SYMCOMP 2025
Lisbon, 10-11 April 2025


# PRELIMINARY SIMULATION RESULTS OF A MOLTEN SALT THERMAL STORAGE TANK FOR CONCENTRATED SOLAR POWER

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**Keywords:** Computational Fluid Dynamics, Thermocline tank, Porous media, Packed-bed

**Abstract** *Molten salt thermal storage systems play a critical role in concentrated solar power (CSP) plants, ensuring energy storage and dispatchability. Among these, thermocline tanks offer the potential for cost reduction, compared to the standard thermal storage system implemented in CSP plants: a two-tank solution (for hot and cold fluid, individually). This paper presents initial results from a Computational Fluid Dynamics (CFD) simulation of the 2.86 $MWh_{th}$ thermocline-tank installed at the EMSP – Évora Molten Salt Platform. The tank incorporates a filler material to enhance thermal stratification. The CFD model integrates the transport equations for mass, momentum and energy, along with closure models to account for the pressure drop imposed by the presence of the filler material and the heat transfer between the molten salts and the filler material. Validation of the model is conducted using experimental data from the literature. The simulation investigates the thermal performance of the tank during the discharging phase, where the axial temperature at the centerline of the tank was monitored periodically. The results were obtained for a simplified geometry of the tank as more improvements can still be made in future work to ensure the accuracy of the model.*

## 1. INTRODUCTION

Thermal energy storage systems (TES) are an essential technology to increase the efficiency of the integration of intermittent renewable energies. For optimal operation and improvement of the system efficiency, a study of the storage system is essential. In the study and implementation of a system of this type, it is necessary to consider the conditions of production (variability of the solar radiation between day and night, the climate of the place and the season of the year, among others) and consumption (periods, seasonality and intensity, among others). In solar thermal applications it is very interesting to have a TES mechanism capable of collecting energy at times of high radiation for later use in periods of absence of sun.

In the scope of such studies, computational fluid dynamics (CFD) are helpful and key to pre-prototyping works. This study presents the initial results from a CFD simulation of the 2.86 $MWh_{th}$ NEWSOL dual media thermocline-tank implemented at ESMP – Évora Molten Salt Platform. The work presented intends to be the starting point for a more focused and intricate analysis on the heat and mass transfer phenomena of this category of TES.

## 2. PROBLEM DESCRIPTION AND MODELLING APPROACH

The 2.86 $MWh_{th}$ NEWSOL thermocline-tank implemented at ESMP – Évora Molten Salt Platform consists of a single cylindrical vertical tank filled with molten-salts, which serve as heat transfer fluid, and slag pebbles that compose the filler material. To facilitate the analysis, the tank simulated in this work is a simplification of the real NEWSOL tank, which is equipped with an inlet and an outlet at the bottom (for cold) and top (for hot) of the lateral wall of the tank. As first analysis and baseline study, in the current model, it is assumed that on a discharging phase, the inlet and outlet are located at the bottom and top of the tank, respectively, occupying all the boundary and creating a plug flow. A simple schematic of the simulated tank as well as the computational domain is shown in Figure 1.

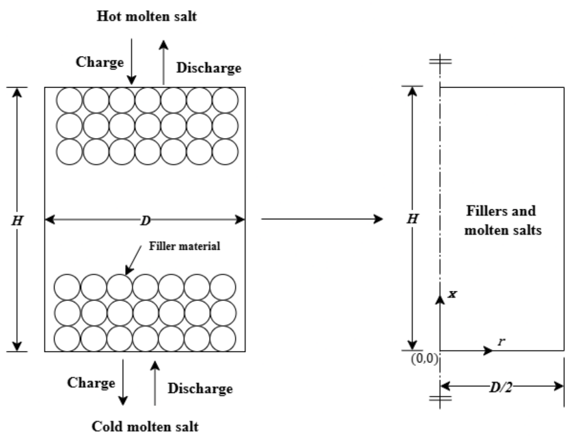


Figure 1. Schematic diagram of the simplified simulated tank and computational domain.

In the following subsections, a transient, two-dimensional, CFD model is presented to account for the flow, heat and mass transfer phenomena within the packed-bed NEWSOL thermocline tank. The thermal non-equilibrium model is considered to account for the different temperatures of molten salt and solid fillers. The following assumptions are taken to simplify the analysis:

- The fluid flow and heat transfer are symmetrical about the axis. As such, the governing equations for transport within the tank become two-dimensional.
- The flow of molten salt through the packed-bed region is laminar and incompressible.
- The solid fillers behave as a continuous, homogeneous, and isotropic porous medium, and the solid medium is not described as independent particles.

## 3. GOVERNING EQUATIONS

Transient, two-dimensional governing equations based on the volume-averaging approach [1] are presented to model the heat transfer and fluid flow inside the NEWSOL thermocline tank.

### 3.1. Continuity equation

$$\frac{\partial(\varepsilon\rho_l)}{\partial t} + \nabla \cdot [\rho_l \vec{u}] = 0 \tag{1}$$

where $\varepsilon$ is the bed porosity, $\rho_l$ is the density of molten salt and $\vec{u}$ is the superficial velocity vector of the fluid where $\vec{u} = \vec{u}_r \overrightarrow{e_r} + \overrightarrow{u_x}\,\overrightarrow{e_x}$.

### 3.2. Momentum equation

$$\frac{\partial(\rho_l \vec{u})}{\partial(\varepsilon t)} + \frac{\nabla\cdot(\rho_l \vec{u}\vec{u})}{\varepsilon^2} = \nabla\cdot(\mu\nabla\vec{u}) - \nabla p + \rho_l \vec{g} - \left(\frac{\mu}{K} + \frac{C_F \rho_l}{\sqrt{K}}|\vec{u}|\right)\vec{u} \tag{2}$$

where $\mu$ is the molten salt dynamic viscosity, $p$ is the pressure, $\vec{g}$ is the gravitational force and $\left(\frac{\mu}{K} + \frac{C_F \rho}{\sqrt{K}}|\vec{u}|\right)\vec{u}$ is a packed-bed momentum source term where the first-term is a viscous loss term and the second one an inertial loss term. $K$ is the permeability of the packed-bed and $C_F$ the inertial coefficient. Both parameters are calculated through empirical correlations, as follows [2]:

$$K = \frac{d_p^2 \varepsilon^3}{150(1-\varepsilon)^2} \tag{3}$$

$$C_F = \frac{1.75}{\sqrt{150\,\varepsilon^3}} \tag{4}$$

where $d_p$ is the filler material particle diameter.

### 3.3. Energy equation for the molten salt

$$\frac{\partial(\varepsilon\rho_l c_{p,l} T_l)}{\partial t} + \nabla\cdot\left(\rho_l c_{p,l}\,\vec{u}\,T_l\right) = \nabla\cdot\left(k_{l,\mathrm{eff}}\nabla T_l\right) + h_{ls}\,a_{ls}\,(T_l - T_s) \tag{5}$$

where $c_{p,\mathrm{l}}$ is the molten salt specific heat, $T_\mathrm{l}$ and $T_\mathrm{s}$ are the molten salt and solid fillers temperature, respectively, $k_{\mathrm{l,eff}}$ is the fluid effective thermal conductivity, $h_{\mathrm{ls}}$ is the interstitial heat transfer coefficient between the fluid and solid fillers and $a_{\mathrm{ls}}$ is the interfacial area density, which is calculated as follows, assuming that the filler particles are spherical:

$$a_{\mathrm{ls}} = \frac{6(1-\varepsilon)}{d_\mathrm{p}} \tag{6}$$

### 3.4. Energy equation for the solid filler

$$\frac{\partial\big((1-\varepsilon)\rho_\mathrm{s} c_{p,\mathrm{s}} T_\mathrm{s}\big)}{\partial t} = \nabla \cdot \big(k_{\mathrm{s,eff}} \nabla T_\mathrm{l}\big) + h_{\mathrm{ls}}\, a_{\mathrm{ls}}(T_\mathrm{s} - T_\mathrm{l}) \tag{7}$$

where $\rho_\mathrm{s}$ is the solid filler density, $c_{p,s}$ is the solid filler specific heat and $k_{\mathrm{s,eff}}$ is the solid filler effective thermal conductivity.

## 4. EMPIRICAL CORRELATIONS AND HEAT TRANSFER PARAMETERS

### 4.1. Effective thermal conductivity, $k_{\mathrm{eff}}$

For the effective thermal conductivity of molten salt and solid fillers we considered the application of an equivalent to the parallel model to obtain these parameters. In [3] more can be found regarding this model.

### 4.2. Interstitial heat transfer coefficient, $h_{\mathrm{ls}}$

The volumetric interstitial heat transfer coefficient is an important parameter to account for in packed bed porous media modelling when a non-equilibrium model approach is being used as it makes the link for the heat transfer between the solid fillers and the heat transfer fluid. This parameter is often obtained by experiments where an empirical correlation is formulated depending on the specific parameters of each simulation (e.g., Reynolds and Prandtl number, porosity of the packed bed, etc.). For the current numerical model, the heat transfer coefficient used is a fixed value of $204.21\ \mathrm{W/(m^2\ K)}$ calculated from Eq. (8) for a reference temperature of 170 ºC, which is the inlet temperature for the discharge cycle and based on the following empirical correlation which is well suited for a wide range of Reynolds numbers and packed bed porosities [4].

$$h_{\mathrm{ls}} = \frac{k_\mathrm{l}\left[2+1.1\, Re_\mathrm{p}^{0.6} Pr^{1/3}\right]}{d_\mathrm{p}^2} \tag{8}$$

where $Re_\mathrm{p}$ is the particle filler Reynolds number, and $Pr$ is the Prandtl number.

## 5. MATERIAL PROPERTIES

The molten salt used in NEWSOL tank is a mixture of 60 wt% $\mathrm{NaNO_3}$ and 40 wt% $\mathrm{KNO_3}$ where its thermophysical properties are temperature-dependent and can be found at [5]. As for the solid fillers (slag pebbles), except density, which is constant, the other thermophysical properties used in the model are also temperature dependent and can be found at [6].

## 6. BOUNDARY CONDITIONS

For each process (charging/discharging) the boundary conditions are given as follows:

### 6.1. Charging process

Top inlet: $\dot{m}_{\mathrm{in}} = \rho_{\mathrm{l,in}} \cdot A_{\mathrm{in}} \cdot u_{x,\mathrm{in}} = 5.3\ kg/s, u_{r,\mathrm{in}} = 0,$ and $T_{\mathrm{l}} = T_{\mathrm{s}} = T_{\mathrm{in}} = 170℃$ (9)

where $\dot{m}_{\mathrm{in}}$ is the inlet mass flow of molten salt, $\rho_{\mathrm{l,in}}$ is its density calculated at the inlet temperature, $T_{\mathrm{in}}$, $A_{in}$ is the surface area of the inlet, and $u_{x,\mathrm{in}}$ is the inlet velocity, normal to the inlet area.
Bottom outlet: outflow boundary condition where:

$$\partial\vec{u}/\partial x = 0,\ \partial T_{\mathrm{l}}/\partial x = 0,\ \partial T_{\mathrm{s}}/\partial x = 0 \tag{10}$$

Exterior Wall: a constant heat flux, $q_{\mathrm{w}}$, is imposed at the wall considering the conductive heat transfer through the layers that constitute the lateral wall of the tank and the convective heat transfer between the exterior surface of the wall and the exterior environment. The following equation is used to calculate the imposed heat flux:

$$q_{\mathrm{w}} = \frac{T_{\mathrm{avg}} - T_{\infty}}{\frac{1}{\mathrm{h_{conv}}} + \sum_{i=1}^{n}\left(\ln\left(\frac{R_{\mathrm{l}}+t_1}{R_{\mathrm{l}}}\right) + \ln\left(\frac{R_{\mathrm{l}}+t_1+t_2}{R_{\mathrm{l}}+t_1}\right) + \cdots + \ln\left(\frac{R_{\mathrm{l}}+t_1+\cdots+t_n}{R_{\mathrm{l}}+e_1+\cdots+e_{t-1}}\right)\right)} \tag{11}$$

where $T_{\mathrm{avg}}$ is the average fluid temperature between the maximum and minimum temperatures inside the tank, $T_{\infty}$ is the ambient air temperature considered to be 25 ℃, $n$ is the number of wall layers (1 is the steel liner, 2 is the thermal concrete, 3 is insulation layer, and 4 the structural concrete layer), $R_{\mathrm{l}}$ is the tank inner radius and $t_n$ the thickness of the $n^{\mathrm{th}}$ layer. $h_{\mathrm{conv}}$ is the heat transfer coefficient taken from an empirical correlation for incompressible flow over a cylinder [7]:

$$Nu = h_{\mathrm{conv}} D / k_{\mathrm{air}} = 0.632\ Re_{\mathrm{D}}^{1/2} Pr^{1/3}, \quad Re_{\mathrm{D}} = \frac{u_{\mathrm{air}} D}{\nu_{\mathrm{air}}} \tag{12}$$

where $Nu$ is the Nusselt number, $D$ is the diameter of the tank, $u_{\mathrm{air}}$ is the air velocity, assumed as $5\ \mathrm{ms}^{-1}$, and $k_{\mathrm{air}}$ and $\nu_{\mathrm{air}}$ are, respectively, the thermal conductivity and the kinematic viscosity of air at the ambient temperature. $Re_D$ is the Reynolds number based on the tank diameter and $Pr$ is the Prandtl number.

Symmetry boundary condition: Since, for the purpose of this work, an axisymmetric model was considered, a symmetry boundary condition was assumed in the tank along its axis.

### 6.2. Discharging process

Bottom inlet: same conditions as in eq. (9)
Top outlet: outflow boundary condition with the same conditions as in eq. (10).
Exterior wall: the same conditions as in eqs. (11) and (12).
Symmetry boundary condition: same conditions as described for the charging process.

## 7. NUMERICAL METHODS

The governing equations described above are solved using the finite volume method [8] and the CFD commercial software ANSYS Fluent v. 2024 R2 [9]. As already described, these equations are solved considering the volume-averaged equations for a porous medium and the non-thermal equilibrium model to account for the local temperature differences between the molten salt and the solid fillers. Gravity is set on the axial direction. The SIMPLE algorithm is employed for the pressure-velocity coupling [10]. The pressure term is discretized by a second order scheme, and momentum and energy equations are discretized by the second order upwind scheme. A first order implicit method is employed for discretization of the transient term. The under-relaxation factors are set to 0.3, 1, 0.7, and 0.5, for pressure, density, momentum and energy, respectively. The simulations are performed for a time-step of 1 s and a mesh with 4000 elements. The governing equations are solved for each time step until the residuals for continuity and momentum equations reduce to less than $10^{-3}$, and $10^{-6}$ for the energy equation.

## 8. MODEL VALIDATION

The current model was validated with the experimental results of Pacheco et. al. [11] and the numerical results of Cabello Nuñez et. al. [6].

### 8.1. Validation with Pacheco et al.'s experimental results

In Pacheco et al.'s experiments, a molten-salt thermocline thermal storage system for parabolic trough plants was analysed and compared with the standard two-tank molten salt system [11]. The tank considered is a 2.3 $\mathrm{MWh_{th}}$ thermocline tank with a length of 5.9 m and a diameter of 3 m. Quartzite rocks were used as filler material and molten salt with the same chemical composition and thermophysical properties as mentioned in the material properties subsection were used. Other geometric parameters and properties used for validation with Pacheco et al.'s experiments can be found at [4]. The validation is performed for the axial temperature profiles of the molten salt in the storage tank at each 30 minutes of a discharging cycle. A good agreement between the experimental and numerical results is obtained even though some deviations exist. The average error percentage between the numerical and experimental results for each 30 min profile is approximately $\pm$ 1%, and the standard deviation and RMSE are also of the same order of magnitude, which indicates that the heat and mass transfer inside a packed bed thermocline tank can be well predicted by this current numerical model.

### 8.2. Validation with Cabello Nuñez et al.'s experimental results

Cabello Nuñez et al. [6] performed a numerical analysis of a hybrid thermal storage system composed of a single medium and a dual medium thermocline tank which used slag pebbles as filler material and molten salt as heat transfer fluid. Both tanks had a 20×20 $m^2$ design and the simulations used in the validation were conducted for the dual medium tank. Other geometric parameters and properties used in the model for this validation can be found at [6]. During the charging process the temperature at the bottom of the tank was monitored, and when the outlet temperature at this location increased by 30 ℃ the process was ended and immediately the discharge process started. The same monitoring activity occurred for the discharging phase but at the top of the tank. The validation is performed for the first full cycle of operation where the axial temperature of the molten salt in the storage tank at the end of the charge and discharge process is compared. The simulation is conducted for a time-step of 1s and a mesh of 8000 elements. The validation shows good agreement between the experimental and numerical results even though there are some deviations. The average error between the experimental and numerical results is around 3% for the charge and 1.5% for the discharge.

## 9. RESULTS AND DISCUSSION OF PRELIMINARY CFD SIMULATION

In the present work, preliminary results for the simplified NEWSOL tank geometry were carried out. A simulation is performed for a discharge cycle where the molten salts enter at the bottom of the tank at 170 ºC and with a mass flow rate of 5.3 kg/s. The full discharge cycle lasted 96 minutes. A uniform temperature distribution through all the tank and equivalent to the maximum temperature in the tank at the end of a charge cycle (490 ºC) was considered as initial condition. Additionally, the fluid was initially at rest. The results obtained can be seen in Figure 2 where the axial temperature of the tank taken at the centerline is presented for each 24 minutes of the simulation. As shown, a transient thermocline evolution inside the tank was observed. In this case, at the end of the discharge cycle, one can highlight that the temperature at the outlet of the tank (approximately 440 ºC) is inferior to the temperature taken at the same location during the whole cycle, which is the maximum temperature at the end of a charge cycle (490 ºC).

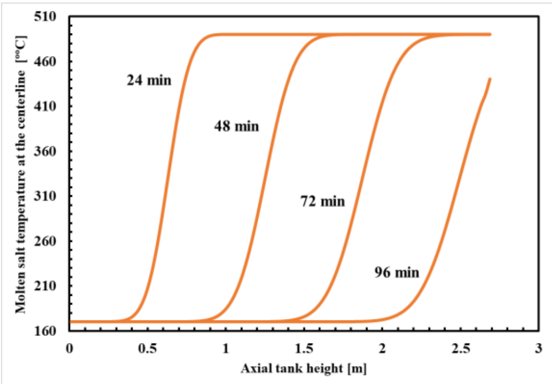


Figure 2. Simplified NEWSOL tank geometry preliminary simulation results.

## 10. CONCLUSIONS

In this study, a transient, two-dimensional numerical model is presented to perform preliminary CFD simulations of the 2.86 $MWh_{th}$ NEWSOL thermocline-tank installed at the ESMP – Évora Molten Salt Platform. The model was successfully validated with experimental and numerical results from the literature. Then, the model was employed to obtain preliminary simulation results regarding a discharge process of the packed bed NEWSOL thermocline tank. It is found that the simulation presents results according to what is expected where a transient thermocline evolution in the tank is observed, although the available output energy at the end of the discharge cycle is inferior to what is possible to retrieve through all the cycle. The simulations presented in the work are preliminary. For a start, mesh and time-step independence studies are being carried out to ensure the accuracy of the predictions. Additionally, improvements to the model can still be made. For example, more realistic initial conditions will be considered and the treatment of the heat transfer between the tank walls and the exterior will be improved. Nevertheless, these preliminary results show the potential of the proposed model to simulate the NEWSOL thermocline tank.

## 11. ACKNOWLEDGEMENTS

The authors acknowledge Fundação para a Ciência e a Tecnologia (FCT) for its financial support via the project LAETA Base Funding (DOI: 10.54499/UIDB/50022/2020) and the PhD grant 2024.01497.BD (Júnior Mané).

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