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Literature Review of Computational Fluid Dynamics Modelling of Thermocline Tanks

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Abstract: *A thermocline tank consists of a thermal energy storage system that allows the continuously operation of a Concentrated Solar Power plant even during periods of solar intermittency, making it a complementary and crucial asset in this type of systems. Accordingly, it is important to conduct a thorough evaluation of the system performance and using computational fluid dynamics (CFD) to such purpose as become increasingly popular. Consequently, understanding which phenomena are considered relevant in CFD modelling of thermocline tanks, the parametric studies already conducted and the identification of some opportunities for future work in this area becomes crucial to accelerate knowledge about a renewable energy production system that can provide some answers to the troublesome times we live regarding energy consumption. The present paper conducts a systematic literature review in the area of CFD modelling of thermocline tanks. For this purpose, the PRSIMA (Preferred Reporting Items for Systematic Reviews and Meta-Analyses) methodology is described and used.*

Keywords: *Computational Fluid Dynamics, Thermocline Tanks, Numerical Modelling, Concentrated Solar Power, PRISMA Methodology*

1. Introduction

Thermal storage systems (TES) can be used in various applications such as commercial buildings, industrial processes and renewable energy systems. This type of system can help reduce energy use costs, improve the efficiency of energy systems, and help integrate intermittent renewable energies into the power generation industry. There are several types of thermal storage systems, including the following: [1]

- ***Latent heat storage*** - uses phase changes in materials to store and release heat, usually through melting or solidification;
- ***Sensible heat storage*** - stores energy in a substance with a high heat capacity, such as water, which can then be heated or cooled whenever necessary;
- ***Thermal energy storage tanks***- stores thermal energy in a reservoir with a heated fluid, such as water or molten salts, which can be used whenever necessary;

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- ***Underground thermal energy storage (UTES)*** – stores energy in the soil, using underground pipes filled with water or another fluid.

Typically, a concentrating solar power (CSP) plant has an integrated TES system with a capacity to continuously supply energy to the system even during periods of solar intermittency. [1] [2] [9] CSP plants have a solar field installed upstream the TES system, and an organic Rankine cycle (ORC) unit operating downstream with the goal of producing electricity. The most commonly TES system used in CSP plants are the two-tank solution in which a tank stores the hot heat transfer fluid (HTF) and the other tank stores the cold HTF. [2, 3] [9]

Another solution that has been increasingly studied worldwide is the one-tank system in which both the hot and cold fluid are stored in the same tank. This type of system account with thermal buoyancy effect to maintain thermal stratification, hence creating a high thermal gradient separation zone between the high and low temperature regions. This high thermal stratified zone is usually called thermocline, and controlling the thickness of such zone is one of the most crucial aspects to bear in mind when studying these systems. Compared to the two-tank solution, the thermocline system offers a reduction in installation costs of 20 to 37 %, hence the growing interest shown worldwide in analysing these systems. [2 - 11] [13 - 21] [23 - 29].

Sensible heat storage systems (SHS) are the most commonly TES systems used in CSP, in which energy is stored by heating a fluid with high heat capacity, keeping it stored at a high constant temperature. There are two main SHS systems: *single-medium tanks* (SMT), that use only one material to store thermal energy based on its temperature, and *dual-medium tanks* (DMT), that use two materials to store and transfer heat throughout the system. In SMT the thermal energy is directly transferred to the storage medium and is stored as sensible heat.

To reduce costs mainly associated with the large volume of HTF required in SMTs to keep the systems always operational, DMTs are also employed in thermocline tanks in which a storage material is used to store the thermal energy, and another material serves as a heat transfer fluid to transfer energy to and from the storage material. Some examples of storage materials are quartzite, ceramic fillers, slag pebbles or phase change materials (PCM) [2, 24, 29]. The tank filled with solid storage material usually constitutes a porous medium, typically a packed-bed in which the HTF exchanges heat with the storage material during the successive charging and discharging cycles. Therefore, the analysis of the thermophysical properties of the storage material, as well as the heat transfer phenomena between the HTF and storage material are significant since the thermal performance of the system is highly dependent on these aspects.

In literature there are many types of HTF used in thermocline tanks (e.g. synthetic oils, water, pressurized air [14] [20, 21, 23] [25]), but the HTF considered to be the best selection considering the necessary balance between capacity, cost, efficiency and the possibility of usage at high temperatures are molten salts. [2] [5] [9] [12] [22] During a charging cycle a loop is formed in which the HTF heated upstream of the thermocline tank in the solar field flows to the top of the tank, supplying energy to the storage material, leaving the tank towards the solar field already cooled. In the discharge phase a loop is formed where the cooled HTF from the ORC unit downstream the thermocline tank enters at the bottom of the tank, receiving energy from the storage material and returning once again to the ORC unit, exiting through the top of the tank. Due to high accuracy achieved in numerical simulations using CFD, this technology is becoming increasingly popular to assess the thermal performance of thermocline tanks as well as its optimal designs and configurations. [2, 12, 22] Succinctly, CFD can be used to model different designs and configurations of thermocline tanks with a view of optimizing the efficiency of the system and also avoiding costs associated with experimental tests. [1, 2, 8, 19] CFD can also be used to analyse the flow of HTF throughout the system and assess the mass and heat transfer between the HTF and the storage material, both at charge and discharge phases also with the view of optimizing these parameters to improve the efficiency. Accordingly, this paper aims to carry out a systematic review of CFD modelling of thermocline tanks using the PRISMA (*Preferred Reporting Items for Systematic Reviews and Meta-Analyses*) methodology, with the focus on describing the numerical models most usually employed to characterize heat and mass transfer phenomena, identifying which operating conditions have already been discussed and mentioning some conclusions of those studies.

2. PRISMA Methodology

This paper is based on the standard systematic literature review, which allows to define a relevant field of research for the proposed theme while also enabling a structured approach, which is rigorous, transparent, minimizes the bias on the chosen articles, and ensures a replicability and a compatibility value. The PRISMA methodology, which is reproducible, easy to follow, and provides valuable information about the current state of the art, was applied to this literature review. The process is started with the selection of the keywords to insert into the database (1). This database was selected during the month of April of 2024. Following, the papers are extracted (2), and the abstracts are analysed to ensure their compliance with the main theme (3). Finally, the documents are fully analysed (4). The PRISMA 2020 flowchart will be used to document the process throughout all of these phases. The database used for this research was Elsevier's Scopus.

As the literature review was quite specific, several keywords were used, and they were divided into *concept* and *context*. Starting with the *concept*, the keywords "Numerical" AND "Study" AND "Molten salt" AND "Modeling" (OR "Model") AND "Thermocline tanks" were used, along with the *context* field of "thermal energy storage" OR "thermocline tanks". Initially, the intent was to provide articles from 2019 onwards, but as the research revealed a small number of results, that was extended to articles from 2014 onwards, therefore, articles published in the last ten years. Additionally, only articles in English were selected, and only journal papers, articles and reviews were relevant. A total of 61 papers was obtained in the Scopus database. Along with these 61 documents, a further sixteen were found during research made on other sources, namely, Google Scholar, and were labelled as relevant to the work being conducted and, therefore, added to the list of papers.

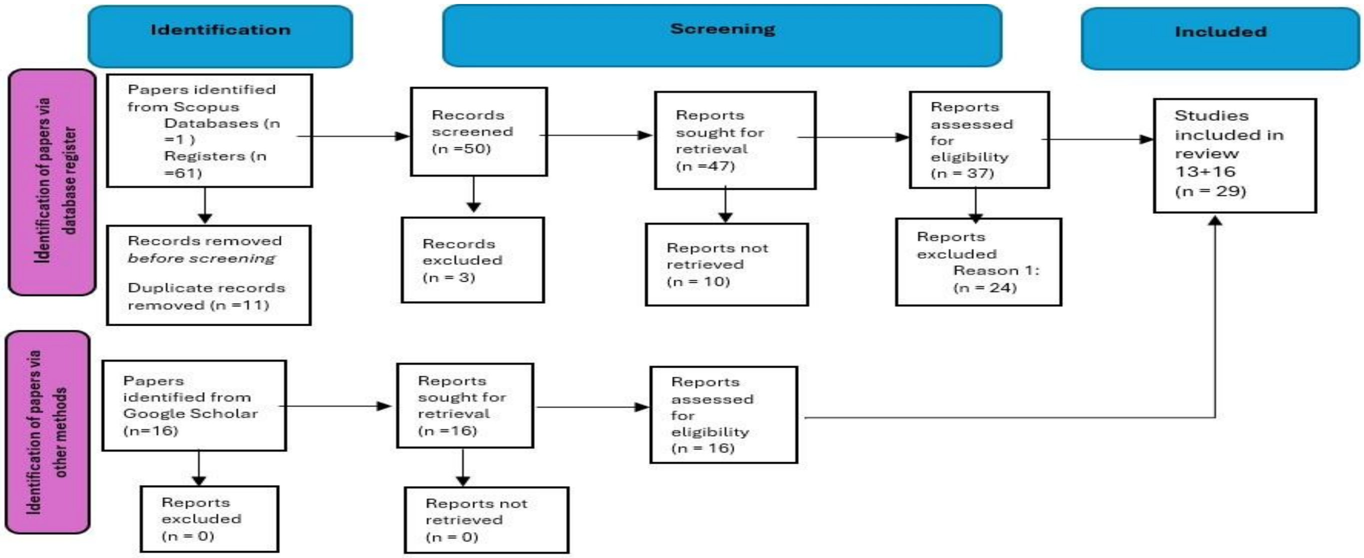

Fig. 1: PRISMA workflow diagram applied.

From the original 61 results, 10 were immediately discarded, as they were duplicates. After that, another 3 papers were excluded based on the titles that had a mislead direction. Despite the majority of the 61 articles being retrieved and analysed, a significant part of them were excluded based on the content of the abstract. In fact, despite a big number of the discarded articles mentioning 2 relevant themes to this paper (latent heat and water heating), they went in a different direction. That explains the 24 discarded articles after the reading of the abstract. With the 13 left, and adding on to the 16 articles from external sources, a final of 29 articles were obtained to be analysed.

3. Numerical Modelling

3.1. Mathematical modelling

The numerical modelling described in this section is related to a *dual-medium* thermocline tank which is usually the most employed one-tank solution in CSP plants. [2 – 11] [13 – 21] [23 – 29. There are two main numerical CFD models found in the literature to simulate thermocline tanks: one dimensional dispersion – concentric based models (1D D – C) and two – dimensional models (2D axisymmetric models). [2][4]. Both models make early assumptions regarding thermal or non-thermal equilibrium between the HTF and the storage material. If one assumes non-thermal equilibrium, then usually two energy conservation equations are employed in which each one is used to calculate the transient HTF and storage material temperatures, respectively. If one assumes thermal equilibrium then only one energy conservation equation is needed, and it is assumed that the HTF and the storage material are mixed. Generally in CFD modelling of DMTs, the tank is filled with a porous bed consisting of solid fillers, the flow of molten salts is assumed to be laminar and incompressible, the distributors are not included in the computational domain, the flow is imposed at the inlet of the filler region, the solid fillers are assumed to be spherical particles with homogeneous, continuous and isotropic properties, the top and bottom surfaces of the thermocline tank are considered being adiabatic, and radiation heat transfer between the fluid and solid, and between particles in the bed is usually neglected. The continuity and momentum equations are also coupled to the energy conservation in CFD modelling of thermocline tanks, where the porosity effect is taking into account in each equation. Normally, the molten-salt used in these systems consists of a mixture of 60 wt% NaNO3 and 40 wt% KNO3 and thermophysical properties such as density, heat capacity, thermal conductivity and thermal viscosity are temperature dependent. [5] The thermophysical properties of the solid fillers are usually assumed to be constant throughout the entire process and are previously known. The temperature of cold and hot molten salts in CSP plants usually varies between 290ºC and 500ºC, respectively [2 – 11] [13 – 21] [23 – 29], and both temperatures are usually defined as boundary conditions along with the inlet molten salts flow rate at the top of the tank. Boundary conditions are also assumed at both charge and discharging phases, usually heat fluxes and adiabatic conditions. [2 – 11] [13 – 21] [23 – 29]. It is costume to also assume an energy equation for the outer thermal insulation layer and steel tank wall thickness where it is assumed that heat is transferred by conduction through the insulation layer and steel thickness. A complete and comprehensive description of each of the terms mentioned above and which make up the mathematical models that allow the CFD modelling of *dual-medium* thermocline tanks can be found in the several articles that compose the literature review of this paper (e.g. mathematical model description found in [2] [3] or [5]).

3.2. Numerical method

Among the commercial CFD software available, ANSYS FLUENT is the most employed to simulate these systems [3] [5] [8 - 11] [14 - 18] [21, 27, 29]. In this case, the Finite-Volume Method (FVM) is used to numerically solve the governing equations described in section 3.1. The pressure-velocity coupling field is solved by the SIMPLE algorithm and sometimes UDF (User – defined functions) code is coupled to the software to account for a solid-packed bed in the porous zone. [5, 11, 13-16, 21, 29] In most of the CFD studies the convective fluxes are discretized by a second order upwind scheme and the transient terms are discretized through a first order implicit scheme [4 - 11] [13 – 21] [24 – 27] [29].

4. Operating parameters analysed in CFD studies

In CFD studies analysed in this review, there are a number of parameters that have been studied in order to optimize the thermocline tank system, even though the obtained results still need to be validated and further analysed. Among the parameters mentioned in the literature to have the most influence on the system's performance are those regarding system configuration, energy transfer coefficients of both the HTF and the storage material and the inlet conditions of the HTF [22]. Regarding energy transfer parameters, the following stand out: the diameter and heat capacity of solid fillers, the heat capacity of HTF, and the porosity and permeability of the porous medium. [2 – 10] [11 - 21] [23 - 29] Regarding the inlet conditions, the analysis of inlet flow rate as well as hot and cold molten-salts temperature stands out. [2, 5, 7] The study of the geometric parameters involving the ideal height/diameter (H/D) ratio, as well as the effect of slope walls have also been discussed in the available literature [2, 11, 19, 23, 28]. In [2], a CFD study was conducted to evaluate the effect of eight parameters on the system's performance, including the effect of the cooled molten salts temperature, the porosity of the packed bed, the diameter, thermal conductivity and heat capacity of the fillers along with the inlet flow rate of the molten salts. It was found that a higher molten salt inlet flow rate increased the efficiency of the discharging phase, but had no effect on the charging phase, and as the temperature of the cooled salts increased, the thickness of the thermocline decreased. The effect of the porosity of the packed bed on the thermocline thickness was more evident during the discharge phase that the charge phase and these parameters had little effect on the molten salts' outlet temperature. The influence of the fillers size was found to have the same degree of impact as the porosity of the packed bed, although it was found that a smaller diameter of the fillers could increase the rate of heat transfer between the HTF and the fillers. On the other hand, varying the thermal conductivity of the fillers had little impact on the system. In [3], increasing the inlet flow rate of HTF (molten salts in this case) also increased the rate of heat transfer by convection, reducing the discharge phase time, thus improving the system. In [4], the authors reach similar conclusions. In [5], it was found, as in [2], that a smaller size of fillers could increase the rate of heat transfer between the fillers and the HTF (in this case, molten salts), reducing the time needed for heat exchange in the tank. In [15], it was found, as in [2], that decreasing the difference between the heated and cooled molten salts increased the efficiency of the discharge process and that possibly this thermal gradient had more influence on the behaviour of the system than the inlet molten salts flow rate. This conclusion was also reached in [18]. In [6], it was settled that the heat capacity of both the HTF and fillers is the most influential parameter regarding system's performance.

A list of the CFD models analysed in this review according to storage materials, heat transfer fluid, operating conditions, type of model and employed CFD software used are exhibited in Table 1.

TABLE 1: Models selected from the literature and respective assumptions applied.

Reference	Heat Transfer Fluid (HTF)	Storage Material	Type of model	CFD Software	Operating Conditions
[2]	Molten Salts	Quartzite	2D axisymmetric	-	566 – 723 K
[3, 5, 11, 15 – 17, 29]	Molten Salts	Quartzite	2D axisymmetric	FLUENT and UDFs	From 290ºC to 565ºC
[4, 13]	Molten Salts	Quartzite	1D D - C	Matlab	293ºC – 450ºC
[6]	Several types (molten salt included)	Quartzite	2D axisymmetric	OpenFOAM	554 – 664 K
[7, 24]	Molten Salts	Quartzite and several PCMs, respectively	2D axisymmetric	In house - code	From 290ºC to 500ºC
[8]	Molten Salts	Quartzite	3D model	FLUENT	563 to 651 K
[9]	Several Types (molten salts included)	Quartzite	2D axisymmetric	FLUENT	300ºC – 410ºC

[10, 18, 27]	Molten Salts	Quartzite	2D axisymmetric	FLUENT	From 290ºC to 500ºC
[14]	Water	-	1D conservation equations	FLUENT	25.9ºC – 50.9ºC
[21, 23]	Pressurized Air	-	1D and 2D models	FLUENT and UDFs and Matlab, respectively	From 20ºC to 300ºC
[25]	Synthetic Oil	Quartzite	1D model	Matlab	290ºC to 400ºC

5. Conclusions

In this paper a systematic literature review on CFD modelling of thermocline tanks was conducted. For that, the PRISMA methodology was employed and added to external contribution of key papers. Despite the importance and high focus on the theme of solar thermal systems, the CFD models selected were few. It can be concluded that the advantages and disadvantages of the different CFD models are very dependent on fillers thermophysical properties such as thermal conductivity or heat transfer coefficient. Also it is strongly dependent upon the molten-salts inlet flow rate and the thermocline thickness formed inside the tank. The CFD software more commonly employed in these types of studies is ANSYS FLUENT, specifically when a 2D axisymmetric model is used. Both other software, e.g., Matlab, can be used in more simplified models, typically 1D dispersion - concentric models. More studies could be conducted in this research area with focus of optimizing the thermal performance of the system such as investigating the full integrated CSP plant (include the solar field and ORC unit in the CFD study) and also making the inlet conditions transient and not only fixed, as most of the analysed studies did. Also, different designs and configuration of thermocline tanks should be studied to achieve optimal performance of these type of systems. With this review, it as possible to identify key missing areas to research and that there are different methodologies accordingly to the accuracy and complexity of the system in study.

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