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A Simplified Numerical Model to Study the Thermal Behavior of a Cascade LHTES System

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Abstract. To promote the integration of Solar Heat for Industrial processes (SHIP), through the development of innovative cascade Latent Heat Thermal Energy Storage (LHTES) systems, a simplified zero-dimensional model for “shell&tube” LHTES systems that is fast, flexible and sufficiently accurate was set up. This model, programmed in Fortran 90, was developed not only to predict the thermal behavior of a cascade LHTES but also to be usable within a software to evaluate its integration in any plant, including a Concentrated Solar Thermal (CST). The model was validated through a comparison both with a more sophisticated numerical simulation and the experimental results. Finally, the simplified model was applied to a case study to analyse the thermal behavior of a system of three LHTES connected in series.

Keywords: LHTES, Cascaded, Multi-PCM, Simplified Model

1. Introduction

To reduce the carbon impact and move towards a green transition, industries are increasingly turning to renewable energy [1], [2]. For industries with processes that use heat, the production of solar heat by Concentrated Solar Thermal (CST) plants is a promising solution. The variability of the solar resource requires the presence of a Thermal Energy Storage (TES) that is able to give continuity to the supply of heat.To overcome some limitations that prevent the easy integration of Solar Heat for Industrial processes (SHIP), one solution is to develop innovative storage systems such as Latent Heat Thermal Energy Storage (LHTES) systems. This technology has the advantage of an almost constant temperature during melting and solidification of the Heat Storage Medium (HSM), with a higher stored energy density. An LHTES system provides maximum performance when operating in a limited temperature range around the melting temperature of the used Phase Change Material (PCM). If, as is often the case, the operating temperature range is wider, multi-PCMs or cascade LHTES solutions can be used. These systems, consisting of same stages with PCMs at different melting temperatures, maintain a relatively high input/output temperature difference and allow a higher heat transfer rate during charging and discharging processes and a stable power output from the plant. Their design for high temperature ranges is complex. The numerous studies in the literature [3], [4], have shown that an adequate numerical model of the LHTES system is the basis for evaluating the performance of the plant and, therefore, setting up its economic feasibility analysis. The aim of this work is to set up a simplified model for “shell & tube” LHTES systems that is fast, flexible, and sufficiently accurate not only to predict the thermal behavior of a cascade LHTES but also to be usable within a tool to evaluate its integration in any plant, including a CST system.

2. Model Description and Implementation

The objective of this work was the development and implementing a software able to simulate in a simplified way the thermal behavior of a cascaded LHTES system consisting of several units connected both in series and in parallel. The simplified model must guarantee very fast response times (a few tens of seconds) and an adequate level of accuracy (error less than 20%). The implementation of this software was made using the Fortran90 programming language and the GFrotran compiler of the GNU Compiler Collection.

2.1 Cascade LHTES System

The cascade LHTES system, considered here, is made up of N_m "modules", hydraulically connected in parallel, each of which is made up of N_{lines} lines connected in parallel and, for each line, N_e LHTES units, connected in series (Figure 1 a). All lines will be identical and the LHTES units of a line can be different according to the PCM they contain, thus being able to also configure a cascade or multi-PCMs system. For the LHTES unit reference was made to an LHTES unit concept, realized and characterized by ENEA in the past years [5], [6]. This solution, named ENEA-TES-LH02 (Figure 1 b,c), is however representative of numerous other concepts of shell&tube type units that can be implemented

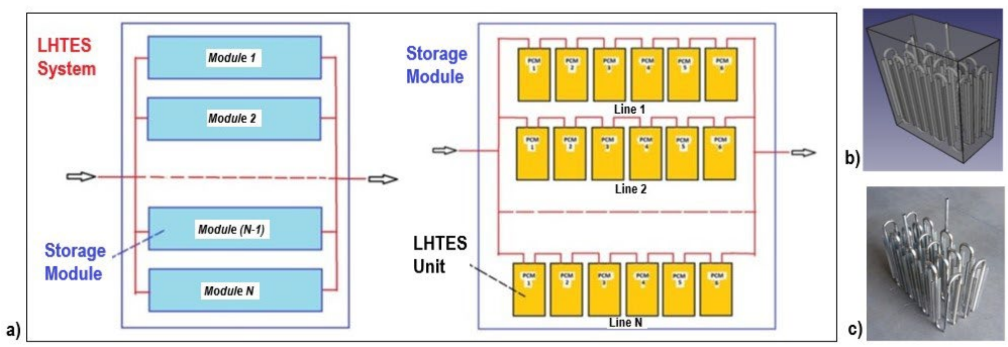

Figure 1. *Cascade LHTES - a) System and Module, b) Unit (project drawing) and c) Unit (as built)*

2.2 Model Description

For the development of a simplified model, it was decided to use a fixed spatial grid scheme, where the movement of the interface of the two phases is plotted through a nodal liquid fraction f that varies between 0 and 1, combined with an explicit solution scheme, based completely on the values of the solution at the previous moment. A simplified zero-dimensional model (0D) based on the "Energy Temperature Transforming" Method (ETTM) and a system with only two components, the Heat Transfer Fluid (HTF) and the Thermal Storage Medium (HSM) was considered. This model has been developed mathematically on the basis of the following assumptions: I) the basic configuration is a classic "shell & tube" (Figure 2); II) The internal heat exchange tube is neglected as it is made of metal, with high thermal conductivity and negligible heat capacity; III) The heat transfer fluid flows inside the tube itself; IV) Phase change material (PCM) fills the annular space around the air chamber; V) the thermophysical properties of HTF and PCM are constant; VI) the external surface of the container is well insulated and in adiabatic conditions.

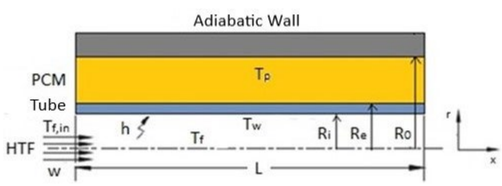

Figure 2. *Thermal storage channel in a tube&shell LHTES unit*

The ETTM/0D model is applied at the individual channel level. There are two basic unknowns: T_{fo}, the HTF inlet temperature, and T_p, the PCM temperature. The heat balance equation for HTF and HSM/PCM can be written:

$$M_f c_f \frac{\partial T_f}{\partial t} = w c_f (T_{fi} - T_{fo}) - h S_s (T_f - T_p) \quad (1)$$

$$M_p c_p \frac{\partial T_p}{\partial t} = h S_s (T_f - T_p) \quad (2)$$

After a few steps and discretizing the previous relations to the finite differences, the following numerical model is obtained, where "i" is used to indicate the current time instant of calculation:

$$^{i}T_{fo} = {}^{i-1}T_{fo} + \Delta t\left[-(a_1 + a_2)^{i-1}T_{fo} + 2a_2{}^{i-1}T_p + (a_1 - a_2)^{i}T_{fi}\right] \quad (3)$$

$$^{i}T_p = {}^{i-1}T_p + \Delta t\left[a_3\left({}^{i-1}T_{fo} - 2^{i-1}T_p + {}^{i}T_{fi}\right)\right] \quad (4)$$

With:

$$a_1 = \frac{2v_f}{L} \quad (5)$$

$$a_2 = \frac{4h}{d_i \rho_f c_f} \quad (6)$$

$$a_3 = \frac{2hd_e}{\rho_p c_p \left(D_0^2 - d_e^2\right)} \quad (7)$$

A model that uses the lumped capacitance method to determine the heat transfer within a storage material, has the characteristic of ignoring the resistance to heat conduction within the solid material. In this case, a corrective factor for the assessment of the convective heat transfer coefficient should be introduced and a coefficient h_e (modified heat transfer coefficient) should be used instead of h. This correction is carried out by applying the procedure proposed by Ben Xu et al. [7]. If we consider a pipe with an internal fluid and an external PCM shell, the following relations can be written (with $\eta = D_0/d_e$):

$$h_e = \frac{1}{\frac{1}{h} + \frac{r_e}{k_p} \frac{(4\eta^2 - 1) + \eta^4(4\ln[\eta] - 3)}{4(\eta^2 - 1)^2}} \quad (8)$$

To account for natural convection, present when PCM is liquid, numerical models with conduction-only heat transfer can use the "effective thermal conductivity method". This method incorporates (via a correlation) the effect of natural convection into the PCM conductivity term. In this method, a correlation for the Nusselt number of the liquid storage medium is used to modify the original thermal conductivity of a stationary PCM in the liquid phase. Effective thermal conductivity is defined as the thermal conductivity that a fluid that is immobile would have to transmit to equate a fluid in motion. Mostafavi et al. [8] proposed a generalized method able to evaluate the various correlation parameters based on the geometric characteristics of the exchanger and the type of used PCM. This method is unfortunately quite complex. The same authors, however, propose a second approach, adopted here, consisting of a constant value for the Nusselt number in the entire operation, calculating a maximum value and applying it to the liquid cells. The effective thermal conductivity is then evaluated through the following relationship, determining the maximum Nusselt number for PCM natural convection conditions:

$$k_{p,eff} = k_{pl} Nu_{NC,max} \quad (9)$$

When the PCM is solid $Nu_{NC,max}$ is 1, instead when the PCM is liquid $Nu_{NC,max}$ = C Ra^n, where C and n are two constant to be determined and Ra is the Rayleigh number.

The ETTM method is based on the adoption of an "apparent specific heat". For the apparent specific heat, during melting, a Gaussian trend was considered with a standard deviation equal to: $\sigma = (T_{m2}-T_{m1})/8$, where T_{m1} and T_{m2} are the starting and ending melting temperature respectively. This standard deviation implies that integration c_{pa} over the entire melting range yields the latent heat H of the PCM with an error of 0.01%. The peak of the Gaussian curve is then: $c_{p,lat,max} = H/(\sigma(2\pi)^{0.5})$, and the contribution of the latent heat is zero outside the melting range. The "apparent specific heat" can then be written as:

$$c_{pa}(T_p) = c_{ps} + (c_{pl} - c_{ps}) * \frac{T_p - T_{m1}}{T_{m2} - T_{m1}} + \frac{H}{\sigma\sqrt{2\pi}} * e^{-\frac{1}{2}\left(\frac{T_p - T_m}{\sigma}\right)^2} \tag{10}$$

The melt fraction, f, is not a state variable in the ETTM method, so it must be evaluated a posteriori, from the temperature reached by the storage medium at a given instant.

The solution of numerical equations in each time step allows to determine the state variables of the system at an instant "i" for the considered element. The time step is defined as: $\Delta t = t_{max}/N_{pas}$, with t_{max} the computational time and N_{pas} number of identical time steps into which the transient is divided. Generally, given the nature of the adopted method, it is better to maintain a time step of the order of 1 second (Δt = 1s).

2.3 Model Implementation

In Figure 3 the block scheme of the "TES_Perf" program, which highlights the interactions between modules, subroutines, and functions is shown. "TESPERF" is the "Main".

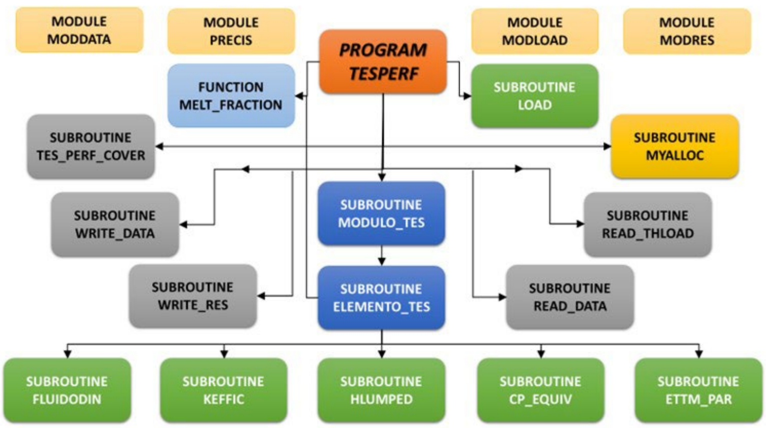

Figure 3. *Block scheme of the calls in "TES-Perf" program*

It is composed by 4 "modules", containing all the in-out data and their precision level, 5 subroutines for I/O functions, 6 subroutines with parameters for setting parameters and initializing variables and, finally, 3 subroutines and a function for the application of the model and calculation of the variables. This program, written entirely in Fortran 90, allows the dynamic allocation of the necessary memory. The input data is read from two text files (one containing the desired heat load history). The output is two files, one containing the summary of the input data and the other the results of the calculation.

3. Code Validation

The model validation was carried out by comparing the main numerical results with those obtained both from a 3D numerical simulation, using the Finite Element Method (FEM) code, CAST3M, and from experimental tests performed on the ENEA-TES-LH02 unit. In both cases the PCM used was “solar salt”.

3.1 Numerical Validation

Numerical comparison between the simplified ETTM/0D model and the FEM/3D simulation was performed separately for the charging and discharging phases. The thermal load history includes an increase of the HTF temperature from 200 to 300°C in 15 min and a holding at 300°C for 5 h and 45 min. For the discharging phase, the history is the same but with inverted temperatures. The 3D FEM mesh represents only half of the unit (symmetry) and is composed of 17205 elements. In Figure 4, the mesh of the half LHTES unit (a) and the distributions on the PCM volume of the temperatures (b) and the rate of melted PCM (c) after about 3 h of transient of the charging phase are shown. The calculation with the ETTM/0D model was performed for the total duration of 6 h with a constant time step of 1 s. Figure 5 shows the comparison of the main results (ETTM/0D vs FEM/3D) for the charging and discharging phases.

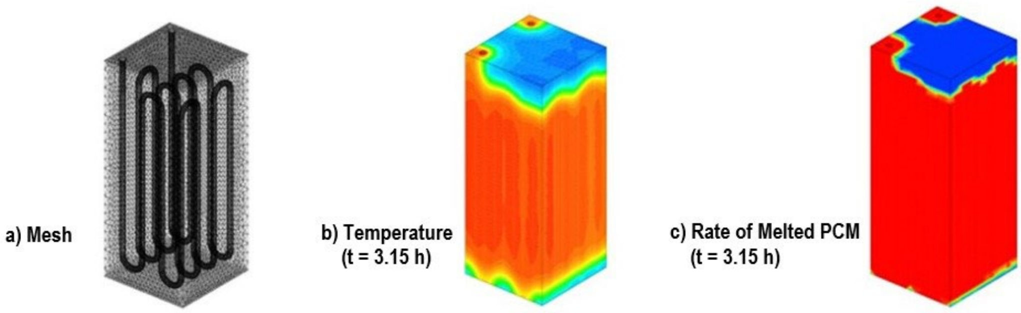

Figure 4. *FEM/3D, charging phase – a) Mesh, b) PCM temperatures and c) melted PCM (t = 3.15h)*

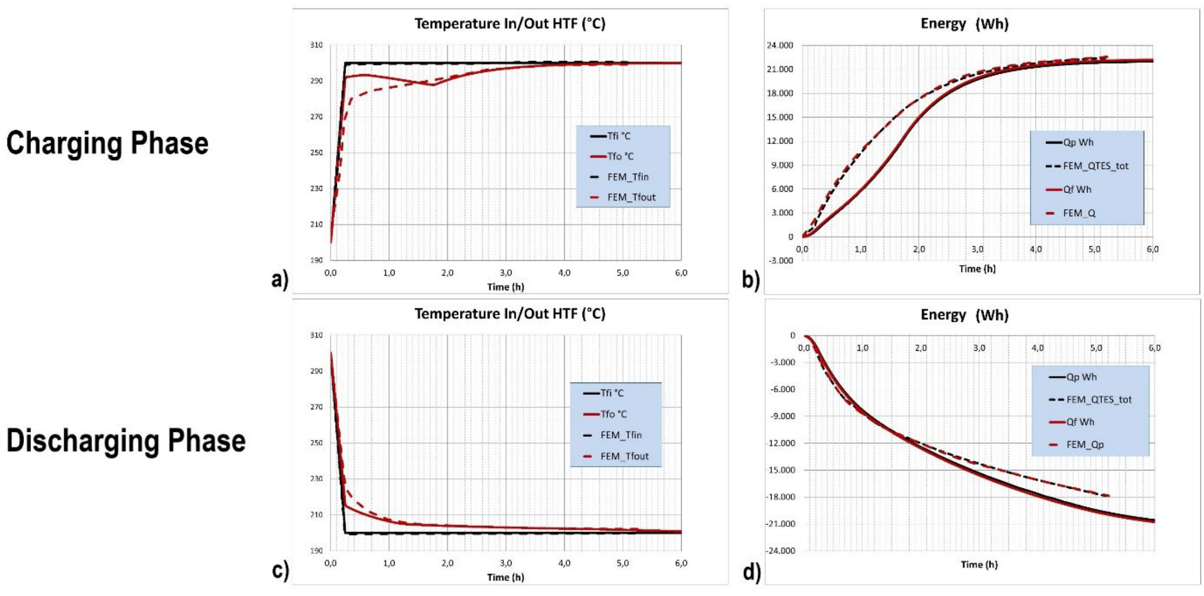

Figure 5. *0D/ETTM (solid lines) vs FEM/3D (dotted lines) - a), c) T_{HTF} In/out; b), d) Energy HTF*

3.2 Experimental Validation

Here are reported the results of the comparison between the simplified ETTM/0D model and an experimental test conducted in ENEA on the ENEA-TES-LH02 prototype (Figura 1) [9]. In this test, a complete charge/discharge cycle of the system was conducted. Note that in the model the HTF inlet temperature was set to the trend of the inlet temperature measured during the experimental test. Furthermore, the thermal losses, which are present in the experimental test, were neglected in the simulation. The calculation with the ETTM/0D model was performed for a total duration of 12 h, with a constant time step of 1 s. Figure 6 reports the comparison between the results of ETTM/0D model and the experimental test for a charge/discharge cycle.

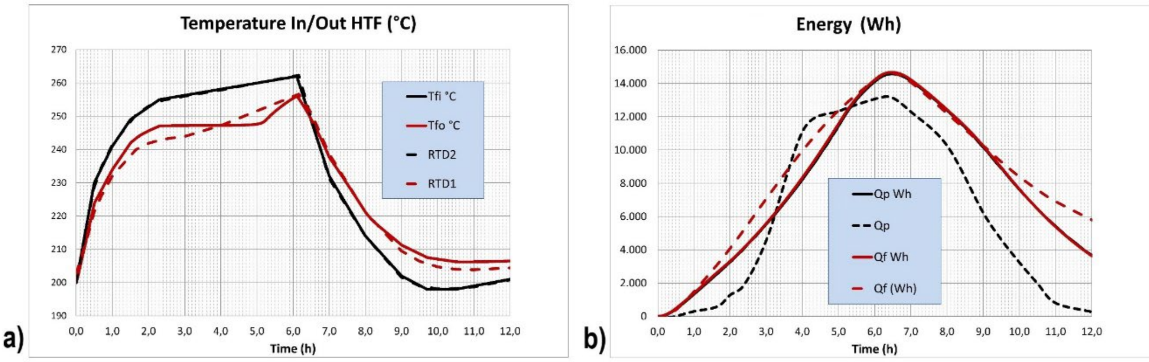

Figure 6. *ETTM/0D (solid lines) vs Experimental test (dotted lines): a) T_{HTF} in/out; b) Energy HTF*

3.3 Main Results

From the comparisons of the results, some considerations can be made. The largest discrepancies are evident in the first hour of both the charging and discharging phases of TES, but they are not such as to distort the overall behavior of the system. These differences are because in this period the phase change of PCM (solar salt) occurs. In fact, in the 0D model the whole mass of PCM is characterized by a single temperature and, consequently, its phase change starts and ends simultaneously in the entire PCM.

4. A Study Case

The ETTM/0D model was applied to a study case in which the thermal behavior of a system composed of three LHTES units connected in series was analyzed. An operating range between 200°C (T_{min}) and 400°C (T_{max}) was considered. The HTF used is a diathermic oil, Therminol 66. Three PCMs were considered (Table 1): PCM1: KOH; PCM2: $NaNO_3$ and PCM3: $NaNO_3$–KNO_3 (60%-40% wt - solar salt) [10][11].

Table 1. *Main physical properties of the 3 selected PCMs.*

		PCM1	PCM2	PCM3
PCM type		KOH	$NaNO_3$	$NaNO_3$-KNO_3 60-40%wt
Melting temperature	°C	380	306	223
Density	kg/m^3	2044	1908	1920
Specific heat – solid/liquid	J/(kg °C)	1400 / 1400	1780 / 1700	1430 / 1540
Latent heat	J/kg	149000	175000	105000
Conductivity – solid/liquid	W/(m °C)	0.5 / 0.5	0.6 / 0.51	0.78 / 0.45
Dynamic Viscosity	kg/(m s)	0.0028	0.0028	0.0025

PCMs have been selected to have a melting temperature within the design operating range and sufficiently far, at least 15-20°C, from the operating limit temperatures, this to contain the charging and discharging time. Furthermore, to optimize the overall exergy efficiency, the melting temperatures follow a geometric regression [12]: $T_{m1}/T_{m2}=T_{m2}/T_{m3}=1.15$, with T_m in Kelvin. Five different cases were considered. In the first three cases, the same PCM was used in all three units (Case1-PCM1, Case 2-PCM2 and Case 3-PCM3), while in the last two cases, a cascade system was tested, using all three PCMs (Unit 1-PCM1, Unit 2-PCM2 and Unit 3-PCM3). In the first four cases, each thermal storage system consisted of three identically shaped units connected in series (PCM volume: $0.161m^3$). In the last case (Case 5), the three storage units had different volumes ($V_{Unit1}=0.5V_{Unit2}$ and $V_{Unit3}=2V_{Unit2}$). In this case the system had a thermal capacity of about 135 kWh. In Figures 7 and 8, respectively for the charging and discharging phases, the results obtained for the various study cases are compared and, in particular: the inlet and outlet temperatures, the power transmitted by the HTF and the accumulated energy. The charging and discharging phases are strongly influenced by the temperature difference between the HTF inlet temperature and the melting temperature of the PCM, the heat exchange engine. The closer these are, the more the evolution of the single phase slows down and the system delays its charging or discharging. Case 1, in charging, and Case 3, in discharging, are evidence of this. Cases 4 and 5, including an element with PCM 1, are also affected by this effect. The thermal powers provided by the systems (in discharging) range from 23 to 40 kW: the highest values are obtained using a cascade system (cases 4 and 5) with the maximum value corresponding to a cascade system in which the volumes of the elements have been varied as a function of the PCM used (Case 5). This seems to highlight what has been reported in the literature: a cascade system is able to improve the HTF-PCM heat exchange and this improves by appropriately calibrating the quantity of the various PCMs. Cascade systems also show another characteristic: they have a very similar charge and discharge efficiency and, indeed, the discharge phase is higher than the charge efficiency, unlike single PCM systems. Naturally, the efficiency in absolute value was lower than cases 2 and 3 because the complete fusion of PCM1 is not obtained anyway.

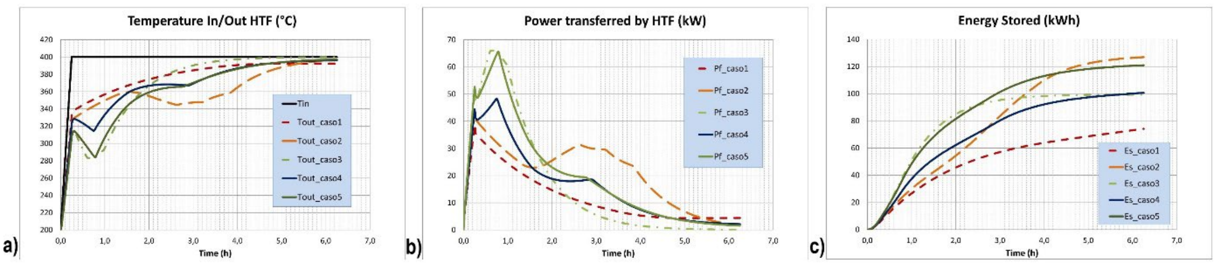

Figure 7. *Charging phase - a) T_{HTF} In/Out, b) Power transmitted by the HTF; c) Energy Stored*

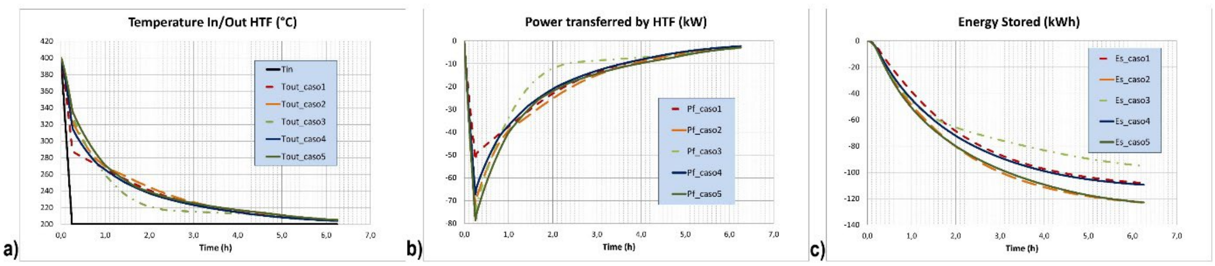

Figure 8. *Discharging phase - a) T_{HTF} In/Out, b) Power transmitted by the HTF; c) Energy Stored*

5. Conclusions

In this work, a simplified 0D model to predict the thermal behavior of a LHTES cascade system has been developed and implemented in an application. This model is based on the "Energy Temperature Transforming Method" (ETTM) and includes some correction to account for the lumped capacity and the effective thermal conductivity of the PCM. This application has very fast execution times (a few tens of seconds) and provides results with errors of less than 20%, as confirmed in the code validation phase. Despite this error, the model seems to be well set, as demonstrated by the temperature trends, consistent with the physical behavior and data comparison, and by the charge/discharge times. The obtained results are very good considering the simplicity of this model. The simplified model was then applied to some case studies to evaluate the performance difference of an LHTES system, consisting of three serially connected units, when using a single PCM or three different PCMs. The analysis confirmed that a cascade system can increase the performance of the LHTES system.

Data availability statement

Data supporting the result of this article can be found in the deliverables of the Project “Network 4 Energy Sustainable Transition – NEST” (https://fondazionenest.it).

Author contributions

Nicolini Daniele: conceptualization, methodology, validation, visualization, writing-original draft; Miliozzi Adio: conceptualization, methodology, software, formal analysis, supervision, data curation, review and editing.

Competing interests

The authors declare that they have no competing interests.

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