Università degli Studi di Cagliari

Dipartimento di Ingegneria Meccanica, Chimica e dei Materiali

CRS4 – Center For Advanced Studies, Research and Development in Sardinia

Internship Activities Report:

CFD simulation of sloshing in a cylindrical tank

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18/02/2019 – 18/05/2019

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1. Introduction

The main purpose of this report is to illustrate the activities carried out during the internship at *CRS4*. The object of the work is the study of liquid sloshing on a tank with the use of computational fluid dynamics (CFD); it was created a numerical simulation on Simcenter STAR-CCM+ software, starting from a study performed by researchers of the *von Karmann Institute for Fluid Dynamics*.
The internship took place between February and May 2019, in the CRS4 facilities located at the *Science and Technology Park (Polaris)* for a total of 150 hours (6 CFU). All activities were supervised by Dr. Vincent Moreau, senior researcher at CRS4, and Prof. Tiziano Ghisu, academic tutor, with the help of Dr. Manuela Profir.

2. CRS4 Research Center

The *CRS4* (*Center For Advanced Studies, Research and Development in Sardinia*) is an interdisciplinary research center founded by the Sardinia Autonomous Region in 1990, whose sole shareholder is the regional agency Sardegna Ricerche. Located in the Comune of Pula, within Science and Technology Park (Polaris), is one of the top-level research centers in Italy, whose activities ranging from high performance computing and energy to biosciences.
This internship was guided by the HPC for Energy and Environment team (led by Dr. Ernesto Bonomi), under the supervision of Dr. Vincent Moreau of the Smart Energy Systems group (program head: Dr. Luca Massidda).
The ***H****igh* ***P****erformance* ***C****omputing for Energy and Environment* team is involved in a wide range of research activities, with the aim of answering to today's challenges on energy production, sustainable management of natural resources and industrial innovation, with a multidisciplinary analysis of problems, in particular with the use of numerical modeling of physical phenomena.
The *Smart Energy Systems* group is focused on applied research into all energy resources and technologies for industry, households and services. (1)

3. Sloshing phenomenon

3.1 Generalities

The term *sloshing* refers to the movement of the free surface of a liquid within a partially filled container, if the container is subject to movement; the free liquid surface can experience different type of motions, depending on type of disturbance applied and shape of the container. The

appearance of waves and rotational movements, especially in resonance conditions, introduce non-linear loads on the containers, which are difficult to predict. The study of this phenomenon therefore has a certain importance in some engineering sectors, such as aerospace, civil, automotive and energy. (2)

3.2 The case of MYRRHA

To assess the seismic safety of HLM (Heavy Liquid Metals) nuclear reactors, the characterization of sloshing assumes a significant importance: the movement of an earthquake is transferred to the liquid coolant, which oscillates inside the partially filled tank, bring consequent additional forces on walls and structures. To investigate these aspects, the von Karmann Institute of Fluid Dynamics (VKI) researchers carried out an experimental study and a CFD investigation in the framework of the MYRRHA project (Multi-purpose hYbrid Research Reactor for High-tech Applications). (3)

MYRRHA is a multi-purpose experimental nuclear reactor (Figure 1), driven by a particle accelerator (Accelerator-Driven System) and designed to use Lead-Bismuth-Eutectic (LBE) alloy as liquid coolant.

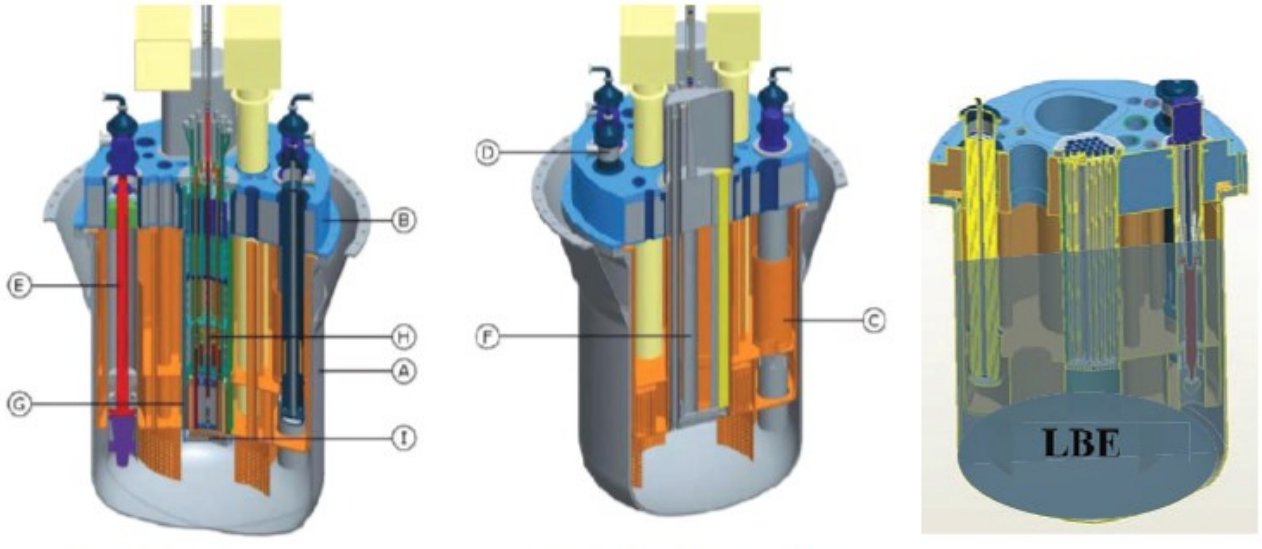

Figure 1 - Scheme of MYRRHA nuclear reactor and level of LBE coolant

MYRRHA is currently under development at the SCK•CEN, the Belgian Nuclear Research Centre; the project has several purposes, including the test of materials and new technologies for nuclear fission and nuclear fusion, the production of radioisotopes for nuclear medicine and the

development of technologies allowing the reduction of nuclear waste through transmutation. (4)
The investigation of the VKI focused on a scale model of MYRRHA: a cylindrical container partially filled with liquid (water or mercury) and subjected to a sinusoidal monoaxial excitation; both laboratory experiments and CFD simulations with the OpenFOAM software, were carried out.
The aim of this internship is to recreate the VKI simulation with the CFD software STAR-CCM+, comparing the results obtained with the VKI experimental results.

4. Preliminary phase

The first days of internship were spent learning basic skills, necessary to continue the work. First, due to the lack of personal experience in this regard, it was necessary to become familiar with the main commands of Linux / Fedora, the operating system on which the architecture of the HPCN (High Performance Computing Network) of CRS4 is based.
In parallel, the basic Simcenter STAR-CCM + software tutorials were performed, focusing on the following sections:

- Geometry: create a 3D-CAD model;
- Mesh: setting meshers, parameters and checking quality of the mesh;
- Incompressible flow: some cases with variety of flow and geometries;
- Multiphase flow: various simulations with Eulerian multiphase turbulent flows model and Volume Of Fluid (VOF) multiphase model.

As a source of additional information is used The Steve Portal, the STAR-CCM+ customer support portal made available by Siemens for this internship, which contain the software guide too. (5)
The VKI report (3) has also been analyzed in detail, in order to highlight the parameters and methods to be used in the simulation.

5. Activities

The activity report presented here follows the classic workflow of a simulation in STAR-CCM +; the subdivision is based on the various branches of the software simulation tree (Figure 2).

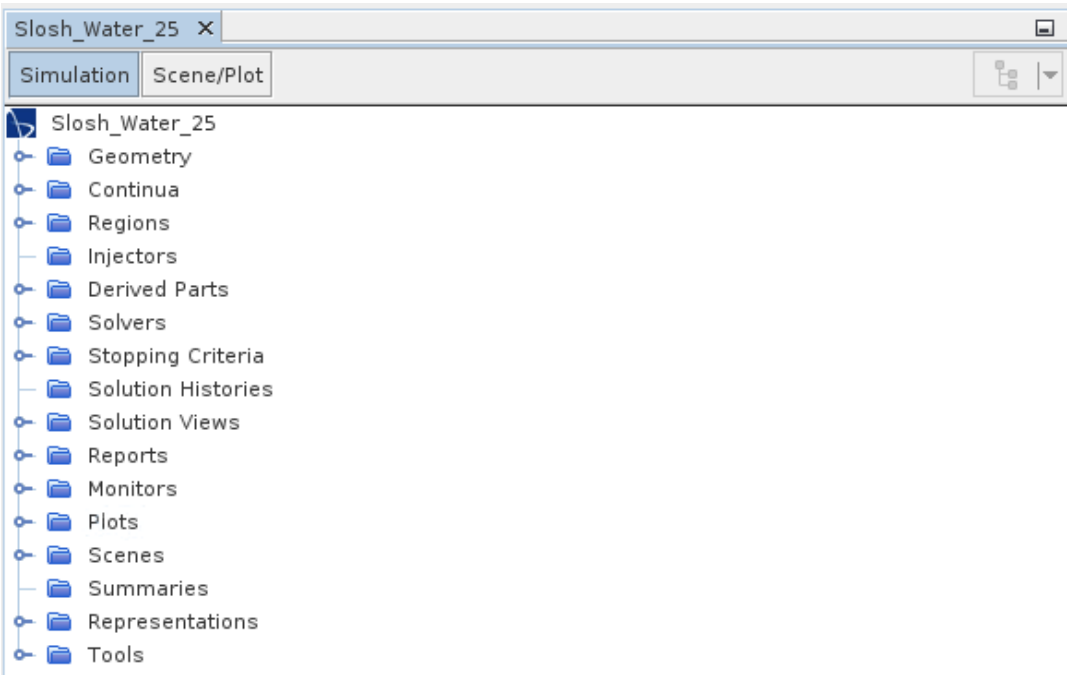

Figure 2 - STAR-CCM+ simulation tree

5.1 Geometry and motion

The system geometry is the same from the VKI report: a cylindrical tank aligned with the z-axis. The radius of the tank is $R = 0.06\ \mathrm{m}$ and the height of the tank mode $H = 0.235\ \mathrm{m}$. To respect the similarity of the problem the liquid height is $h = 0.135\ \mathrm{m}$, keeping the same height/radius ratio as in MYRRHA $(h/R = 2.25)$ with a scale of 1/66. All the boundaries are set to wall type.

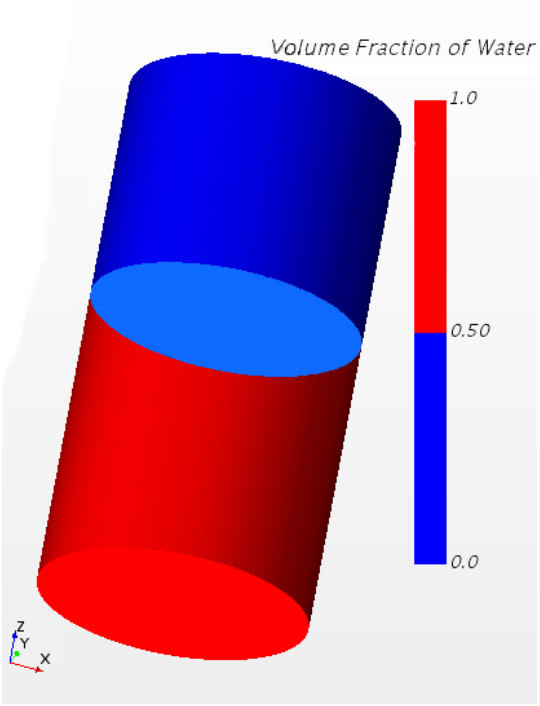

Figure 3 - Cylindrical tank with initial distribution of liquid $(h/R = 2.25)$

The tank is subjected to a sinusoidal excitation along the x-axis, $X = X_0 \sin(\omega t)$. By differentiating this expression, the translational velocity is obtained (5.1):

$$v = X_0 \omega \cos(\omega t) \tag{5.1}$$

with:

$X_0 = amplitude$

$\omega = 2\pi f = angular\ frequency$

The sloshing phenomena has its apex in the case of resonance; natural frequency is dominated by geometric parameters (tank radius and liquid height) while it's little influenced by liquid properties like surface tension, then it's possible to neglect them in this calculation and use the following expression for an upright cylindrical tank (5.2):

$$\omega_{m,n}^2 = \frac{g\xi_{m,n}}{R} \tanh\left(\frac{\xi_{m,n} h}{R}\right) \tag{5.2}$$

where for antisymmetric modes $m = 1$: $\xi_1 = 1.841$, $\xi_2 = 5.335$, … . For the first mode the natural frequency is $f = 2.77$ Hz.

This value is used to calculate the angular frequency $\omega = 17.4\ {}^{\mathrm{rad}}/_{\mathrm{s}}$; two different amplitudes X_0 of excitation are applied: 0.0025 m and 0.005 m.

5.2 Physics

Physic models used in this simulation are listed below (Figure 4):

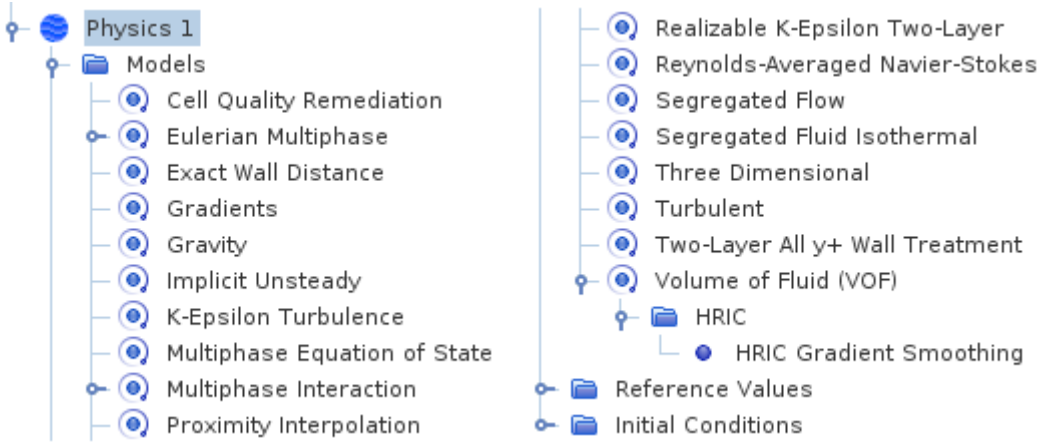

Figure 4 - Physic models used in simulation

The main model of this simulation is the *Volume Of Fluid* (**VOF**): it's a multiphase model useful for solving problems with mixtures of immiscible fluids and free surfaces. It predicts the position and movement of the surface between different phases using the field function of phase volume fraction α_i, defined as (5.3):

$$\alpha_i = \frac{V_i}{V} \tag{5.3}$$

where $\mathrm{V_i}$ is the volume of phase i in the cell and V is the volume of the cell. Therefore, for a cell can occur one of the following configuration:

$\alpha_i = 0$	$\rightarrow$	The cell is completely void of phase i
$\alpha_i = 1$	$\rightarrow$	The cell is completely filled with phase i
$0 < \alpha_i < 1$	$\rightarrow$	Presence of interface in the cell

The sum of volume fractions of all phases in a cell must be equal to 1. Material properties of fluid in the interface-containing cell are defined as properties of a mixture fluid of the phases, and calculated with a weighted average.

The phase mass conservation equation drive the distribution of phase i:

$$\frac{\partial}{\partial t}\int_V \alpha_i \, dV + \oint_A \alpha_i \, \mathrm{v} \cdot d\mathrm{a} = \int_V \left(S_{\alpha_i} - \frac{\alpha_i}{\rho_i}\frac{D\rho_i}{Dt}\right) dV - \int_V \frac{1}{\rho_i} \nabla \cdot \left(\alpha_i \, \rho_i \, \mathrm{v}_{d,i}\right) dV \tag{5.4}$$

where $\mathbf{a}$ is the surface area vector, $\mathbf{v}$ is the mixture velocity (mass-averaged), $\mathbf{v_{d,i}}$ is the diffusion velocity, $\boldsymbol{S_{\alpha_i}}$ is a user-defined source term of phase i and $^{D\rho_i}/_{Dt}$ is the Lagrangian derivative of the phase densities ρ_i.

For a simulation of two VOF phases (like in this simulation) the volume fraction transport is solved for the first phase only. Then, the volume fraction of second phase is deducted for each cell, taking into account that the sum of the phases in a cell must be equal to 1.

The *High Resolution Interface Capturing* (**HRIC**) sub-model was used to maintain sharp interface between the phases. It can be activated when the Convection parameter is set to 2nd-order, and contain four main settings:

- Sharpening Factor: if $\neq 0.0$ introduce an additional term at the transport equation to reduce numerical diffusion of the simulation. Can assume values from 0.0 to 1.0: in this simulation it was set to 0.3 ;
- CFL_l: lower limit of Courant number. In this simulation was set to 8.0;

- CFL_u: upper limit of Courant number. In this simulation was set to 10.0;
- HRIC Gradient Smoothing: smoothed gradient to reduce spurious oscillation that can occur in the volume fraction field, especially when the mesh has a large aspect ratio. In this simulation this parameter was enabled.

Unlike in the VKI report, turbulence was considered in this simulation, using a *Reynolds Averaged Navier-Stokes* (**RANS**) model and a *Realizable K-Epsilon Two-Layer* as eddy viscosity model. The Two-Layer approach uses an algebraic relation that solves k and binds ε with the distance from the wall, in the regions of near-wall flow, dominated by viscosity:

$$\varepsilon = \frac{k^{3/2}}{l_\varepsilon} \tag{5.5}$$

where l_ε is a length scale function.

Due to the difficulties in using the LBE in the laboratory, the VKI experimental and numerical investigations were carried out with water and mercury, also in order to investigate the effect of liquid properties on sloshing. (3)

In this internship the simulation was carried out only with water. The properties of the materials used for this simulation are listed below (Table 1):

Table 1 - Properties of materials ($\mathbf{T_{ref} = 293\ K}$)

Fluid phase	***Density*** $\boldsymbol{\rho}\ [\mathbf{kg/m^3}]$	***Dynamic viscosity*** $\boldsymbol{\mu}\ [\mathbf{Pa \cdot s}]$	***Surface tension*** $\boldsymbol{\sigma}\ [\mathbf{N/m}]$
Water	997.561	$8.8871 \cdot 10^{-4}$	0.072
Air	1.81415	$1.85508 \cdot 10^{-5}$	

A dynamic *Kistler correlation* was selected for model the contact angle between the liquid phase and the wall boundary instead of the default static value. This method is suitable for inertia-dominated or capillary-dominated flows and require three parameters: equilibrium contact angle (in this simulation was set to $90°$), advancing contact angle (set to $100°$) and receiding contact angle (set to $80°$). To reduce some parasitic currents on the free surface it was activated the *Interface Momentum Dissipation* (set to 0.1).

5.3 Mesh

In the first phase of the work various preliminary meshes were used, in order to highlight any errors in the model settings or inconsistencies in the results. For the final mesh it was decided to

replicate the configuration of the VKI report: a trimmer volume mesh, with base size of 0.0016 m and 765768 hexahedral cells (Figure 5).

Figure 5 - Mesh used in the simulation

Surface Remesher model was used: it performs a retriangulation of the geometry surface in order to obtain a better volume mesh. In addition, the *Prism Layer Mesher* was used: this model generates a layer of orthogonal prismatic cells near the walls and boundaries, in order to obtain a better accuracy of the flow solution; geometric progression was used to distribute the layers.
The main parameters of the mesh are listed below (Table 2):

Table 2 - Final mesh parameters

Type	Trimmed	***Prism layer thickness***	45% BS
Base size	0.0016 m	***Surface curvature***	36 points/circle
Relative minimum size	25% BS	***Surface growth rate***	1.2
Relative target size	100% BS	***Growth rate***	Fast
Maximum cell size	100% BS	***Cells***	765768
Prism layer number	3	***Interior faces***	2271064
Prism layer stretching	1.3	***Vertices***	780681

5.4 Model strumentation

The instrumentation of the model represents an important part of the work since it allows to extrapolate the data necessary for the analysis of the results obtained.

In this simulation the model has been instrumented with derived parts (such as points or surfaces) to keep track of the following parameters:

- Monitor: max elevation of free surface;
- Monitor: volume integral of water over Z0 (Z0 = initial water height) (Figure 6);
- Monitor: water mass error (%);
- Plot on scalar scene: volume fraction of water;
- Plot on scalar scene: Courant number;
- Plot on vector scene: velocity vector on free surface.

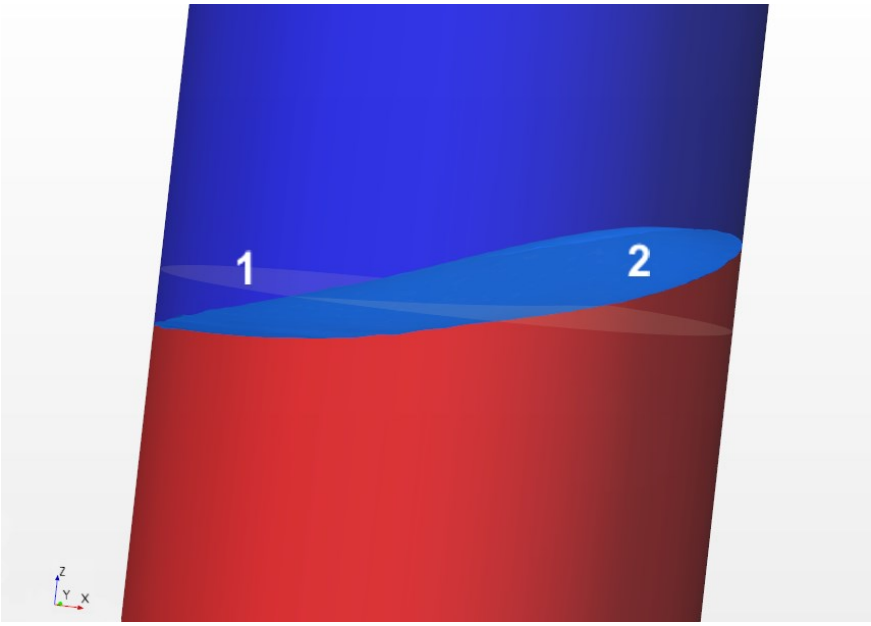

Figure 6 - Free surface: Z0 initial height (1) and position during the simulation (2)

It was initially planned to include other instrumentation tools to detect other parameters of interest (e.g. momentum, velocity vector on the ZY plane, vorticity, etc.) but it wasn't possible due to the timing and unforeseen events that occurred.

5.5 Simulations and results

The entire design and setting phase of the simulation models was carried out on a local computer, while the final simulations were performed on the CRS4 cluster, using 40 cores for each simulation.

The main parameters used for the solvers are listed below (Table 3):

Table 3 - Main solvers parameters used in final simulation

Implicit unsteady: time-step	0.004 s
Implicit unsteady: temporal discretization	1st order
Segregated VOF – Single step: under relaxation factor	0.9
Segregated VOF – Single step: relaxation scheme	Gauss – Siedel
K-Epsilon turbulence: under relaxation factor	0.8
K-Epsilon turbulent viscosity: under relaxation factor	1

A first attempt at simulation in the final configuration highlighted the problem of the numerical error on the water mass: the water level tends to be reduced at each iteration, and after a few seconds of physical time the decrease is perceptible in the scalar scene even at sight.

In order to compensate this effect, a correction factor has been introduced: a source of water mass that reintroduces the lost water mass, whose value is calculated as the difference between the initial water mass and the water mass value monitored after each iteration.

After this correction water mass error is contained in an acceptable range ($< 1\%$), like shown in Figure 7 and Figure 8.

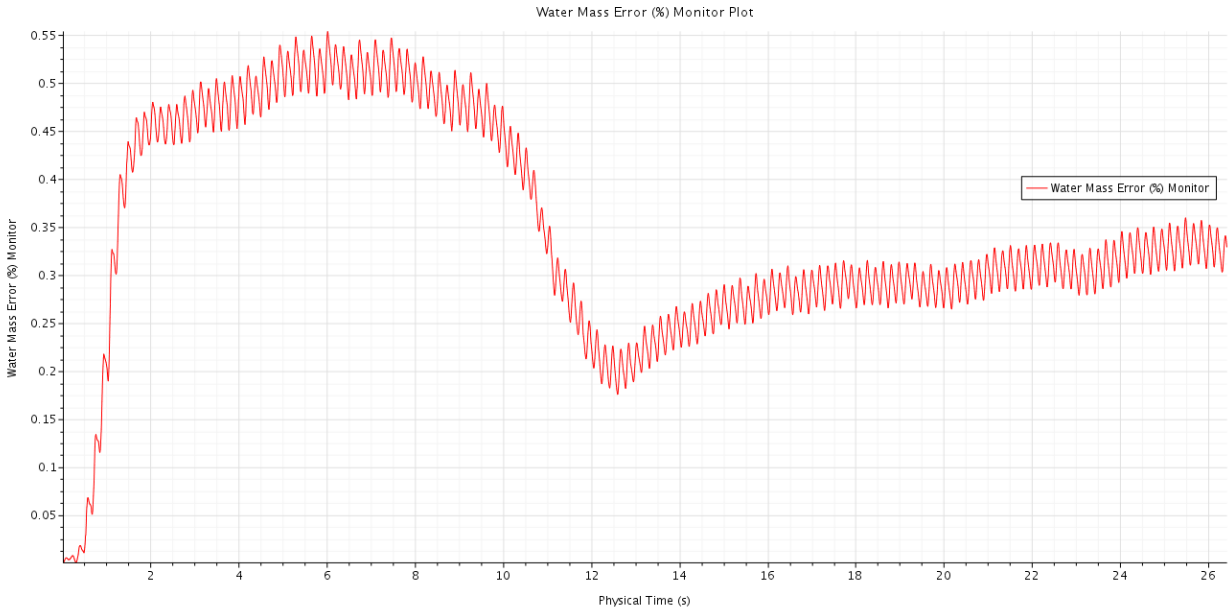

Figure 7 - Water mass error (%) in final simulation with X_0=0.0025 m

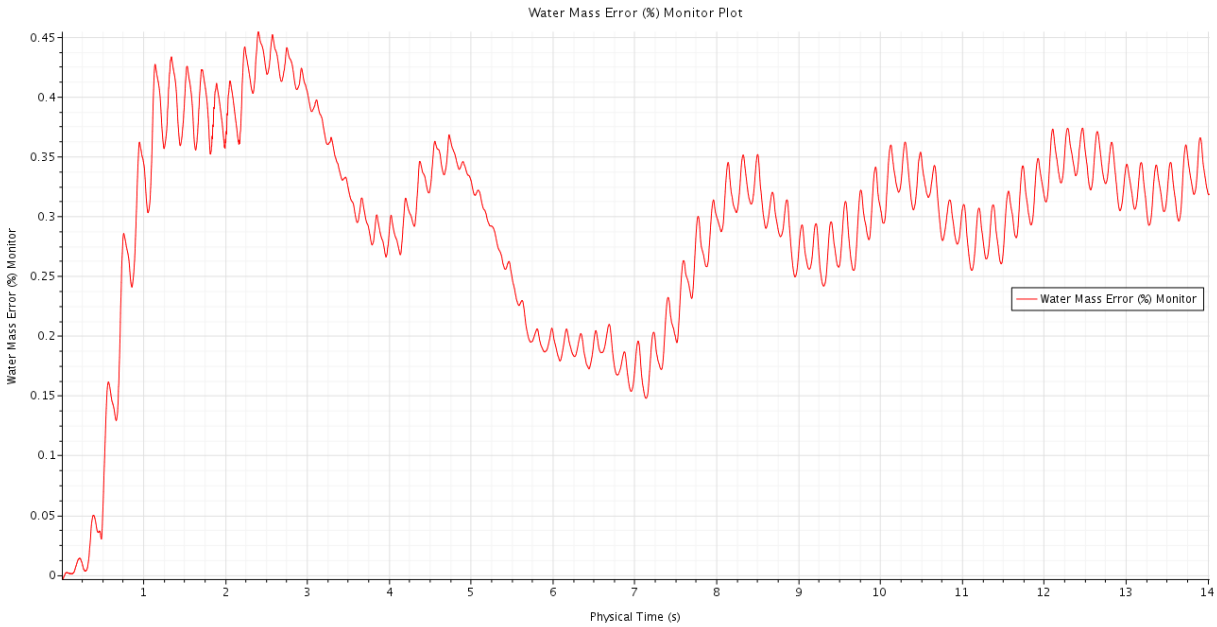

Figure 8 - Water mass error (%) in final simulation with X_0=0.005 m

A second simulation attempt resulted in another problem: the source of water mass, previously described, wrongly poured the liquid phase throughout the domain, including the air phase zone, causing anomalies in the numerical solution, such as unnatural splashes and sprays, visible in Figure 9.

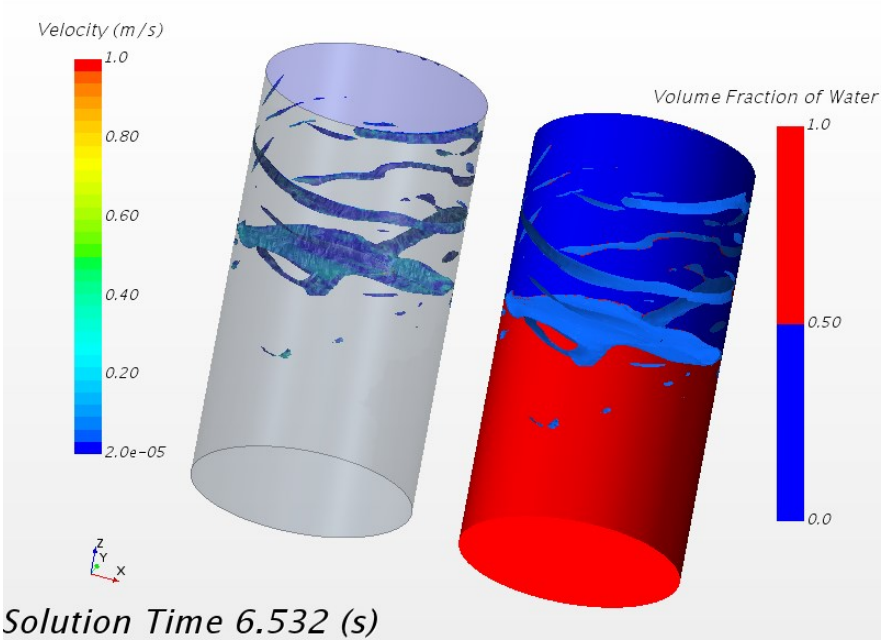

Figure 9 - Unnatural splashes caused by wrongly water mass error correction

To solve this problem the correction factor has been modified, allowing the reintroduction of the missing water mass only in an area of the domain where the liquid phase is present, sufficiently far from the free surface to avoid disturbing effects.

Once these issues were overcome, the final simulations were carried out. In both cases analyzed two different behaviors occurred. In a first phase the liquid oscillates along the x-axis, with a certain elevation; then, gradually, it starts to rotate clockwise. This swirling behavior is typical of liquids moving in symmetrical tanks and its appearance also occurs in the VKI experimental results. In the lower amplitude case the water starts to rotate at 8.728 s of physical time, while in the case of higher amplitude the rotation start at 4.774 s of physical time, like shown in Figure 10.

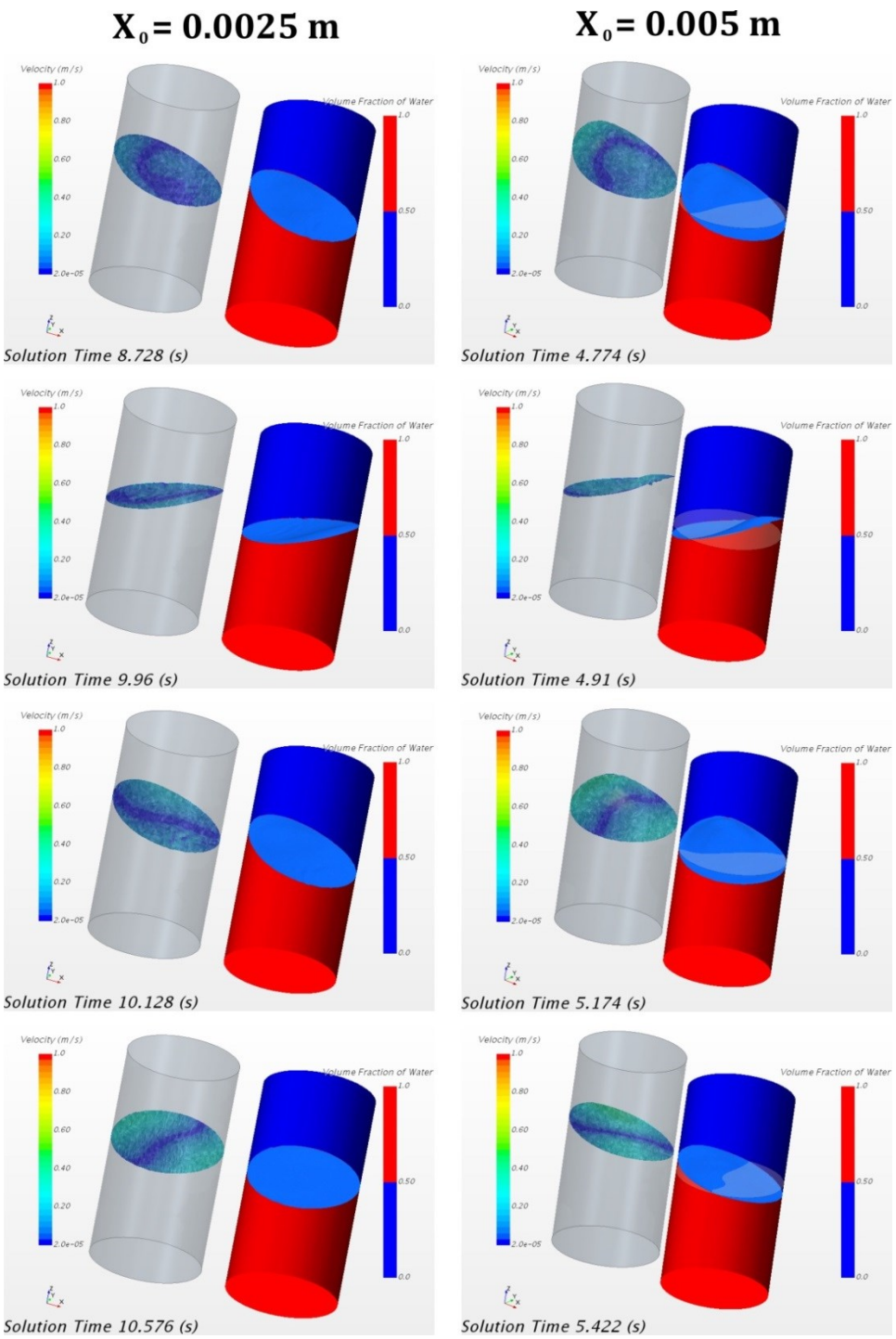

Figure 10 - Swirling phenomena: lower amplitude (left) and higher amplitude (right)

Maximum elevation of free surface for the two cases is shown on Figure 11 and Figure 12:

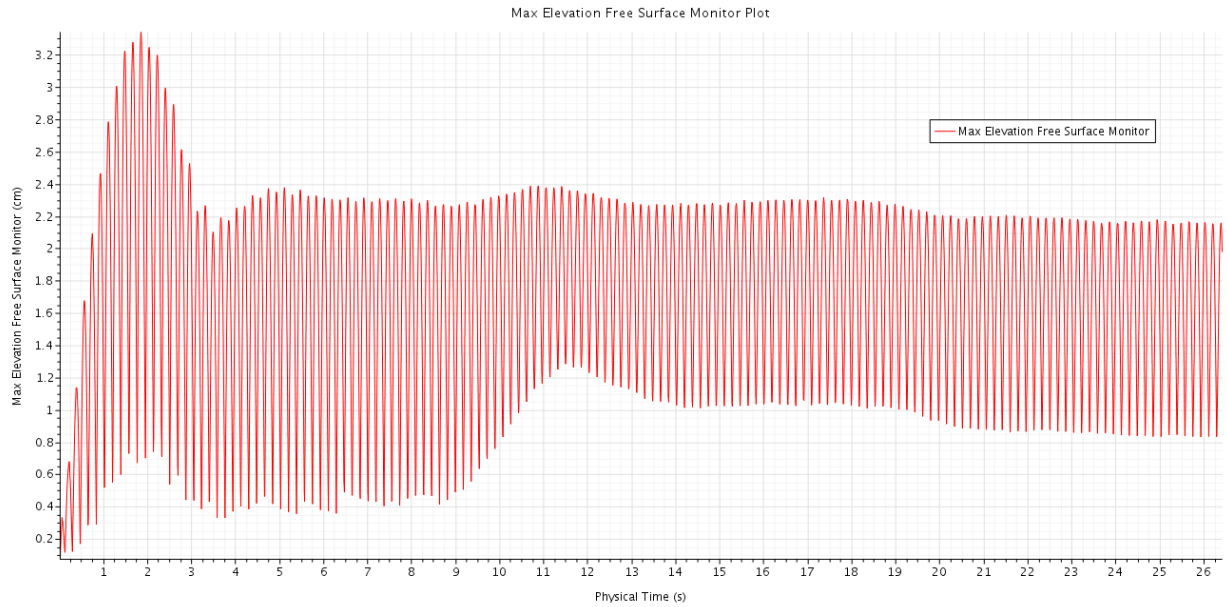

Figure 11 – Maximum elevation of the free surface (X_0=0.0025 m)

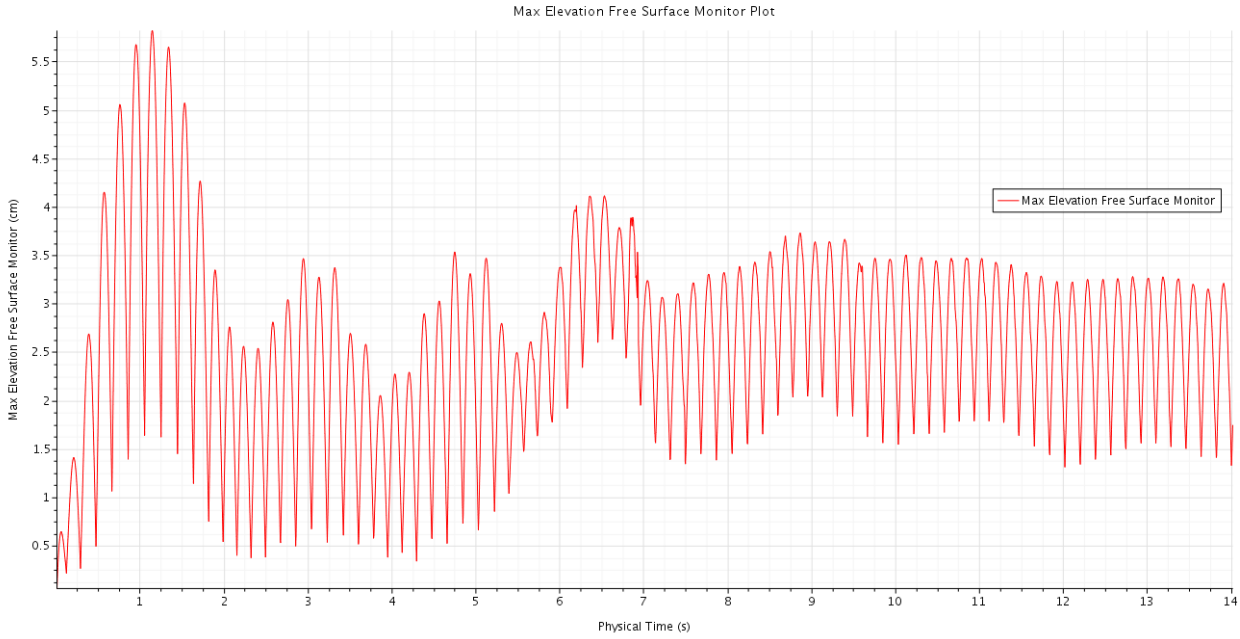

Figure 12 - Maximum elevation of the free surface (X_0=0.005 m)

For the lower amplitude case the max elevation is about $3.3\ \mathrm{cm}$, while in the case of higher amplitude is about $5.8\ \mathrm{cm}$. In both cases the value of maximum elevation is obtained in the first oscillations; during the swirling phase the elevation of free surface stabilizes at a lower value, with cycles of light growth and decrease at low frequency. This behavior is in line with the VKI experiment results, even if the values of maximum water elevation are slightly different.

In both cases the free surface ripples less than it does in the VKI experimentations results, with visible effects especially in the higher amplitude case, during the swirling phase (Figure 13).

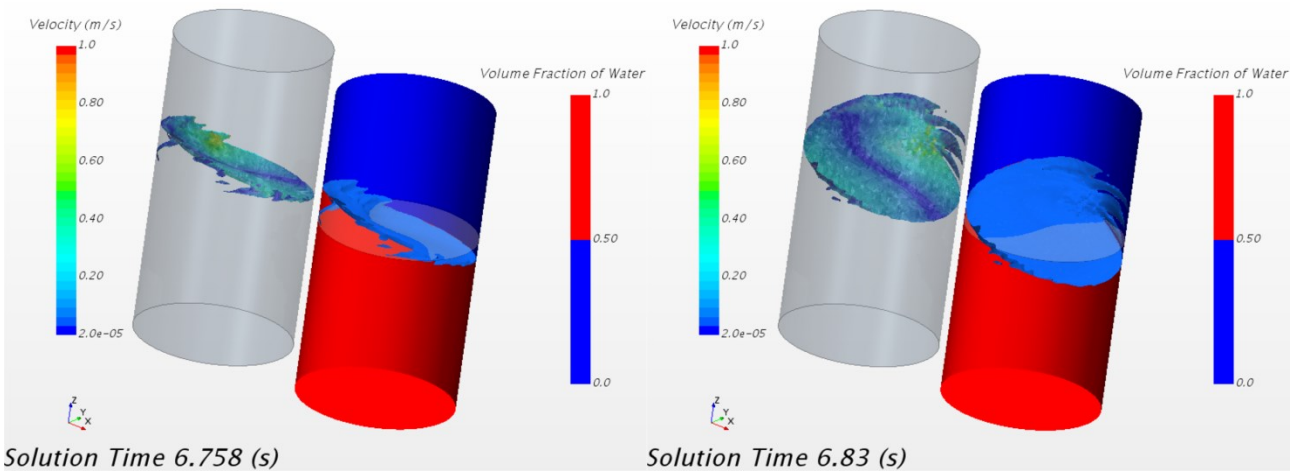

Figure 13 – Perturbation of the free surface during swirling phase (X_0=0.005 m)

6. Conclusions

In this internship at CRS4 the phenomena of sloshing in a cylindrical tank partially filled with water was studied using the STAR-CCM+ software. Not all the scheduled tests and simulations were performed, due to unforeseen events that occurred during the period of the internship (which caused a reduction of the time available), but some main goals has been achieved, finding a good correspondence with the results of the von Karmann Institute study, used as reference.

The simulation shows that VOF method is capable to predict this particular fluid behavior. For a complete study of sloshing phenomena it will be necessary to investigate more in-depth the incidence of some parameters on it (e.g. surface tension, liquid / wall contact angle, different fluid). It will also be indicated to operate simulations with a smaller time-step, necessary to bring out even the smallest aspects of the fluid behavior, and try different physics models to find an optimum solution between results resolution and reduction of numerical errors.

The experience of this internship has been very positive and enriching, from curricular and personal point of view; carried out in a professional working context, it has been the occasion to have a first fleeting contact with the fascinating world of research and to put into practice what was learned in the classroom. An experience of this type is recommended to all colleagues because it gives valuable knowledge and skills that can certainly be spent in the future career of an engineer.

References

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(3) Myrillas K., Planquart P., Buchlin J., Schyns M., "*CFD and experimental investigation of sloshing parameters for the safety assessment of HLM reactors*", NURETH-16, Chicago, IL, 2015

(4) Baeten P., Schyns M., Fernandez R., De Bruyn D., Van den Eynde G., "*MYRRHA: A multipurpose nuclear research facility*", EPJ Web of Conferences, vol. 79, p. 03001, EDP Sciences (2014)

(5) https://documentation.thesteveportal.plm.automation.siemens.com