CZECH TECHNICAL UNIVERSITY IN PRAGUE

FACULTY
OF MECHANICAL
ENGINEERING

SUMMARY OF DISSERTATION

CZECH TECHNICAL UNIVERSITY IN PRAGUE
Faculty of Mechanical Engineering
Department of Environmental Engineering

Summary of Dissertation Thesis

Stratification in storage tanks for heat pumps

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Doctoral Study Programme: Mechanical Engineering

Study Field: Environmental Engineering

Supervisor: doc. Ing. Tomáš Matuška, Ph.D.

Dissertation thesis statement for obtaining the academic title of "Doctor" abbreviated to "Ph.D."

Prague March 2024

Title in Czech language: Stratifikace v zásobnících tepla pro tepelná čerpadla

This doctoral thesis is an outcome of a full-time doctoral study programme at the Department of Environmental Engineering , Faculty of Mechanical Engineering, Czech Technical University in Prague.

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The thesis was set out on:

The defense of the dissertation thesis will take place on:

at the meeting room no. B1-819 of the Department of Environmental Engineering of the Faculty of Mechanical Engineering of the CTU in Prague, Technická 4, Praha 6, before the Board for the Defence of the Doctoral Thesis in the branch of study Environmental Engineering.

The thesis is available in the Department of Science and Research of Faculty of Mechanical Engineering, CTU in Prague, Technická 4, Praha 6 - Dejvice.

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SHRNUTÍ

Pro zajištění vysoké kvality akumulace tepla a vysoké účinnosti při jeho získávání se v zásobnících tepla často využívá tepelného vrstvení (stratifikace). Motivace pro využití stratifikace spočívá v tom, že mísení vrstev v zásobníku může být během provozního cyklu minimalizováno tak, že na konci ohřevu objemu zásobníku může být z horní části odebírána voda o vysoké teplotě, čímž se dosahuje vysoké tepelné účinnosti na straně odběru, zatímco v dolní části může být odebírána voda o nízké teplotě a tak udržena vysoká účinnost na straně jímání obnovitelného tepla. Výzkum stratifikace zahrnuje posouzení široké škály konceptů, které se vyskytují okolo ústředního tématu zásobníků tepla, především jejich návrhu a modelování.

Tato práce je zpracována jako „Disertace publikacemi“. K průvodnímu textu této práce je připojeno celkem 5 publikací (článků), které představují 3 hlavní výzkumné studie. Celkem 4 články jsou publikovány v recenzovaném impaktovaném časopise ležícím v prvním kvartilu (Q1), zatímco 1 článek je publikován v recenzovaném impaktovaném časopise ležícím v prvním decilu (D1).

V první studii je představena jak experimentální tak numerická práce. Samotná studie je založena na systematické a komplexní rešeršní práci, např. bylo diskutováno použití více-uzlového a „plug-flow“ přístupu k modelování různých rozložení teploty. Modely byly kategorizovány jako lineární, stupňovité, spojitě-lineární a obecné třízónové modely pro rozložení teploty. Následně byla demonstrována dynamika degradace teplotního gradientu a ovlivňující parametry v pohotovostním i dynamickém režimu. Kromě toho byl ukázán přehled současných metod a postupů k vyhodnocování stratifikačního chování a jeho kvantifikaci. To zahrnuje geometrické parametry, uvažování konstrukčního návrhu, jako návrh vtoku, poměr rozměrů nádrže či specifikace materiálu stěny a také provozní parametry pro omezení mísení. Praktické techniky a metody byly představeny novým způsobem a rozšiřují základ praktických aplikací a výzkumných postupů.

Na základě rešerše bylo dále kvantifikováno turbulentní mísení na základě teplotního profilu, MIX čísla a Richardsonova čísla. Pro nalezení optimálních provozních podmínek v režimu vybíjení zásobníku byly vytvořeny různé CFD modely a experimentálně ověřeny na vlastním laboratorním zkušebním zařízení pro různá nátoková zařízení. Hodnocené parametry pak zahrnují průtok, rozdíl teplot ΔT a dále konstrukci nátoku do zásobníku, takže mezi nimi byla stanovena vzájemná závislost. Výsledky numericky prokázaly, že provozní podmínky zásobníku lze optimalizovat vhodnou volbou konstrukce nátoku. Tato výzkumná zjištění mohou sloužit jako vodítko pro optimalizaci návrhu zásobníku tepla, konkrétněji návrhu založeného na vhodném nátokovém zařízení integrovaném s konkrétním zdrojem tepla, neboť teplotní stratifikace a *COP* zdroje tepla, tj. například tepelného

čerpadla, jsou neodmyslitelně korelovány. Tepelná čerpadla jsou zařízení s vysokým průtokem a nízkým ΔT, na rozdíl od solárních systémů jako zařízení s nízkým průtokem a vysokým ΔT. Vhodná volba nátokového zařízení pro konkrétní provozní podmínky zdroje tepla je proto kritická.

Druhá studie je zaměřena především na vývoj vhodného exergetického modelu kvantifikujícího degradaci stratifikace v zásobníku tepla na základě druhého termodynamického zákona, který byl sledován pro přizpůsobení rovnic vyjadřujících entropii a exergii. Nové modely prošly přísným validačním procesem. Nejprve byla provedena experimentální validace, poté byl využit přístup založený na datech za použití LSTM neuronové sítě. LSTM model reprodukoval výsledky vypočtené nově vyvinutým exergetickým modelem, a výsledky vypočtené kvantitativním přístupem odpovídají výsledkům datového přístupu. Součástí procesu validace modelu bylo porovnání výsledků s pracemi jiných autorů. Stejně důležitým bylo i podrobení dat časové řady analýze statistické nejistoty z pohledu Gaussova rozdělení. Bylo zjištěno normální rozdělení nejistoty s 95 % datovými body v rozmezí 5% nejistoty. Nakonec, byly tyto rovnice přizpůsobeny datové vrstvě, aby bylo možné v reálném čase zaznamenávat výsledné stratifikační chování při akumulaci tepla a topného faktoru *COP* tepelného čerpadla během cyklu nabíjení/vybíjení zásobníku tepla. Takové vyhodnocení v reálném čase poskytuje lepší pohled na energetickou účinnost systému OZE jako zdroje tepla a může tak být pomocí expertům a výzkumníkům.

Ve třetí studii je demonstrováno použití inteligentní datové vrstvy pro vyhodnocování a predikci výsledného chování stratifikovaného zásobníku tepla integrovaného s tepelným čerpadlem. Modelování dat, jejich získávání, zpracování a transformace se provádí dynamicky. Byla vyvinuta metoda k využití rámce datové vrstvy k vizualizaci energetické účinnosti akumulace tepla v reálném čase tak, aby vyhovovala exergetickému modelu podle druhého termodynamického zákona. To umožňuje expertům intuitivně porozumět energetické účinnosti jejich zařízení pomocí nového datového řetězení. Datová vrstva vyhodnocuje degradaci vrstvení (ve smyslu generování entropie) pomocí nového modelu podle druhého termodynamického zákona odvozeného v této třetí studii. Kromě entropie také vypočítává *COP* tepelného čerpadla při různých provozních parametrech.

SUMMARY

To assure high quality thermal storage and high efficiency of its acquisition, thermal stratification is often employed in thermal storage tanks. The motivation of stratification lies in the fact that mixing of layers can be minimized during operational cycle of the tank so that high temperature water could be taken at the load end, thus maintaining high thermal efficiency at demand side, while low temperature water can be drawn at lower bottom, thus maintaining the high efficiency at renewable heat collection side. The investigation of stratification entails the assessment of a wide variety of concepts to be embodied around the central theme of the thermal storage, especially its design and modelling.

This thesis is put forward as “Thesis by publication.” In total 5 papers, which represent three main research studies, are attached together to accompanying text in this thesis. Meaning, 4 papers are published in first quartile (Q1) peer-reviewed impacted journal, while 1 paper is published in first decile (D1) peer-reviewed impacted journal.

In the first study both experimental and numerical work is presented. The study is based on systematic comprehensive review work. For instance, multi-node and plug-flow approach to model various temperature distribution models are resurfaced. These models are categorized as linear, stepped, continuous-linear and general three-zone temperature distribution models. Subsequently, the dynamics of thermo-cline decay and influencing parameters both during standby and dynamic mode were demonstrated. In addition, a survey of state-of-the-art methods and practices to ascertain the performance improvement and its quantification were illustrated. This includes geometrical parameters – such as, structural design incorporation, essentially – inlet design, tank aspect ratio and wall material specification, and also, operational parameters to curb down the inlet mixing. Practice techniques and methods which were presented here in a novel way, extend towards the ground of practical application and research procedures.

Furthermore, based on review, quantification of turbulent mixing was achieved on the basis of temperature profile, MIX number, and Richardson number. Various CFD models were developed and experimentally validated on the own laboratory test rig in order to find the optimal working conditions in discharge mode for different inlet devices. The evaluated parameters include flow rate, ΔT, and design of inlet device (diffuser), henceforth a direct interdependence between each was thus established. The results proved numerically that the tank working conditions can be optimized by proper selection of inlet device. These research findings can serve as guidelines to optimize the storage tank design, more specifically, inlet device-based design integrated with heating system, as thermal stratification and *COP* of heating system i.e. heat pumps, for example, are inherently

correlated. Heat pumps are high flow rate and low ΔT devices, while, solar systems are low flow rate and high ΔT devices. Thus, the suitable choice of inlet device for a particular operating condition is critical.

Second study is mainly focused on development of suitable exergetic models quantifying stratification decay of thermal storage based on second law of thermodynamics which was observed in tailoring the entropy and exergy equations. The new models underwent strict validation process. Firstly, experimental validation was achieved. Secondly, data driven approach using LSTM neural network was utilized. The LSTM model reproduced the results calculated by newly developed exergetic model thus the results calculated by quantitative approach is validated by data driven approach. Finally, the results were also compared with the work of other authors as a part of validation process. Equally important, time series data thus collected underwent statistical uncertainty analysis. Probability distribution of error in terms of Gauss distribution was analyzed. It was observed that the uncertainty was normally distributed with 95% data points falling under 5 % uncertainty range. In conclusion, it was made possible to fit these equations to the customized data layer in order to stream in real time the end to end stratification performance of thermal energy storage, and *COP* of heat pump during charge/discharge cycle. This real time evaluation gives a better perspective about the energy efficiency of RES system and thus could help experts and researchers.

In the third study, application of intelligent data layer for evaluating and predicting end to end performance of heat pump integrated stratified thermal energy storage system is demonstrated. The data modelling – acquisition, curation, and transformation is done in situ (dynamically). A method was developed to utilize of data-layer framework to visualize in real-time energy efficiency of thermal storage, in other words, to fit the developed second law of thermodynamics-based exergy model. This will help experts to intuitively understand the energy efficiency of their devices using novel data pipeline. The data layer evaluates stratification decay (in terms of entropy generation) using the novel second law model derived in the third study. In addition to entropy it also calculates *COP* of the heat pump at different operational parameters.

Contents

Nomenclature

c	thermodynamic specific heat capacity (J/kg·K)
E	energy content of j^{th} fluid layer
g	acceleration due to gravity (m/s^2)
h	height (m)
L	characteristic length pertaining to tank (m)
M_E	moment of energy (J·m)
M_{exp}	moment of energy of experimental tank (J·m)
$M_{ful\text{-}mix}$	moment of energy of fully mixed tank (J·m)
M_{str}	moment of energy of perfectly stratified tank (J·m)
MIX	MIX number (dimensionless)
Ri	Richardson number
v	velocity component in y direction (m/s)
V	volume (m^3)
y_j	vertical distance between nodes (mm)
T	temperature (^{o}C)
t	time (sec)
$T_{hp,out}$	heat pump output temperature (^{o}C)
$T_{hp,in}$	heat pump inlet temperature (^{o}C)
T_i	temperature of i^{th} layer (^{o}C)
ξ	exergy (kJ)

Greek

β	coefficient of thermal expansion (1/K)
ρ	fluid density (kg/m^3)
Δs	thermodynamic entropy production (J/K)
v_{hp}	heat pump flow rate/circulation pump flow rate m^3 /s
η	Stratification efficiency

Introduction

Background and motivation

Thermal energy storage (TES) is the essential part of renewable energy systems. This is because it is the only solution against noncoincidence of supply and demand, especially with solar systems. Improving the performance of this central component can significantly decrease the auxiliary energy demand for both the space and domestic hot water heating. For designing or performing building energy simulations of heating systems including the storage tanks it is essential to adopt the integrated and dynamic simulation approach. According to Campos Celador et al. [1], storage tank models can help to determine the annual saving and subsequent decision-making to increase it right at the design phase of the system. Stratified storage tank is a cost-effective building heat storage technology which facilitates the reduction in auxiliary heating demands, reduction in primary energy savings, discounting the consumer costs, while promoting the lower carbon footprints [2, 3]. The simple concept of thermal stratification lies in the fact that colder water being denser than hot water is withdrawn from the bottom and is circulated to the energy collection side (source side). This increases the efficiency of energy collection especially with renewables – solar thermal and/or heat pump, as it increases with decrease in inlet water temperature. Consequently, hot water is made to enter at the top of the tank which promotes the stratification.

High performance of such TES employing water as storage medium is undeniably indispensable. For this purpose, an effective TES device should satisfy these technical prerequisites (Fig. 1):

- Thermal stratification: the water tank should be able to sustain hot and cold water separately without any physical barrier, in other words, continuous or stepped temperature distribution of water across the height of the tank should be practiced.
- Mixing of hot and cold volume of water induced due to different operational cycle's viz. charging and discharging should be minimized.
- The tank design should minimize the dead water weight.

- The tank design should minimize the heat losses.

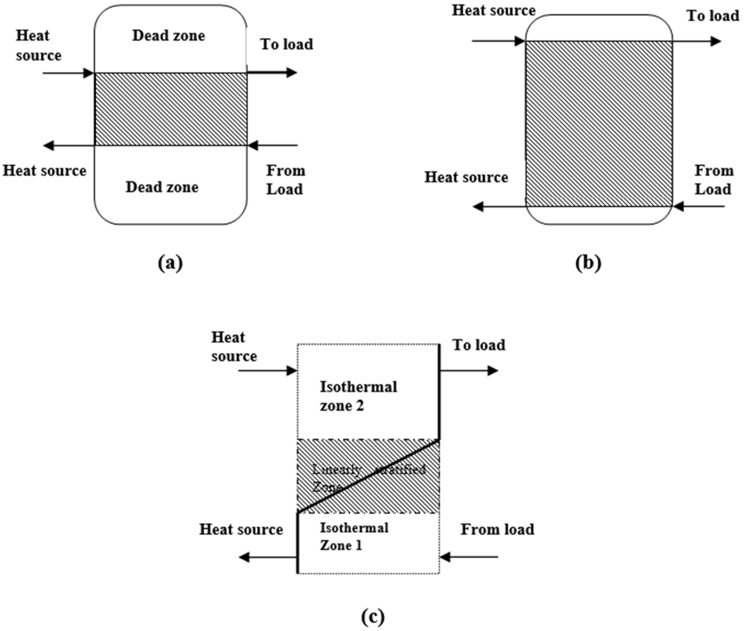


Fig. 1. (a) and (b) Different positions of inlets and outlets in storage tank, and (c) indication of thermal stratification in the same.

Two counteracting forces i.e. buoyant forces and gravity are responsible for movement of the newly introduced fluid inside tank. High density or low temperature fluid layers have the tendency to settle down as early as possible, while low density or high temperature layers have the propensity to move towards the upper hot layers. In addition, the momentum with which water is introduced into the bulk impacts the core fluid and hence decides how it will react with rest of the fluid layers. After the fluid layers are settled at their respective positions, thermal stratification is built up forming a thermocline region which can be described by different temperature distribution models such as linear, stepped or three zone model. This thermocline serves as the thermal barrier to separate the hot and cold-water regions. Hot water is extracted from the upper part to feed the load, while cold water is extracted from the lower region to circulate to the energy addition loop. Thus, thermal stratification is maintained within the tank during the different operation cycles. Nevertheless, this stratification starts to fade away due to different hydrodynamic and/or thermal contingencies which need to be controlled.

Stratified water tanks can either be directly heated or indirectly heated by addition of a heat exchanger between energy source and the tank. Directly heated water tanks are highly effective at thermal exchange, however they are weak at maintaining the stratification due to high mixing and turbulence. Henceforth, they are usually equipped with different structural design changes viz. inlet stratifiers, baffle plates, diffuser systems etc. In addition, the performance of the immersed type thermal system can be significantly improved by correctly crafting the inner arrangement of the coils. The simulation results validated by experimental findings by Celador et al. [4] concluded that sophisticated inner arrangement can improve the performance and effectiveness of hot water preparation up to 15%.

The primary purpose of the thermal energy storage is to maximize the availability (or exergy) in the form of useful energy gain [5]. Energy and Exergy analysis both are used to quantify the performance of the TES. Exergy analysis, on the other hand, is a second law based thermodynamic investigation which provides gain over energy analysis in a way – firstly, it puts into account the temperature differences for the same energy content storages – this is particularly required for stratified storages as they sustain spatial temperature variations or thermocline, which could be stepped or linear [6]. Secondly, it considers the causes and location of quantitative losses due to mixing of fluids at different temperatures, and losses towards the environment. The working of TES moreover is governed by operating cycles, typically, energy addition, storage, and energy removal cycles. Careful thermal management and control of these cycles could result in increased performance of the thermal recovery.

Yaici et al. [7] performed a CFD analysis to evaluate the influence of geometrical and operational parameters on performance of the tank in charging mode. The results confirmed that a controlled optimization between both geometrical and operational variables is rudimentary for an appropriately designed storage tank. Geometrical factors include aspect ratio representing the effect of varying tank height with fixed diameter and vice versa, and also inlet and outlet position with respect to the top and bottom wall of tank. The operational parameters include mass flow rate, inlet temperature variation and the effect of initial water temperature variation. The results concluded that the low mass flow rate instills increased level of thermal diffusion, axial wall conduction, and thermal conduction within the hot and cold-water layers, due to increase in thermal exchange time – thus, increasing the thermocline thickness and decreasing the stratification.

Objectives

This Ph.D. thesis investigates the behavior of thermal energy storage (TES) experimentally and with the help of simulation. The point of focus throughout this thesis is the thermal stratification assessment carried using pre-established indices found in the literature, using own custom built second law model and also using CFD code. The three specific objectives of this thesis are:

1. Design and simulate the methodology to separate the good from the bad operational parameters during TES operation from the view of stratification quality and thus efficiency of renewable heat sources connected to TES.
2. Design and validate own custom built second law model to quantify the availability of the energy that is being added and subsequently removed during charge and discharge cycle of TES.
3. Design and build an intelligent IoT stream processing unit to fit the second law model previously developed and predict the second law stratification efficiency in real time.

Solution Methods

Investigation of stratification efficiency of TES can be done by either energy or exergy analysis. Energy analysis uses first law of thermodynamics. This entails various stratification indices such as MIX number, Richardson number etc. These stratification numbers consider the temperature gradient rather than the exergy/entropy as in the case of second law modelling. Study 1 revolves around this strategy to evaluate TES stratification behavior. In this study quantification of turbulent mixing was achieved on the basis of temperature profile, MIX number, and Richardson number. Temperature dat was collected using experimental setup as described in Fig. 2.

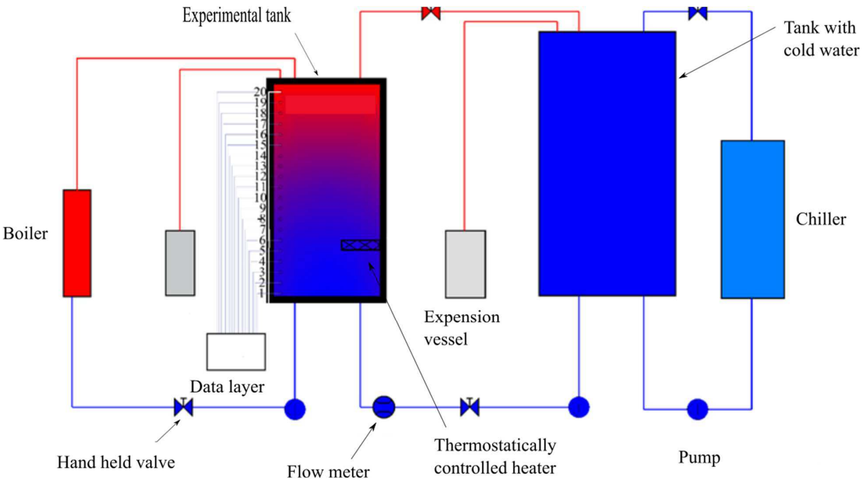


Fig. 2 Schematic of experimental setup

The experimental setup as shown in Fig. 2 consists of primary cylindrical hot water storage tank with following parameters: 397 L in volume, 550 mm diameter and 1905 mm overall height. The tank is connected to the secondary tank with chilled water in order to perform discharging cycles. To measure the vertical distribution of temperature, 20 Pt100 temperature sensors were attached around to the outer surface of tank wall in the vertical direction, dividing the tank into 20 equal fluid layers. Charging of the tank was performed using two methods. Firstly, by thermostatically controlled electric heater which is present in the lower half of the tank, secondly, by an external electric boiler. Experimental tank can be set for various mixed conditions, 60 °C and 50 °C for example. Discharging process is carried out by regulating manually operated valve as shown in Fig. 2. A pump is also used for discharging. In addition, tank with chilled water is connected to the thermostatic chiller to cool it down after each discharging cycle. The evaluated parameters included fluid flow rate, ΔT (between heat pump outlet and TES temperature). These parameters were also investigated for different diffuser design (in CFD analysis), henceforth a direct interdependence between each was thus established. Refer Renewable Energy paper in Study 1 for more information.

CFD models for given designs were developed and experimentally validated on the test rig in order to find the optimal working conditions in discharge mode. This accounted for the operational parameters influencing stratification efficiency in TES. The influence of operational parameters was also recognized in the Study 1 and was further explored in Study 2. The results proved numerically that the tanks working conditions can be optimized by proper selection of inlet device. For instance, slotted type inlet device sustained maximum stratification even in as adverse a condition as of turbulent inflow & low ΔT. Perforated and simple inlet devices were capable of delivering best discharge efficiency only at low flow rate of 200 l/h and were showing insignificant dependency on ΔT. To establish these facts, MIX number and Richardson numbers were recognized earlier in the Study 1. MIX number evaluates the tank on the basis of both vertical temperature distribution and the total energy stored in the tank. Accordingly, it postulates the mixing process in the tank by evaluating the moment of energy of individual water layers. Moment of energy of thermal storage tank is calculated to account for energy location by summation of the sensible energy content up to j^{th} vertical segment, weighted with the height of its location (Eq. 1 & 2). MIX number varies between 0 and 1.

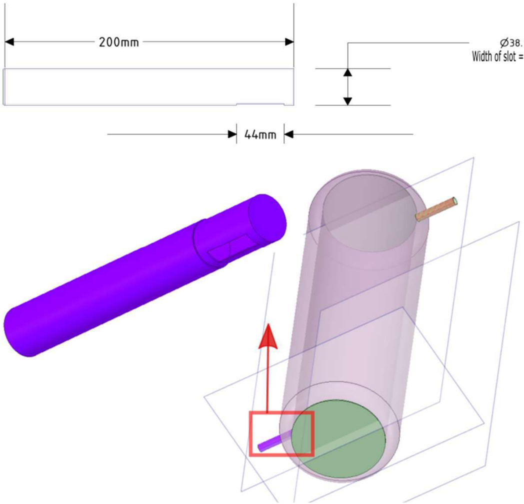
$$M_E = \sum_{j=1}^{j} y_j . E_j \tag{1}$$

$$MIX = \frac{M_{str} - M_{\exp}}{M_{str} - M_{full-mix}} \tag{2}$$

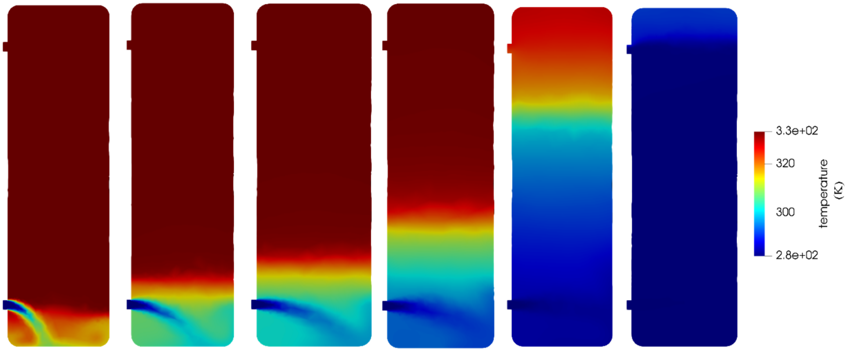
MIX number for 60 – 10 °C (60 °C being TES temperature, and 10 °C being discharge temperature) at flow rates of 200, 400, 600 and 800 l/h discharging flow rate was calculated for each inlet device. MIX for 200 l/h has the lowest ascent, followed by 400 l/h, then 600 l/h; finally, 800 l/h has the highest ascent of MIX number suggesting more intense mixing with 800 l/h discharging rate (refer Fig. 3 in Renewable Energy paper within study 1). Richardson number Ri is a dimensionless number which characterizes the ratio between potential energy required for vertical mixing and the turbulent kinetic energy available for such process (Eq. 3).

$$Ri = \frac{g\beta \Delta TL}{v^2} \tag{3}$$

A small Ri signifies mixed storage, while high Ri number indicates stratified one. Ri is increased as flow rate is decreased from 800 to 200 l/h. For example, Ri at τ^* (dimensionless time) = 0.6 for 800 l/h is nearly 75, while for 200 l/h it is approximately 120, $\tau^* = 0.6$ being the dimensionless time at which 60% of tank volume is already discharged. Numerical solution for one such operational parameter is shown in Fig. 3.



(a)



(b)

Fig. 3 Numerical analysis of TES (a) TES physical model, (b) temperature contours

As narrated the behavior of TES is governed by operating cycles, namely energy addition, storage and retrieval. Evaluating TES for non-transient conditions might not lead to full end to end energy quantification. This is termed as research and performance gap in the current methods. As an advancement to the limitation of current indices, second law models were developed and the data was fitted using the data layer. The model allowed to calculate end to end entropy, exergy and availability of the system. Eq. 4 and 5 represent the derived second law models fitted by data layer. Eq. 4 is entropy change (where *n* is the number of layers), Eq. 5 is exergy, while Eq. 6 is the stratification efficiency of TES. The derivation is depicted in study 2.

$$\Delta s_{total} = \int_0^H \rho(h)\cdot c(h)\cdot (V/n)\cdot \ln\left(\frac{T_{hp}}{T_i}\right) dh. \tag{4}$$

$$\xi = \int_0^t \rho(T)\cdot \dot{v}_{hp}\cdot c(T)\cdot [T_{hp,out}(t) - T_{hp,in}(t)]dt - T_0 \int_0^H \rho(h)\cdot (V/n)\cdot c(h) \ln\left(\frac{T_{hp}}{T_i(h)}\right) dh \tag{5}$$

$$\eta_{st}(ch) = \frac{\int_0^t \rho(T)\cdot \dot{v}_{hp}\cdot c(T)\cdot [T_{hp,out}(t) - T_{hp,in}(t)]dt - T_0 \int_0^H \rho(h)\cdot (V/n)\cdot c(h) \ln\left(\frac{T_{hp}}{T_i(h)}\right) dh}{\int_0^t \rho(T)\cdot \dot{v}_{hp}\cdot c(T)\cdot [T_{hp,out}(t) - T_{hp,in}(t)]dt} \tag{6}$$

To validate the second law models an experimental setup with water-water heat pump and water storage tank 397 L as investigated TES has been arranged. Speed controlled heat pump has nominal heat output 6.1 kW and coefficient of performance 4.78 at B0/W35 conditions and 50 Hz. In addition, an intelligent data layer was developed which collected and fitted the previously developed second law models. The data modelling – acquisition, cleaning, and transformation is done in situ (dynamically). Data-layer framework visualized real-time energy efficiency of TES using second law models developed in Study 3. Data layer served as the entry point for all the sensors connected to the TES integrated with heat pump system. For this task novel data layer was devised and programmed using Raspberry Pi-4 systems (Fig.4). Wide range of computing packages was observed which is not limited to PostgreSQL (to store/retrieve dynamic data that is being collected from sensors (RTD, current loop, Modbus)), Pandas/Numpy (to do all the scientific data computing, parsing, transformation, and curation), MatPlot-Lib/Seaborn for an in-situ animated visualization of the stratification decay. This considerably improved the intuitive understanding of stratification decay in real time, thus improving the advanced laboratory testing of HP integrated TES systems serving as information addition to the practice. The data layer consists of two Raspberry Pi (Raspi1 & Raspi2) mini computers, both running on Raspbian – Debian Linux operating system. Raspi1 stores temperature data from 19 Pt100 sensors located at various locations of the test bench, while Raspi2 stores the flow rate data, all in real time. Each 5th second the data is logged into each of the Raspi's PostgreSQL-DBs tables. In addition, a short code snippet running in Raspi1 also fetches wattmeter readings. Wattmeter data is used to measure the performance factor of the heat pump. All the data is used to fit together second law model to calculate the exergy/entropy and thus stratification efficiency. Raspi1 also retains 'Flask server' which is constantly logging the data on web-based application server (Fig. 5). The process diagram of data layer is described in more detail in Fig. 6.

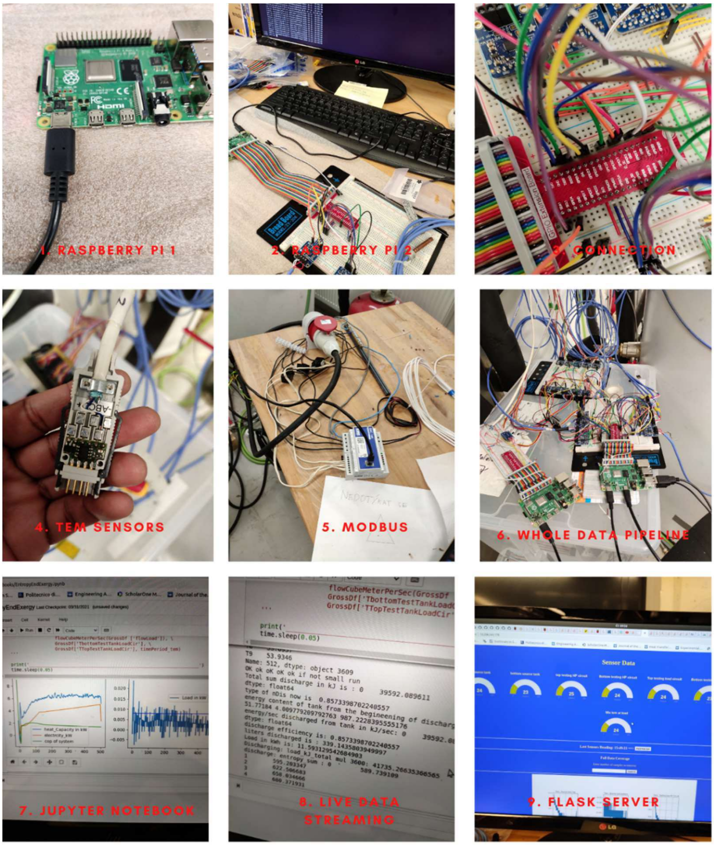


Fig. 4 Intelligent data layer

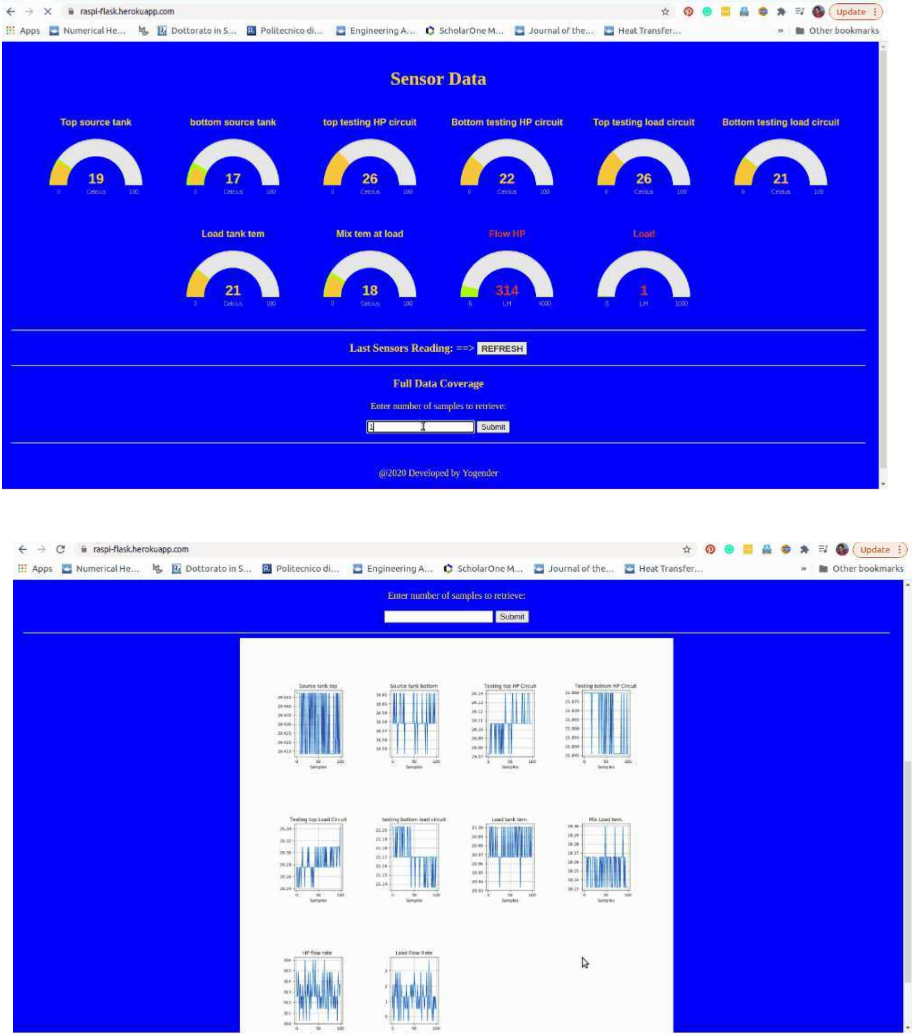


Fig. 5 Flask server

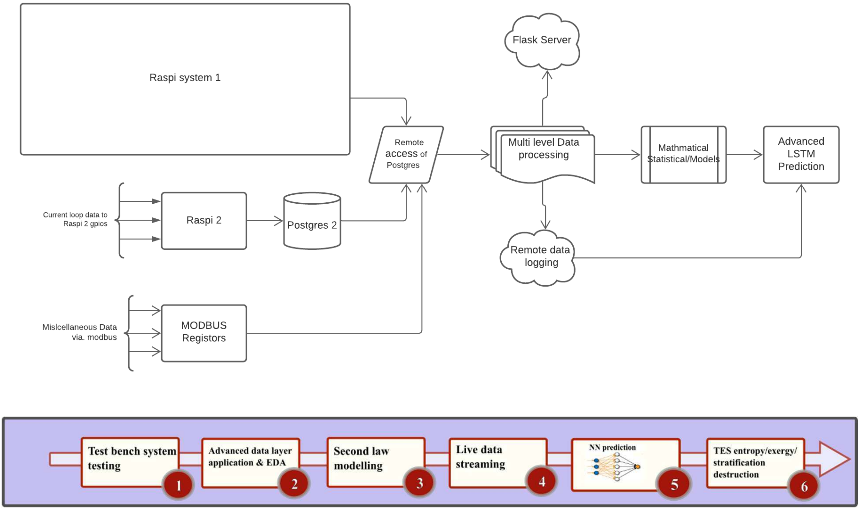


Fig. 6 Detailed process diagrams for data layer

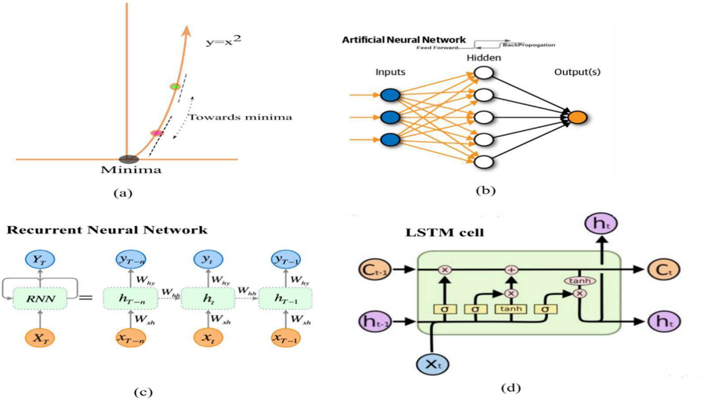


Fig. 7 NN architecture [8, 9]

Data layer was also equipped with hyper tuned neural network models to predict the stratification efficiency during each operating cycle. This incorporate applied deep learning (DL) framework utilizing long short-term memory (LSTM), and multilayer perceptron (MLP) to model the layered temperature and to predict the entropy generation during charging and discharging loop (Fig. 7b-d). Fig. 7 shows the architecture of the neural network used for prediction.

This is another non-traditional way of evaluating TES other than first or second law modelling. Neural networks in this fashion served as the entry point of the data produced by second law model that was developed and used during study 3. The results predicted by neural networks corroborated the results obtained by second law model. In this way, the neural network modelling validated the results of second law models. Model training and weight adjustment use a technique called stochastic gradient descent. In this technique, the network repeatedly determines the coefficient of the loss function where it has its local minima (Fig. 7a). Fig. 8 shows information flow with regards to LSTM modelling and quantitative model fitting by data layer.

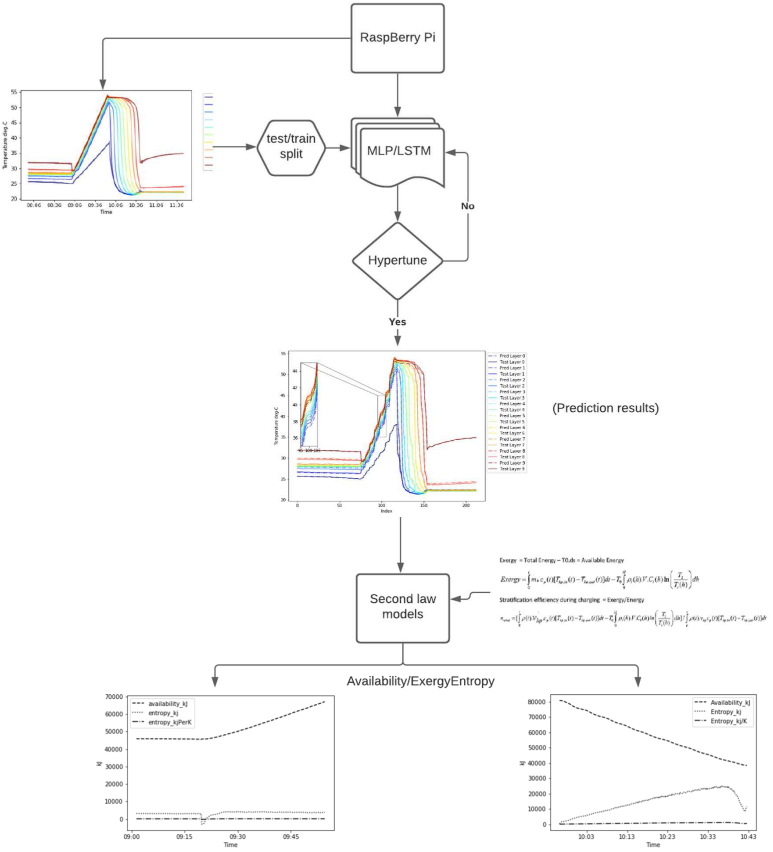
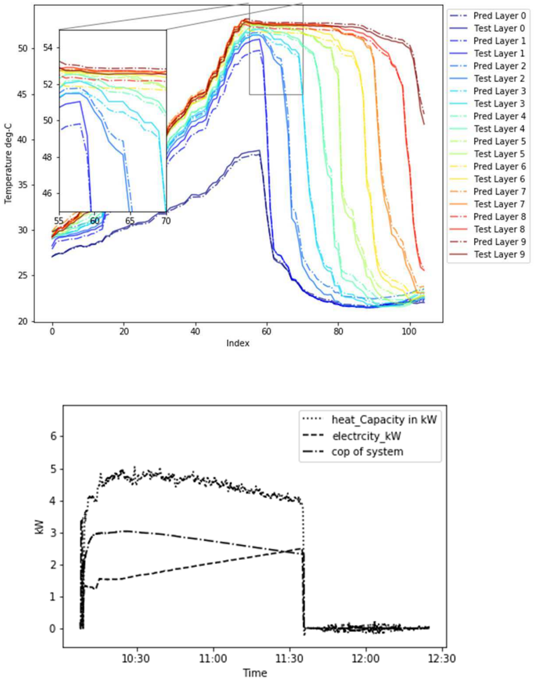


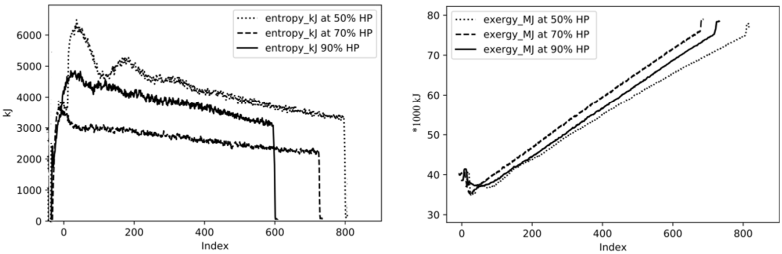
Fig. 8 Complete workflow of data layer from data injection to model fitting and prediction



(a)

(b)

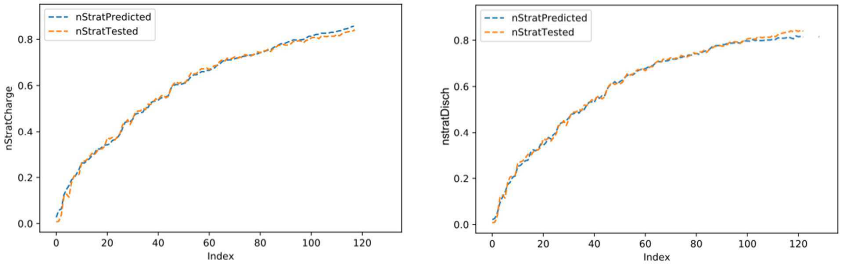
Fig. 9 Data collected by data layer, (a) temperature distribution, (b) heat pump parameters



(a)

(b)

Fig. 10 During charging at different heat pump compressor speeds (a) entropy generation, (b) exergy in TES



(a) (b)

Fig. 11 Stratification efficiency (validation) during (a) charge, and (b) discharge

Fig. 9 shows the work of data layer. The sooner the data layer collects the data from experimental setup, it dynamically plots the temperature profile of TES and heat pump parameters. Heat pump parameters include heat capacity, electricity consumption, and *COP* of the heat pump. These data points are collected for charge and discharge cycles. Fig. 9 also shows the predicted values of temperature. Fig. 10 shows the work of second law models developed in this thesis. Entropy and exergy generation in the TES at different compressor speeds were calculated during charge and discharge cycles. Fig. 10 however shows the results of second law models during charging. Entropy generation was found to be highest at slowest compressor speed.

The credibility of results obtained was ascertained at each stage. Ingested data in the data layer underwent linear regression to ascertain credibility of collected sensor data. Afterwards, statistical error distribution was performed (ref. Fig. 6 in the Renewable Energy paper within study 1 and Fig. 7 in Journal of Energy Storage paper within study 2). Second law models were validated using data driven as well as quantitative approach. Refer Fig. 11, Fig. 15 and Fig. 17 in the Journal of Energy Storage within Study 2 for validation using data driven approach. Finally, neural network modelling was validated itself. Fig. 12 in the same paper shows the parameters such as mean squared error and validation mean squared error. Validation is also shown in the Fig. 11.

Thesis Organization

This thesis is presented as "Thesis by publication". Five papers are bundled together to prepare this thesis. One paper among these is published in D1 (Decile 1), while four are published in Q1 (Quartile 1).

Objective coverage by Study 1: *Design and simulate the methodology to separate the good from the bad operational parameters during TES operation.*

(Design of operational parameters, stratification quantification, experimentation and CFD analysis are addressed by paper 1 & 2)

- **Paper 1:**

  Yogender Pal Chandra, and Tomas Matuska. Stratification analysis of domestic hot water storage tanks: A comprehensive review, Energy and Buildings 187 (2019) 110-131

  (Q1 – top 25%, Impact Factor: 7.201)

  DOI: https://doi.org/10.1016/j.enbuild.2019.01.052

  Citations (WoS): 63

  Yogender Pal Chandra: 80% contribution. Investigation, Data curation, Formal analysis, Software, Validation, Writing - original draft, Visualization.

  Tomas Matuska: 20% contribution. Conceptualization, Methodology, Writing - review & editing, Supervision, Project administration, Funding acquisition

- **Paper 2:**

  Yogender Pal Chandra, and Tomas Matuska. Numerical prediction of the stratification performance in domestic hot water storage tanks, Renewable Energy 154 (2020) 1165-1179

  (Q1 – top 25%, Impact Factor: 8.634)

  DOI: https://doi.org/10.1016/j.renene.2020.03.090

  Citations (WoS): 35

  Yogender Pal Chandra: 80% contribution. Investigation, Data curation, Formal analysis, Software, Validation, Writing - original draft, Visualization.

  Tomas Matuska: 20% contribution. Conceptualization, Methodology, Writing - review & editing, Supervision, Project administration, Funding acquisition

Objective coverage by Study 2: *Design and validate the custom built second law model to quantify the availability of the energy that is sbeing added and subsequently removed during charge and discharge cycle of TES*

- **Paper 3**: Yogender Pal Chandra, Gwang Jim Kim, Tomas Matuska. Second law performance prediction of heat pump integrated stratified thermal energy storage system using long short-term memory neural networks, Journal of Energy Storage 61 (2023) 106-699

  (Q1- top 25%, Impact factor: 8.907)

  DOI: https://doi.org/10.1016/j.est.2023.106699

  Citations (WoS): 1

  Yogender Pal Chandra: 80% contribution. Investigation, Data curation, Formal analysis, Software, Validation, Writing - original draft, Visualization.

  Gwang Jim Kim: 1% contribution. Conceptualization, Methodology

  Tomas Matuska: 19% contribution. Writing - review & editing, Supervision, Project administration, Funding acquisition

Objective coverage by Study 3: *Design of intelligent IoT stream processing unit to fit the second law model previously developed*

- **Paper 4:** Yogender Pal Chandra, and Tomas Matuska, Intelligent data systems for building energy workflow: Data pipelines, LSTM efficiency prediction and more, Energy and Buildings 267 (2022) 112135

  (D1 – top 10%, impact Factor: 7.201)

  DOI: https://doi.org/10.1016/j.enbuild.2022.112135

  Citations (WoS): 0

  Yogender Pal Chandra: 80% contribution. Investigation, Data curation, Formal analysis, Software, Validation, Writing - original draft, Visualization.

  Tomas Matuska: 20% contribution. Conceptualization, Methodology, Writing - review & editing, Supervision, Project administration, Funding acquisition

- **Paper 5:** Yogender Pal Chandra, and Tomas Matuska. Energy modeling of thermal energy storage (TES) using intelligent stream processing system, Energy Reports 8 (2022) 1321 – 1335

  (Q1 – top 25%, Impact Factor: 4.937)

  DOI: https://doi.org/10.1016/j.egyr.2022.08.012

  Citations (WoS): 0

Yogender Pal Chandra: 60% contribution. Investigation, Data curation, Formal analysis, Software, Validation, Writing - original draft, Visualization.
Tomas Matuska: 40% contribution. Conceptualization, Methodology, Writing - review & editing, Supervision, Project administration, Funding acquisition

Results & Achievements of objectives

Research gaps and performance gaps were identified during Study 1. The ***first objective*** of this Ph.D. thesis was design, operational parameters, stratification quantification, using experimentation and CFD analysis. This is presented in ***Study 1***. In this study, quantification of turbulent mixing was achieved on the basis of temperature profile, MIX number, and Richardson number (indices observed in ***Study 1***).

Research gap:

- The research gap was observed during ***Study 1***. More specifically, MIX number was picked and utilized to quantify the stratification in TES experimentally. *Study 1* extended the work of Haller et. al [1,3] in terms of experimental investigation of the same. In addition, CFD methods and models were developed to collect, model, and curate the data and were validated using experimental results. Their work was further extended by investigating MIX number for various TES operational and inlet design characteristics.
- G. Rosengarten et. al [2] proposed second law approach in characterizing TES with application to solar energy water heater. Their work was further extended by simplifying their model, customizing it for temperature dependent thermophysical properties and applying it in real time mode in both charge and discharge cycle. These models were later customized for our TES use-case. This is presented in the ***Study 2.***

Performance gap:

- Energy disbursement in renewable energy system is a transient state process. A streaming data layer edge device was developed which analyses the energy efficiency of renewable energy system in real time. This is very novel approach in such analysis.
- G. Rosengarten et. al [2] analyzed renewable energy system in single discharge cycle. This dissertation focuses on automated analysis of full charge and discharge cycle giving more insight into energy disbursement from electric grid to load.

Results: The evaluated parameters include flow rate and ΔT, henceforth a direct interdependence between each was thus established. Various CFD models were developed and experimentally validated on the test rig in order to find the optimal working conditions in discharge mode. The results for different diffuser designs proved numerically that the tank working conditions can be optimized by proper selection of inlet device. For instance, slotted type inlet device sustained maximum stratification even in as adverse a condition as of turbulent inflow & low ΔT. Perforated and simple inlet devices were capable of delivering best discharge efficiency only at low flow rate of 200 l/h and were showing insignificant dependency on ΔT. However, as flow rate is increased, ΔT dependency increased. Seeing the compounded benefits of slotted inlet devices and decreased ΔT, it was concluded that slotted inlet device delivered comparatively better thermal performance at both adverse conditions i.e. high flow & low ΔT and high flow & high ΔT, however, failed to outshine the rest of the inlet devices at low flow rate & low ΔT, and low flow rate & high ΔT. These research findings can serve as guidelines to optimize the storage tank design, more specifically, inlet device-based design integrated with heating system, as thermal stratification and *COP* of heating system (heat pumps), for example, are inherently correlated. Heat pumps are high flow rate and low ΔT devices, while, solar systems are low flow rate and high ΔT devices, Thus, opting for accurate choice of inlet device for a particular operating condition is critical.

*The **second objective*** of this Ph.D. thesis was to design and validate the custom built second law model to quantify energy/exergy dispersal during TES charging and discharging. This is presented in ***Study 2.*** To quantify the system performance, second law efficiencies (exergy, and entropy) of TES along with *COP* of heat pump system were introduced. It also proposes optimized modelling framework of one complete charge/discharge cycle which can further be appended over a longer time horizon. A tailored second law-based exergy equations to be fitted to the data layer for real time streaming of entropy/exergy in TES and *COP* was derived. Stratification decay was also predicted using Neural Networks.

Results: Three distinct compressor speeds and tapping rates were studied using this data-streaming edge device and their exergy disbursement was studied in live mode. It was observed that entropy generation was maximum at highest discharge rate of 800 l per hour i.e. 25,000 kJ (while only 3000 kJ for 900 l/h of charging rate). Furthermore, entropy generation has not only impact on stratification efficiency, however also on performance factor of the heat pump. Making it extremely essential to adjust for inlet flow rate and compressor speed ratio. *COP* of 3.2 was obtained at 70 % compressor speed, while at the same time maximum discharge efficiency was registered at lowest discharge flowrate of around 450 l/h.

The ***third objective*** of this Ph.D. thesis was to design intelligent IoT stream processing unit to fit the second law model previously developed. This is presented in ***Study 3***. This study demonstrates the application of intelligent data layer with neural networks for evaluating and predicting end to end performance of heat pump integrated stratified thermal energy storage (TES) system. The data modelling – acquisition, curation, and transformation is done in situ (dynamically). This study is a 'method-based' study to demonstrate the data-layer framework and its application in assessing energy efficiency of renewable energy system by fitting the custom second law exergy models previously developed, all in real time. This real time analysis can help researchers to intuitively understand the energy efficiency of renewable energy systems in high expertise labs.

Results: The data-streaming edge device was comprised of two *Raspberry-Pi* mini computers, running on Raspbian operating system. Both stored and processed the TES and heat pump data in live mode in master slave architecture. The data was stored in Postgres-SQL database, from where it was processed and ingested to custom real time interactive dashboarding system. The data layer streams, end-to-end (from electric gird to user tapped water) exergy balance of heat pump integrated TES system in live mode. This makes sure that the engineer has clear understanding of the percentage of grid output being consumed as entropy during charging/discharging, and what percentage of it is available to user as the tapped water. For that matter, real time dash-boarding was built. Prediction modelling was also performed using deep learning frameworks.

Validation of results:

A neural network model using LSTM was developed and was used to predict the temperature of TES layers and its stratification efficiency. The error range for temperature and efficiency prediction was observed to be 5 % and 2 % respectively (ref. Fig. 17 in the Journal of Energy Storage paper) as shown within Study 2. The LSTM model reproduced the results calculated by exergetic model thus the results calculated by quantitative approach is validated by data driven approach. The data-driven approach is agnostic and makes no assumptions - but does not give any clue how and which inputs influence the output. The quantitative approach works with assumptions but shows clearly the quantitative relationship between input features and the calculated output, thus helps to deepen the understanding of the processes. Data driven approach in theory is bias-free.

In addition, time series data thus collected underwent statistical uncertainty analysis. Probability distribution of error in terms of gauss distribution was analyzed. Error was roughly normally distributed with 95 % of data points falling under 5 % error (ref. Fig. 7 in the Journal of Energy Storage paper).

Conclusion

This thesis emphasizes the importance of thermal stratification in heat storage systems, and how it can improve the efficiency and exergy of the system. A well-stratified tank is able to deliver higher exergy with less heat input compared to a mixed isothermal tank. To achieve this, it is important to maintain a stable vertical temperature gradient during all operation cycles of the tank. This can be achieved through careful monitoring of hydrodynamics and thermodynamics, and the management of inlet-outlet configuration, such as the position, shape, and type of diffuser, hot water inlet, bulk water temperature difference, and draw-off rate. Other parameters such as thermal conductivity and aspect ratio of tank is also important in this regard. The degree of mixing in the tank can be measured through various parameters, which require accurate temperature measurements of each water layer using temperature sensors. The research is furthered to develop calculation methodology for the same.

CFD part of the thesis focuses on the influence of various inlet devices on stratification degradation. Three types of inlet devices (slotted, perforated, and simple) were simulated in a transient manner to understand their performance under different operational conditions, such as flow rate and ΔT. The results showed that the slotted inlet device performed best at high flow rates and low ΔT, which is suitable for heat pump-based storage tanks. However, for solar system-based storage tanks, which require low flow rates and high ΔT, the application of slotted inlet devices did not make much difference in stratification efficiency. CFD model validation was also performed. CFD data was plotted against the experimental data. In addition, mesh independent study was also performed. The study also highlighted the importance of stratification indices, such as temperature evolution, MIX number, and discharging efficiency, in assessing the performance of storage tanks. These indices use first law approach to assess the stratification. Later on, second law approach was used as second objective.

Furthermore, the second law of thermodynamics was considered in developing equations for entropy and exergy. The models and the edge devices allow for real-time monitoring of TES performance and heat pump efficiency during charge/discharge cycles. Advanced deep learning algorithms specifically LSTM neural networks were used to model the data collected by edge device and to predict the TES layered temperature and efficiency. The neural network prediction is considered as data driven approach to evaluate the stratification. And it is also used to validate the quantitative models developed. The error between quantitative and predicted results lied within 5% range. The exergy balance presented in the thesis measures the effective utility of the heat pump integrated with the TES system.

Lastly, a methodology was developed to study the stratification of TES in real-time mode using custom-built data-stream processing edge devices and exergetic (quantitative) models. The study tested a TES integrated heat pump used for a single-family house for stratification efficiency and energy balance, and applied custom exergy models using a custom data streaming edge device to study end-to-end energy expenses. Overall, the study provides a promising approach to real-time experimental based optimization of TES systems.

Overall, these methodologies can be used for high expertise lab testing of TES systems.

Value addition to the theory:

The theoretical aspect of this thesis was to identify a research gap related to TES and stratification indices to quantify thermal stratification in TES. CFD models and algorithms were developed to understand the applicability of temperature distribution and stratification indices to quantify the stratification in TES. This knowledge was later used in experiments. It was found that first law models were static and focused on TES only. In order to evaluate the TES along with heat pump, and that also dynamically and in a transient state manner, second law models were developed. Mathematical equations were derived in the theoretical part of this thesis and were used to measure how well a TES system was stratified. More specifically, thermodynamic models were developed to quantify exergetic expenses in TES integrated heat pump. This methodology of evaluating the TES along with heat pump is proposed as an improvement plan over first law models.

Value addition to the practice:

A real-time performance evaluation and streaming edge device was developed for the heat pump integrated with a thermal energy storage (TES). The edge device observed the exergetic models (previously developed in theoretical part) to demonstrate and quantify the entropy generation in TES and its effects on the *COP* of the heat pump during charging and charging cycles. Optimization of the circulation flow rate and compressor speed was also achieved using the above. Overall, this methodology provides a better perspective on the energy efficiency of renewable energy systems and could help researchers in this field. In short, value addition to practice is the data layer setup in the testing lab, predictive modelling using the data layer and subsequent second law model fitting and validation. Using both the models (theoretical addition) and data layer (practical addition), researchers can gain more inference in renewable energy systems in tightly controlled specialized and high expertise labs.

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Publications related to the title of Dissertation:

1. Yogender Pal Chandra, and Tomas Matuska. Stratification analysis of domestic hot water storage tanks: A comprehensive review, Energy and Buildings 187 (2019) 110-131

2. Yogender Pal Chandra, and Tomas Matuska. Numerical prediction of the stratification performance in domestic hot water storage tanks, Renewable Energy 154 (2020) 1165-1179

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4. Yogender Pal Chandra, and Tomas Matuska, Intelligent data systems for building energy workflow: Data pipelines, LSTM efficiency prediction and more, Energy and Buildings 267 (2022) 112135
5. Yogender Pal Chandra, and Tomas Matuska. Energy modeling of thermal energy storage (TES) using intelligent stream processing system, Energy Reports 8 (2022) 1321 – 1335