NewSOL Project (720985)

Fluent: Case 0

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"Fluent: Case 0"
Internal Report on work developed by LNEG included in Subtask 5.1 "Thermocline concrete tank simulation" for partial fulfillment of deliverable D5.1 "System configuration for thermocline concrete tank".
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1. Overview

In order to implement the simulation of a thermal process in a computational fluid dynamics application, both the geometry (Section 2) and the mesh (Section 3) must be defined, including different mesh zones if needed.

Next, the boundary conditions (Section 4) including inlets, outlets, walls and symmetry planes must also be defined and the materials (filler and fluid) thermal properties must also be included, usually with temperature dependency for the fluids. The thermal properties (Section 5) for fluids include density, specific heat, thermal conductivity and dynamic viscosity. The thermal properties for the solid material include all the previous properties but the dynamic viscosity. On the other hand, a porosity must also be defined considered that the filler material will be described as a porous material.

Afterwards, models (Section 6) to calculate turbulence, radiative heat transfer, etc must be activated and set up and finally, some tests must be performed (Section 7) to ensure that the proposed mesh is up to task.

This document presents all the described steps in order to set up what is called Case 0. In the following work the inlet mass flow and temperature, the heat losses through walls, the materials themselves and their properties, including, porosity and the turbulence and radiative heat transfer models can also be changed.

Everything can change, but the mesh. The only exception to this is to refine the mesh a little bit in particular areas in order to increase detail and mitigate some flow problems and improving the results.

2. Geometry

The geometry for the TES tank was proposed by LNEG in a previous report[1]. However, both constructive and budget limitations defined a different approach to size the TES tank. Moreover, the aimed autonomous working period for an eventual power block also changed.

Thus, by definition of the project coordinator (University of Évora) and according to the minutes from March, 1st, meeting, the dimensions presented in Table 1 apply to the thermal energy storage (TES) tank.

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[1] P. Azevedo (2017), "Thermal calculations for TES tank predesign: EMSP case-study", LNEG's internal report LEN-UER-2017-N02-IR, May, 2017.

Table 1: Thermal Energy Storage (TES) tank dimensions.

Parameter	Unit	Value
Height (including US)	[m]	4,5
Diameter	[m]	2,8
Ullage Space (US)	[m]	0,5
Baskets	-	8
Height	[m]	0,5
Bottom basket	-	Only MS
Top basket	-	Only MS

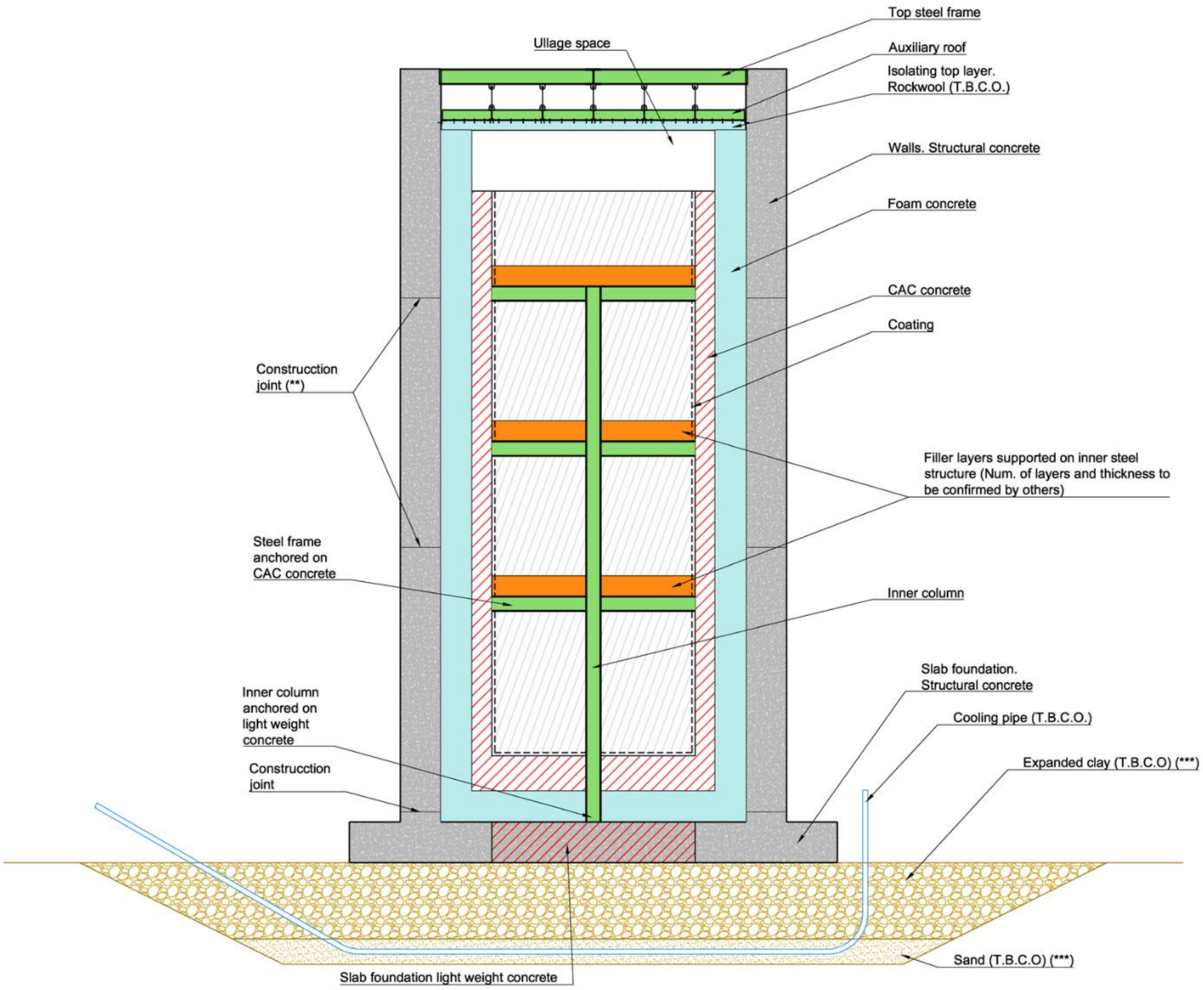

Figure 1: Tank predesign.

The geometry for the CFD work must be defined in 2D. Considering that the case consists of a cylindered tank, the tank must be represented by a radial cut from the center axis to the wall as depicted in Figure 2.

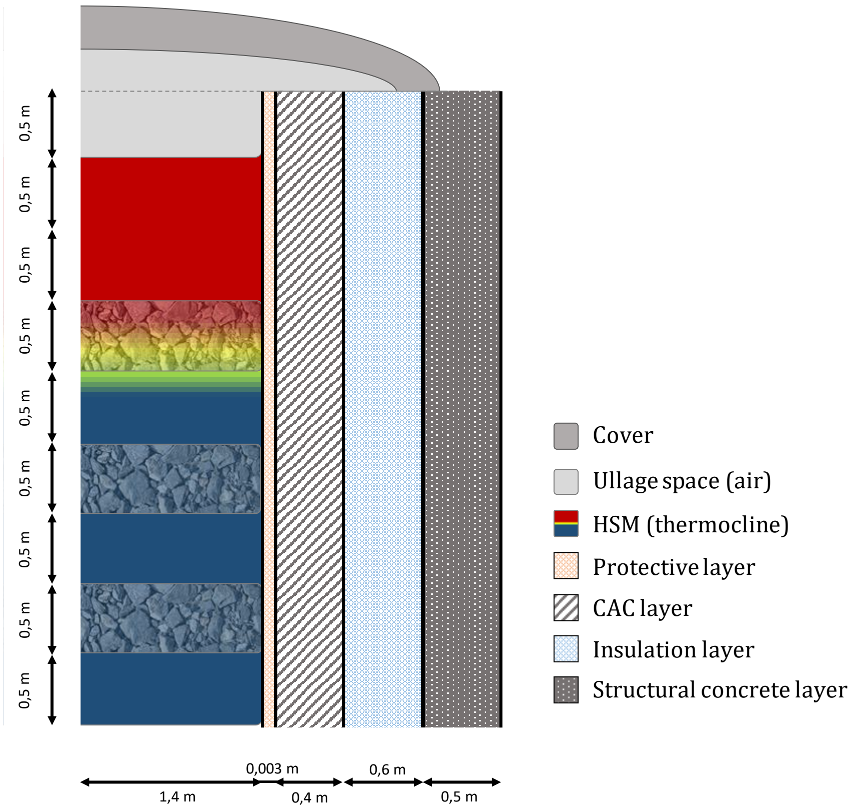

Figure 2: Axial cut to the TES tank.

3. Mesh

Previous experience would lead us to an unstructured mesh to tackle more complex geometries. Moreover, the modelling of chemistry reactivity, mandatory in certain cases, would be greatly improved with the use of an unstructured mesh due to the presence of turbulence in shear walls.

However, the expected geometry for the thermal energy storage tank to be built at EMSP (Évora Molten Salts Platform) and described in Section 2 may, indeed, be very suitable to a structured mesh. Thus, a first attempt in order to determine Reynolds (Re), Grashof (Gr) and Raleigh (Ra) numbers can be made using a structured mesh, as described in IR04[2].

If the wall effect becomes relevant enough for thermal diffusion due to near wall eddies or if the numerical convergence reveals itself hard to achieve, an unstructured solution should then be attempted.

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[2] M. Giestas Lima e P. Azevedo (2017), "Available CFD models assessment", LNEG's internal report LEN-UER-2017-N04-IR, December, 2017.

Generally, the mesh should be tested considering the tools provided to test the mesh. If those tools are not available in Fluent, eventually the tests could be performed in TGrid (an old program from Fluent to test meshes).

Afterwards, the case should be defined with boundary conditions, materials and models (Sections 4 to 6).

The mesh must have different continuous zones, in order to define the presence or the absence of filler material in each zone. These zones will represent the 8 baskets described in Table 1.

The mesh must meet the tests defined in Section 7 of this document. The grid independence test must be considered for the detail of the mesh, namely the definition of the number of cells.

4. Boundary conditions

Walls

The side wall around the tank doesn't need to be defined in what concerns to the used material thermal properties. The only phenomenon to consider is the heat transfer through walls from the inside to the outside. The wall is constituted by multiple layers as presented in Figure 3. However, the study of the heat transfer through the wall was already presented in a previous report[3] and it is not addressed in this document.

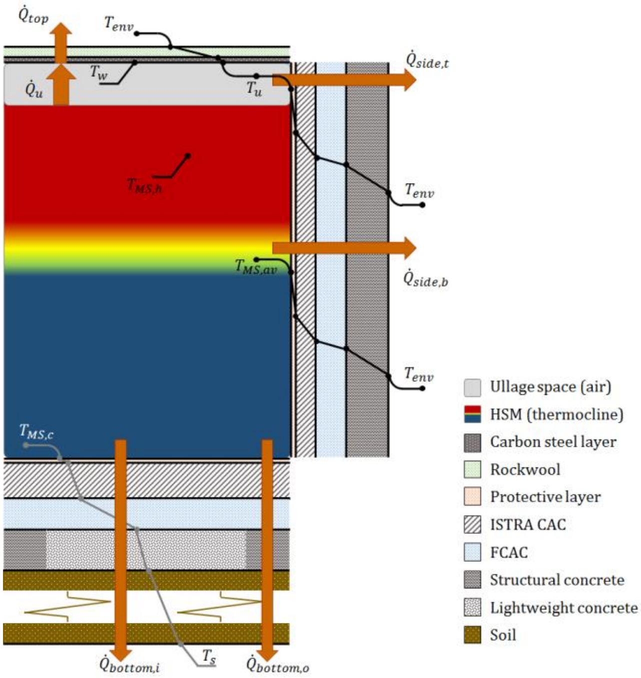

Figure 3: Heat fluxes through the wall.

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[3] P. Azevedo (2017), "Thermal calculations for TES tank predesign: EMSP case-study", LNEG's internal report LEN-UER-2017-N02-IR, May, 2017.

Considering the data presented both in Table 1 and Table 2, the heat transferred per area unit is 82,1 W/m^2. The equivalent thermal conductivity for all the layers in the wall and including the convection in both sides of the wall is 0,171 W/m^2-K.

Table 2: TES working conditions.

Parameter	Unit	Value
Maximum fluid temperature inside the tank (MS)	[ºC]	500
Minimum fluid temperature inside the tank (MS)	[ºC]	200
Fluid temperature outside the tank (Air)	[ºC]	20
Wind velocity	[m/s]	6

Table 3: TES side wall specification (to be confirmed).

Layer	Definition	Thickness [m]	Thermal conductivity [W/m-K]
1	Protective layer	0,003	16
2	ISTRA CAC 0	0,4	2,05
3	FCAC	0,6	0,113
4	Structural concrete	0,5	1,63

Inlet

The top of the computational volume will be considered as inlet or outlet depending whether the tank is charging or discharging, respectively.

According to LNEG's report[4], the inlet mass flow ($\dot{m}_{inlet}$) to consider should be 5,373 kg/s (to be confirmed).

The inlet should be defined as "velocity inlet" and the velocity should be calculated according to (1).

$$v_{inlet} = \frac{\dot{m}_{inlet}}{\rho_{MS@500\,°C} . A_{tank}} \quad (1)$$

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[4] P.Azevedo (2017), "Thermal calculations for TES tank predesign: EMSP case-study", LNEG's internal report LEN-UER-2017-N02-IR, May, 2017.

Where:

$\dot{m}_{inlet}$: inlet mass flow [kg/s];

$\rho_{MS@500\,°C}$: Molten salt density @ 500 °C [kg/m^3];

A_{tank}: Area of the TES tank [m^2];

v_{inlet}: Velocity at the inlet [m/s] in axial direction.

With the parameters considered along this report, the velocity in axial direction is 4,54x10^{-4} m/s.

Outlet

The outlet should be defined as a "pressure outlet".

Symmetry

The left side of the tank does not need to be designed nor meshed, because the boundary condition can be defined as symmetry. This saves cells, cutting the problem down by half.

5. Materials

The materials considered for the definition of the Case 0 are the molten salt from Yara, the Yara MOST, and the slag from S. Domingos Mines, used as filler. In order to consider those materials properly, their thermal properties must be given.

The materials for the walls don't need to be defined considering that the boundary conditions already defined a heat loss through the walls.

Yara MOST

The thermal properties for the Yara MOST molten salt include density, specific heat, thermal conductivity and viscosity. These properties were addressed in a previous report[5].

Density

The density should be defined as a polynomial function (2).

$$\rho(T) = -0{,}91987.T + 2380{,}9 \qquad (2)$$

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[5] P.Azevedo (2018), "Thermal properties", LNEG's internal report LEN-UER-2018-N07-IR, February, 2018.

Where:

T: Yara MOST temperature (ranging from 200 °C to 500 °C) [°C];

$\rho(T)$: Density @ temperature [kg/m^3].

Specific heat

The specific heat should be defined as a polynomial function (3).

$$Cp(T) = -0{,}70121.T + 1799{,}3 \tag{3}$$

Where:

T: Yara MOST temperature (ranging from 200 °C to 500 °C) [°C];

$Cp(T)$: Specific heat @ temperature [kJ/kg-K].

Thermal conductivity

The thermal conductivity should be defined as a polynomial function (4).

$$k(T) = -4{,}0 \times 10^{-6}.T^2 + 2{,}62 \times 10^{-3}.T + 0{,}133 \tag{4}$$

Where:

T: Yara MOST temperature (ranging from 200 °C to 500 °C) [°C];

$k(T)$: Thermal conductivity @ temperature [W/m-K].

Dynamic viscosity

The dynamic viscosity should be defined as piecewise-linear profile, according to Table 4.

Table 4: Dynamic viscosity piecewise-linear profile, dependent on temperature.

Temperature [°C]	Dynamic viscosity [kg/m-s]
140	$12{,}5 \times 10^{-3}$
150	$7{,}8 \times 10^{-3}$
170	$5{,}4 \times 10^{-3}$
200	$3{,}6 \times 10^{-3}$
205	$3{,}6 \times 10^{-3}$
260	$2{,}4 \times 10^{-3}$
300	$2{,}1 \times 10^{-3}$
400	$1{,}4 \times 10^{-3}$
460	$1{,}1 \times 10^{-3}$
500	$1{,}1 \times 10^{-3}$

Although some discrepancies were found between Yara MOST thermal properties and the Hitec XL properties, a commercial molten salt with the same composition, the data provided by Yara was used as received and regressions were made when applicable. This data can be of influence in the expected results.

Slag from S. Domingos Mines

The most common way to represent a packed bed in CFD calculations is to define the filler material as a porous media. Thus, the void space in the material packed bed is an important parameter of the material and it is represented as porosity of the material. The porosity will represent the part of the tank volume that will be filled by molten salts. Hence, the properties of the filler material will largely influence the behavior of the thermal energy storage tank, namely, the storage heat capacity, due to the large difference of specific heats between both molten salts and filler material.

The slag from S. Domingos' mines will be used as a filler material. The slag thermal properties were disclosed by UEvora[5] and Table 5 presents the disclosed data about the filler material.

Table 5: Slag thermal properties.

Property	Units	Value
Fluid porosity	-	50%
Density	[kg/m^3]	3600
Specific heat (Cp)	[kJ/kg-K]	0,444
Thermal conductivity	[W/m-K]	1,7

6. Models

The turbulence and radiation models are important models to be considered. In the initial convergence tests it will be advisable to include the turbulence model. The energy equation must be on although no radiation should be active.

Turbulence model

The turbulence model should be defined only after both Re, Gr and Ra numbers are known. The knowledge of those numbers will allow us to better understand what type of flow will be generated inside the tank, more specifically near the walls. However, although the ease of use presented by the Spalart-Allmaras model, the versatility presented by the SST k-ω seems to represent a better choice for an initial attempt, as described in IR04[2].

Afterwards, the convergence response and the computational expense of both mesh and turbulence model will be assessed in order to define which can be the least expensive solutions without compromising the results.

Radiation model

With regard to the radiation model, several issues must be addressed. The optical thickness is one of the most interesting parameters to consider in order to choose the radiation model. Although, several meters are an appropriate length scale for the domain, radiation will certainly find it hard to reach surfaces across a medium with approximately 50% (v/v) of opaque solid material.

Thus, the most suitable radiation models for that length scale (e.g. P-1 or Rosseland) may very well yield inadequate results if the optical thickness were to be addressed as the mean free path. Therefore, if the appropriate length scale is reduced to a length of few centimeters, eventually other models should be considered (e.g. DTRM, DO or MC).

As concluded in a previous report[2], a model capable of work across a full range of optical thicknesses must be used for a first approach (e.g. DTRM, DO or MC). The computational costs can also be addressed, but the DO model is a good candidate, providing that the packed bed is represented by porous material instead of multiphase material.

Finally, the absorption and/or scattering coefficients of the molten salts and the filler material must also be known and considered. And, although, these data were not provided, they will be asked and, in the meantime, the proposed values (by the CFD package) should be used.

7. Tests

The simplest case should be tested in order to test the convergence of the solution with the proposed mesh. The independence of the grid size will ensure the best results with the minimum computational costs for the models activated and the initial solution independency will ensure that the solution proposed by the model is unique.

All these tests should be conducted in a steady-state case, even if the case will afterwards be defined as transient.

Convergence tests

The initial convergence tests will allow to ensure that the mesh is adequate. The convergence criteria should be as described in Table 6.

Table 6: Absolut criteria for initial residues.

Residual	Absolut Criteria
Continuity	0,001
x-velocity	0,001
y-velocity	0,001
z-velocity	0,001
energy	1e-06
turbulence	0,001

Grid size independence

The mesh should be created with a large number of cells. In this case, a first approach can be 1 cell for each 5 mm. For an orthogonal mesh equals 252 k cells.

Then the mesh should be coarsened and the results compared. When the results start to become different from the previous ones, the minimum reticulation was achieved in the previous iteration.

Initial solution independence

After the previous tests, an initial solution independence test must be conducted in order to ensure that the results yielded are unique for the conditions defined and don’t depend on the initial solution.