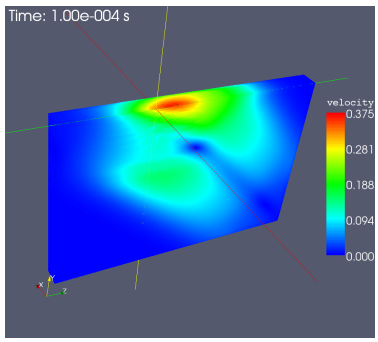
Time	Energy density	Pressure	Velocity magnitude
ms	0 – 1070 J/kg	-1.5 – 30 bar	0 – 0.375 m/s
0.02			
0.04			
0.06			
0.08			
0.1			

Table 1: small model results, tensile limit is considered

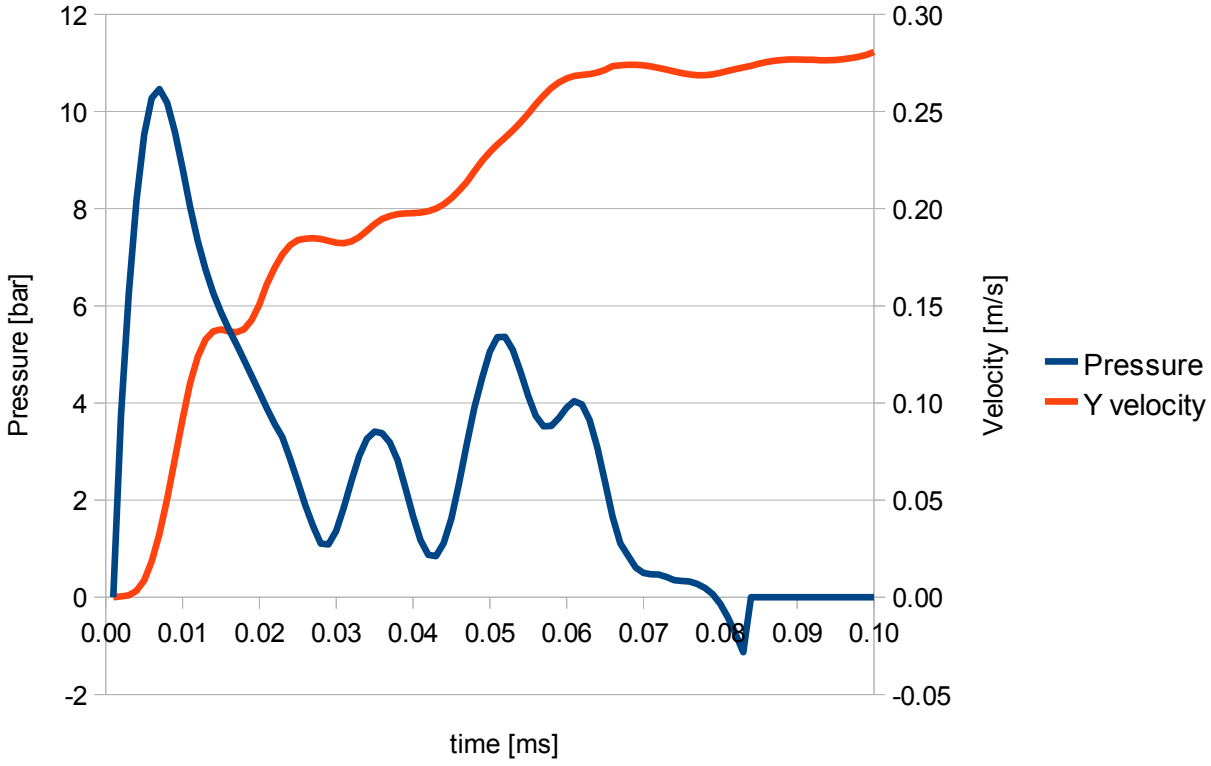


Figure 2: Pressure and vertical velocity for a particle located on the beam axis 5mm below the free surface. The small model with tensile limit is used

4.2 Large model, long run, tensile limit

In this second run a larger model is used, the liquid portion considered is now 80cm long along the z axis and 60 cm high, the particle distance is a bit increased with respect to the previous model to keep the particle number around one million. The simulation is run for 2ms, to cover the effects of a single pulse.

The results of energy pressure and velocity distribution in the model are shown in Table 2. The specific energy grows linearly with time, up to 1ms. In the pressure field the acoustic wave propagation and reflection on the sides of the computational domain is visible, the time required for an acoustic wave to travel through the whole model is much less than the pulse length, and the whole liquid appears under a null pressure state, due to continuity loss at the end of the pulse.

The effect of the pressure wave reflection is visible in the velocity plots also. The distribution of the velocity magnitude field in the volume is similar among the different plots and grows with time. The maximum value of the calculated velocity is for the particles close to the entrance point of the beam on the liquid free surface. It is possible to observe that the first three plots at 0.2, 0.4 and 0.6ms appear similar, and the maximum value of the velocity is more or less constant. The fourth and fifth plots, at 0.8 and 1ms again appear almost identical but with values higher than the previous set.

This behaviour can be verified in Figure 3 also, showing the graph of the vertical component of the velocity for a particle 3.3mm below the free surface at the point of entrance of the beam. The velocity grows rapidly in time until 0.1ms, then it continues growing but at a much lower rate and finally it rises again after 0.6ms until it reaches a maximum before 0.8ms.

Time	Energy density	Pressure	Velocity magnitude
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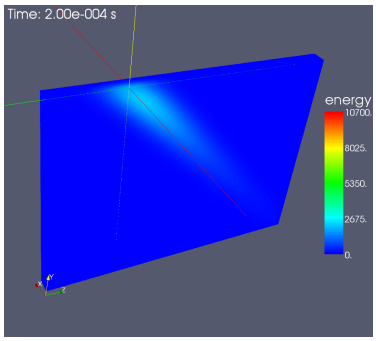
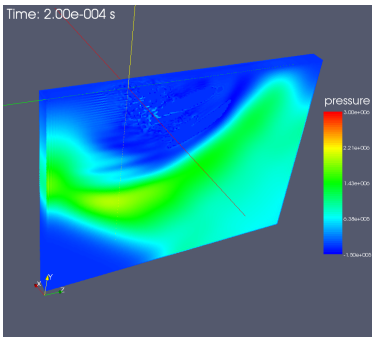
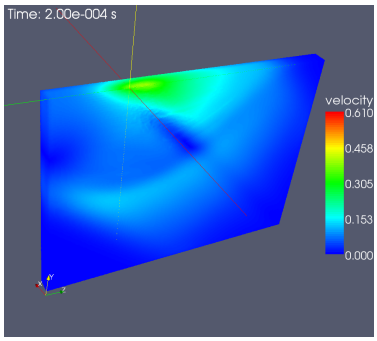
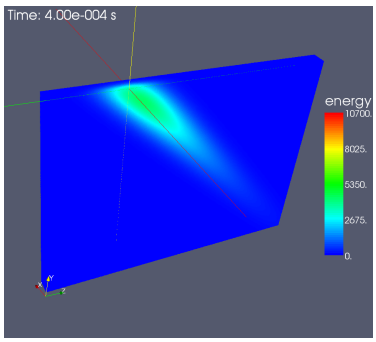
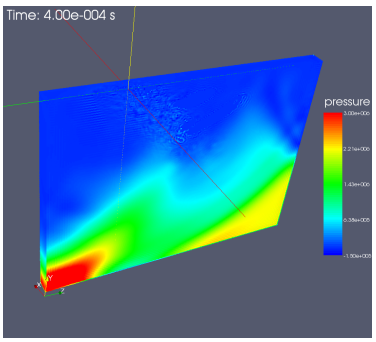
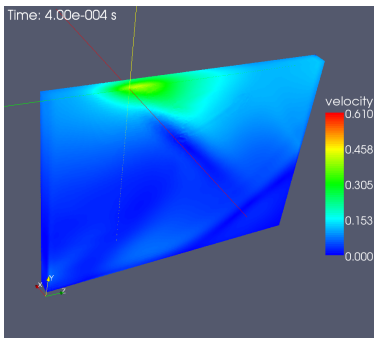
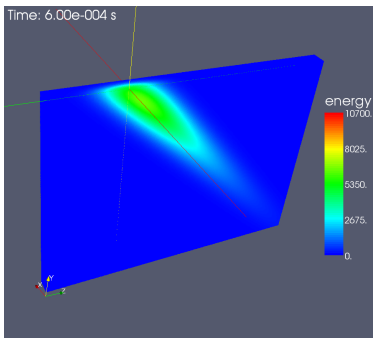
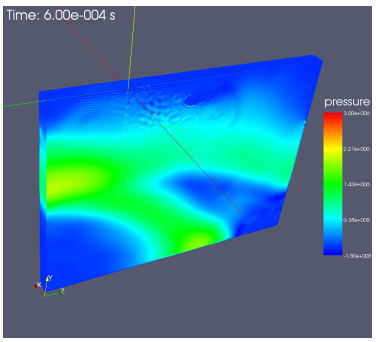
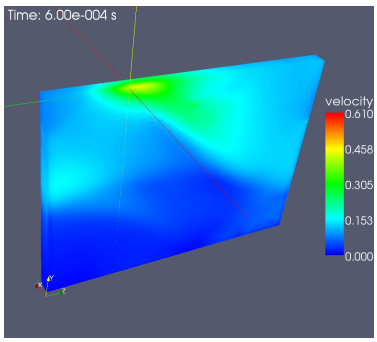
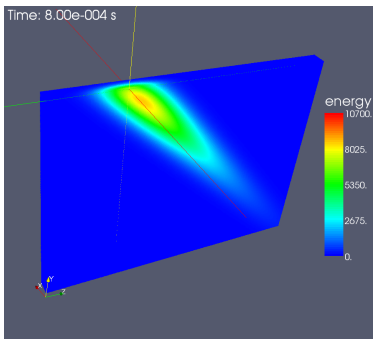
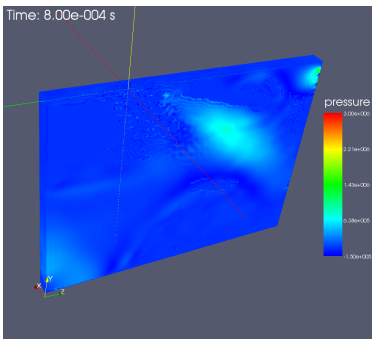
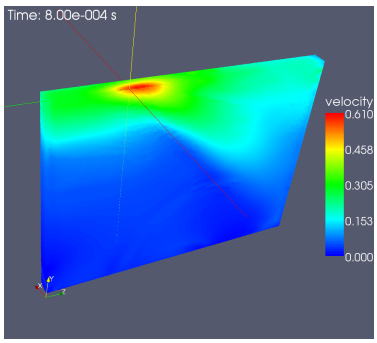
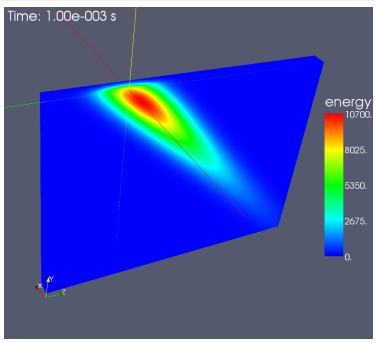
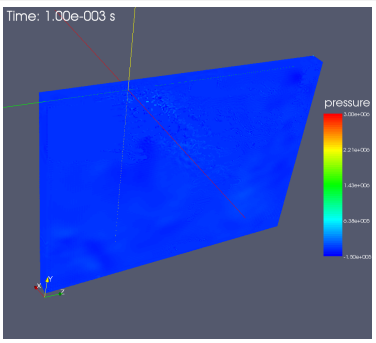
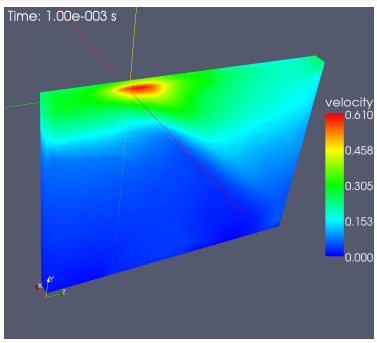
0.2			
0.4			
0.6			
0.8			
1			

Table 2: large model with tensile limit

The first rapid growth is due to the direct pressure wave induced by the beam power deposition in the liquid. The point under exam is close to the most heated area and the time required for the pressure wave to arrive is very short.

The beam pulse is still active and the liquid is heated for 1ms, the velocity of the particle is still positive and is due to the relatively slow thermal expansion of the liquid due to the temperature rise.

Given the velocity of sound in the liquid of 1700m/s, it takes 0.7ms for an acoustic wave to travel twice the depth of the vessel of 60cm. Therefore around 0.7ms we can observe a second “kick” for the liquid on the free surface due to the pressure wave reflected on the bottom.

This pressure wave is positive and compresses the liquid on its arrival, but when it reaches the free surface, the pressure wave should change sign, and be reflected downwards. The liquid anyhow has a tensile limit and cannot withstand high negative pressure values. The acoustic wave loses its energy that is converted in the kinetic energy of the particles, with a calculated maximum value of the splashing velocity of 0.6m/s.

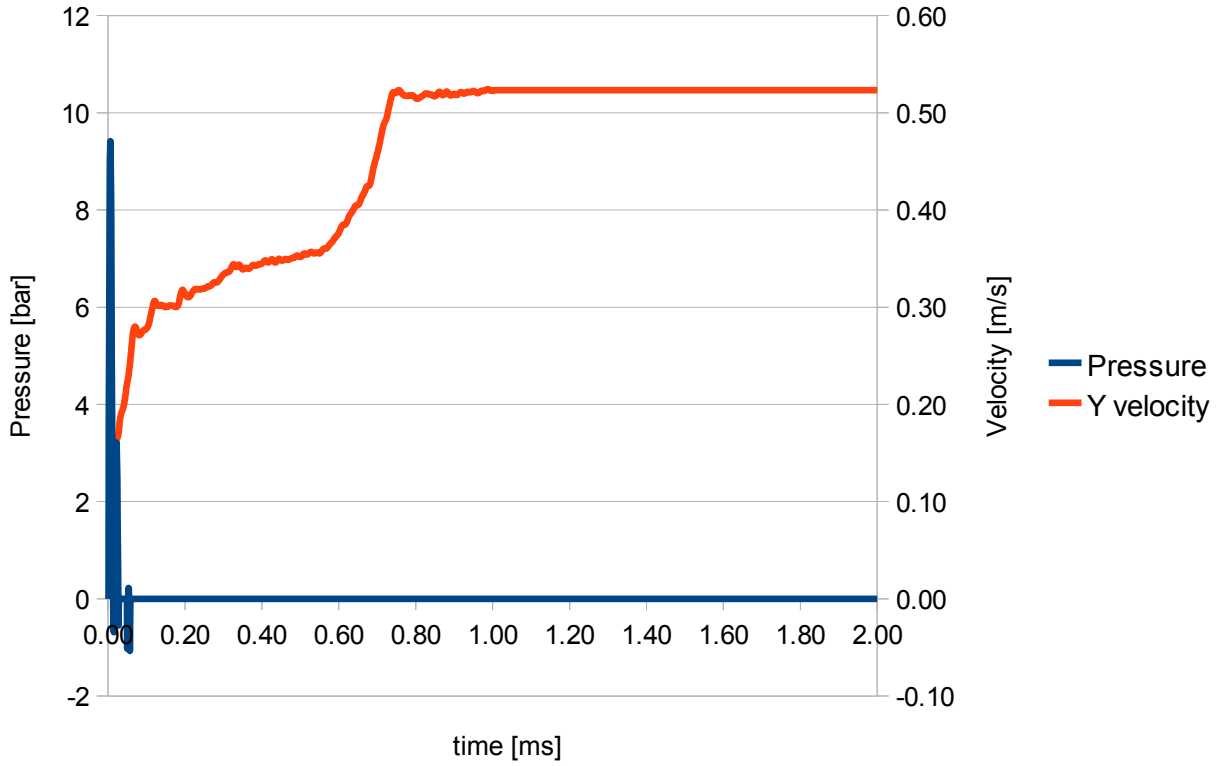


Figure 3: pressure and vertical velocity for a particle located on the beam axis 3.3mm below the free surface. The large model with cavitation is used

4.3 Large model, long run, no tensile limit

Figure 4 Shows the velocity and pressure for a particle 3.3mm under the free surface at the beam entrance. The simulation was run on the same model as before with the same conditions except for the tensile limit that is not included.

It is evident the difference with respect to the previous plot, here the material does not lose its continuity and the acoustic wave is reflected from the free surface, and the velocity of the particle is reduced after the the reflection. The liquid cannot cavitate and splashing is not possible.

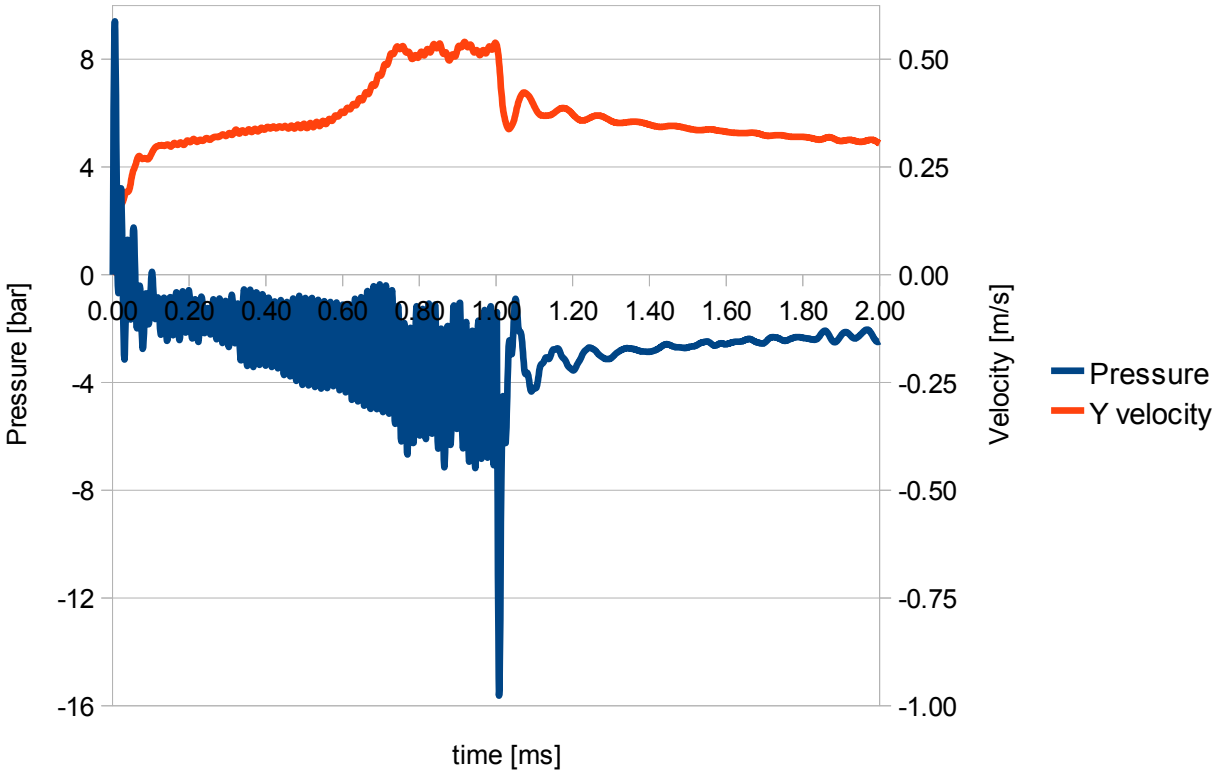


Figure 4: pressure and vertical velocity for a particle located on the beam axis 3.3mm below the free surface. The large model is used but breaking of the material is not allowed

5 Discussion

We want to make some analytical calculations in order to have a term of comparison for the maximum pressure reached inside the liquid due to the beam energy deposition and for the resulting splashing velocity. We take as a reference the analytical work of P. Sievers for elastic waves in solid targets [3].

Among others he considered the case of a partly heated thin rod with finite rise time. An elastic thin rod of length l is heated constantly for a time t_0, in a portion of length l0, the maximum temperature difference reached in the heated part is T_0. The maximum stresses in the rod in an arbitrary long time were:

$$\sigma_{max} = \pm E \alpha \Delta T_0 \qquad if\ c t_0 \leqslant l_0$$

$$\sigma_{max} = \pm E \alpha \Delta T_0 \frac{l_0}{c t_0} \qquad if\ c t_0 > l_0$$

In these expressions σ_{max} is the maximum stress, E is the young modulus, and α is the linear thermal expansion coefficient. The important result is that the maximum stress depends not only on the temperature increase, but also on the size of the heated area that has to be compared with a characteristic length, given by the product of the speed of sound in the material for the duration of the loading. This result can also be interpreted on a time basis, the beam determines an increase of pressure only for the time required to an elastic wave to travel through the heated part of the rod.

If we consider a thin and long rigid cylinder filled with liquid, partially heated, and we repeat the calculations with the symbols previously introduced we get:

$$p_{max} = \pm \rho \Gamma e_0$$

$$p_{max} = \pm \rho \Gamma e_0 \frac{l_0}{c t_0}$$

where p_{max} is the maximum pressure reached in the liquid, Γ is the Gruneisen parameter, c is the speed of sound, e_0 is the energy density in the heated part at the end of the loading time t_0.

To calculate the maximum pressure reached in this simple consideration with a uniform heating we need to know the value of the energy density and the size of the heated part. In our case the heating is not uniform and we do not have a value for the size of the energy deposition, not to mention that our case is three dimensional. We have anyway he total energy deposited in the volume, and if we specify a value for the energy density we would obtain an equivalent volume to have the same total energy and an equivalent size of this volume.

In our case we have a maximum energy density of 11kJ/kg, the average deposited power is 2.3MW, that corresponds to a total deposited energy per pulse of 115kJ. The equivalent length may be thus calculated as:

$$l_0 = \sqrt[3]{\frac{E_0}{\rho e_0}}$$

and we obtain l_0 = 10cm.

The value of ct_0 is 1.74m, that is far higher than the equivalent length of the energy deposition.

The ratio of the two length is 0.057, this means that the maximum pressure is less than the 6% of the maximum theoretical pressure increase of a very fast impulsive load. This is equivalent to say that only the very first portion of the pulse causes a pressure increase in the liquid. The first plateau of the splashing velocity is reached after 0.06ms, approximately the 6% of the loading time. This data is in very good agreement with the results of Table 1 and Figure 2

The maximum pressure results p_{max} = 170bar, still much higher than the maximum found in the simulation of 30bar. But this is an upper bound limit, since the energy is considered to be much more concentrated than in the real case.

A guess of the splashing velocity may be obtained if we consider that the elastic energy of the liquid due to pressure increase is entirely converted in kinetic energy. The mean velocity of the liquid that can be considered as a rough approximation of the splashing velocity is then:

$$\rho \frac{v^2}{2} = \frac{p^2}{2 \rho c} \qquad v = \frac{p}{\rho c} = \frac{\Gamma e_0}{c} \frac{l_0}{c t_0}$$

and with the previous approximations we obtain a value of the splashing velocity of 0.9m/s.

This should be an upper bound for the splashing velocity in these conditions, and is again in good agreement with the numerical results.

6 Conclusions

Several numerical simulations of the fast transient due to a single pulse in a LBE target designed for ESS were run on the SPH code Armando.

The aim of the calculations was to verify the possibility of a splashing phenomenon from the free surface and calculate the value of the splashing velocity.

Splashing is only possible if the liquid may lose its continuity when subject to high negative pressures, and this is simulated adopting a tensile limit for the material model.

The simulations show that the liquid reaches a maximum value of the splashing velocity in a time lower than the pulse duration of 1ms, and the maximum value is 0.6m/s.

A simple analytical model have been developed to cross check the numerical results, a higher bound of the splashing velocity is calculated as 0.9m/s, confirming the numerical results.

The splashing velocity is much lower than the value foreseen due to previous experience with short pulses and is far less dangerous for the design. The maximum height that can reach a free particle with initial speed of 0.6m/s is in fact less than 2cm, and the time required to fall back on the free surface is 0.12s.

Some actions can be taken to improve these results: the reflection of the pressure wave from the bottom of the vessel can be minimized with a proper design and the tensile limit of the liquid, that in any case has to be verified with an experiment, can be optimized by filtering the impurities and small bubbles in the liquid.

7 References

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