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Black box modelling of a latent heat thermal energy storage system coupled with heat pipes

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Abstract. This paper presents black box models to represent a LHTESS (Latent Heat Thermal Energy Storage System) coupled with heat pipes, aimed at increasing the storage performance and at decreasing the time of charging/discharging. The presented storage system is part of a micro solar CHP plant and the developed model is intended to be used in the simulation tool of the overall system, thus it has to be accurate but also fast computing. Black box data driven models are considered, trained by means of numerical data obtained from a white box detailed model of the LHTESS and heat pipes system. A year round simulation of the system during its normal operation within the micro solar CHP plant is used as dataset. Then the black box models are trained and finally validated on these data. Results show the need for a black box model that can take into account the different seasonal performance of the LHTESS. In this analysis the best fit was achieved by means of Random Forest models with an accuracy higher than 90%.

1. Introduction

Heat pipes are devices widely used for increasing heat recovery and improving thermal performance of heat exchangers in different applications [1]. In particular, heat pipes (HP) can be used to enhance the performance of LHTESS (Latent Heat Thermal Energy Storage System) which are increasingly adopted as storage systems in renewable and hybrid power plants. In literature several studies investigated heat pipes potential to increase the thermal conductivity of PCM (phase change materials) and to decrease PCM charging and discharging time [2, 3]. Robak et al. [2] found that inclusion of heat pipes increases PCM melting rates by approximately 60%. Naghavi et al. [3] shown different applications of heat pipes

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coupled with PCM storage systems for low temperature and high temperature solar collectors. Among the other findings, some of the advantages guaranteed by heat pipes are: (i) very low temperature gradients between the two opposite sides of the HPs, so that an almost isothermal heat source is available for the PCM; and (ii) the heat flux through the HPs can be used to provide low heat flux densities within the LHTESS even in presence of large heat flow rates from the heat source/sink [3].

In this study a LHTESS equipped with reversible heat pipes is considered. Such system is embedded in a micro solar CHP (combined heat and power) plant for application in individual dwellings and small business residential buildings for on-site electricity and heat generation (2-kWel/18-kWth), using solar thermal energy at modest temperatures of 250-280°C (as proposed by researchers at Northumbria University [4] and under the European funded H2020 Innova MicroSolar project [5], led by Northumbria). The proposed technology is based on a linear Fresnel mirror solar concentrating collector and a micro Organic Rankine Cycle (ORC) plant [5]. In figure 1 a schematic representation of the micro solar ORC plant is provided.
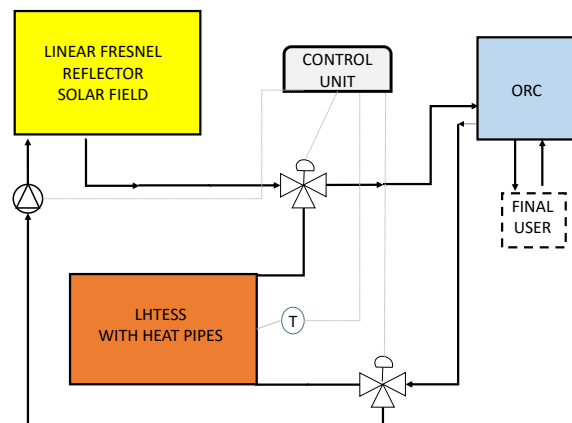

Figure 1. Schematics of the micro solar ORC pant.

The role of the storage system is to store the surplus energy from the solar field and to supply the ORC in case the solar energy is not sufficient. In order to increase the overall efficiency of the plant, in this project new reversible heat pipes are developed by Aavid Thermacore [6]. They are capable of transferring heat at high rate in both directions. This means that heat flows through the heat pipes from the solar circuit to the thermal storage tank with PCM and from the tank to the ORC plant circuit. It is expected that the proposed novel design will significantly increase the specific heat accumulation and storage efficiency. The plant will be tested on the field at Almatret (Lleida, Spain) and, in the meanwhile, a simulation model for the overall micro CHP plant was developed.

Purpose of this paper is to present the modelling of the LHTESS with the embedded heat pipes by means of an accurate but also fast computing model. At this aim, black box models are trained on the basis of a white box model simulation results, representing in detail the real system. This is intended also as a preliminary work to better understand the system behavior and the most influencing parameters, so to easily extend the methodology to the training/validation of black box models by means of experimental data collected during field test.

2. Methods
The LHTESS, as designed by Northumbria University and Aavid Thermacore [4, 6], consists of a rectangular array of heat pipes embedded in PCM and the heat transfer fluid (oil) flows through the heat pipes evaporator /condenser that is not embedded in the PCM, named oil chamber (figure.2).
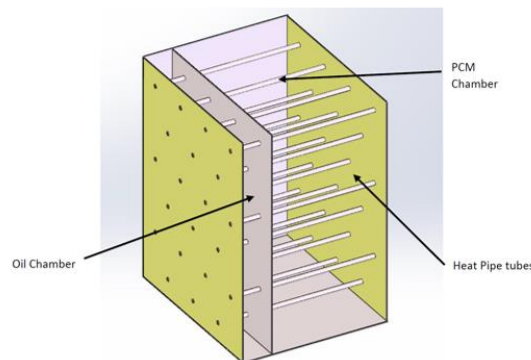
Figure 2. Schematic design of the LHTESS.

Given the complexity of the physical behavior of PCM and heat pipes system (which includes also phenomena such as hysteresis or sub-cooling), its physical representation is challenging. In order to have a good representation of the real behavior and to obtain a tool easy to implement in a comprehensive energy system simulation environment, black box models are a good option. The choice of the black box model structure and its identification procedure is a critical issue. In this work AutoRegressive models with eXogenous inputs (ARX), Nonlinear AutoRegressive networks with eXogenous inputs (NARX) and Random Forest (RF) regression models are considered. The performance of the different black box models, in the validation procedure, is compared to the results of the white box model on the basis of the Root-Mean-Square Error (RMSE) and Normalized Root-Mean-Square Error (NRMSE). In particular, accuracy of results is the key performance parameter taken into account to evaluate the effectiveness of the proposed black box models.

2.1. LHTESS and white box model description

The PCM storage material, investigated by Northumbria University and the University of Lleida [7] is made of the so-called solar salt KNO3(40wt.%)/NaNO3(60wt.%), which has high heat of fusion but low thermal conductivity; its melting temperature is in the range 216-223°C [8]. In a volume of 1.90 m3 there are 3.8 tons of this material to store about 100 kWh of latent thermal energy from the solar field in order to guarantee 4 hours of ORC unit operation during night time. Reversible heat pipes, developed by Aavid Thermacore [6], are charged with a sufficient amount of demineralized water to carry the required power; they are able to withstand a maximum pressure of 100 bar.

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The physically based PCM storage tank model was developed according to the guidelines of the IEA Task 32 report on advanced storage concepts [9]. The PCM is supposed isotropic and isothermal in each time-step. Hysteresis and sub-cooling effects are neglected. The white box model represents the behavior of the heat pipes by means of: (i) a limitation in the maximum power exchanged with the oil because of the limited heat pipes capacity (40 kW) and (ii) a minimum temperature difference between the oil and the PCM equal to 5°C.

The dataset used for training the black box models is represented by the simulation results of the white box model. The white box model is implemented in TRNSYS (an environment for transient representation of thermal systems behavior [10]) within the overall micro-solar CHP plant. A full year of operation of the plant, set in the city of Cagliari in Italy (local coordinates 39° 22' 38.41'' N and 9° 12' 16.61'' E), is considered. Therefore, the operating conditions of the LHTESS during its operation

in the integrated plant are taken into account. The simulation time step is 10 minutes (T_c, sampling period).

The input variables to the black box models are:
- Oil inlet temperature (T_{OIL}^{in});
- Oil inlet flow rate (F_{OIL}^{in});
- Ambient temperature (T_A);
- Direct Normal Irradiance (DNI) of the sun;
- Operation mode of the plant (OM). Indeed, there are 6 different operation modes in the control strategy of the micro solar CHP plant, where the LHTESS can be charged or discharged in different operating conditions.

The input variables are averaged to better reflect their influence on the output variables by a test and trial procedure. Eventually, T_A is filtered by a median filter over a 24 hours period, while T_{OIL}^{in}, F_{OIL}^{in} and DNI are filtered by a median filter over a 2 hours period and OM is filtered by a mode filter over a 24 hours period. The output variables of the black box models, i.e. the variables to be predicted, are:
- Oil outlet temperature (T_{OIL}^{out});
- Temperature of the TES (T_{TES});
- Thermal losses of the TES to the environment (P_{LOSS}).

In figure 3 the input and output variables of the black box models are represented.
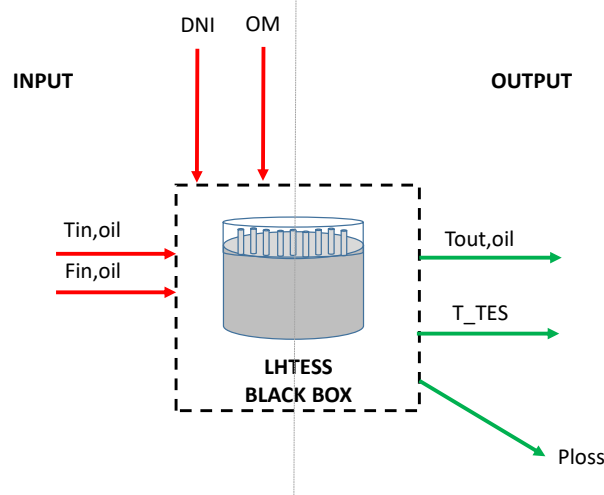
Figure 3. Schematic representation of the Black Box models input and output variables.

2.2. ARX models

The autoregressive model with exogenous inputs is a linear model defined by the equation 1 as in [11]:

$$A(z)y(k) = B(z)u(k) + v(k) \tag{1}$$

with $A(z)$ and $B(z)$ denoting polynomials with respect to time-shift operator z:

$$A(z) = 1 + a_1 z^{-1} + \cdots + a_{na} z^{-na} \tag{2}$$

$$B(z) = b_0 + b_1 z^{-1} + \cdots + b_{nb} z^{-nb} \tag{3}$$

The ARX model considered in this study for simulation can be mathematically represented as:

$$\sum_{i=0}^{n_a} a_i \, \hat{y}(k-i) = \sum_{j=0}^{n_b} b_{1j} \, F_{OIL}^{in}(k-j-n_k) +$$

$$+\sum_{j=0}^{n_b} b_{2j} \, T_{OIL}^{in}(k-j-n_k) + \sum_{j=0}^{n_b} b_{3j} \, T_A(k-j-n_k) + \sum_{j=0}^{n_b} b_{4j} \, DNI(k-j-n_k) +$$

$$\sum_{j=0}^{n_b} b_{5j} \, OM(k-j-n_k) \tag{4}$$

where $k = nT_c$ denotes time, $n \in Z$, sampling period T_c and a_i, b_{1j}, b_{2j}, b_{3j}, b_{4j} and b_{5j} denote the unknown model parameters. n_a, n_b and n_k are the orders of the model (so called hyper-parameters) associated with output, inputs and dead time in the system, respectively. $\hat{y}(k)$ represents the estimated outputs, namely T_{OIL}^{out}, T_{TES} and P_{LOSS}.

2.3. NARX models

The A nonlinear autoregressive network with exogenous inputs is a special case of Recurrent Neural Network (RNN), which proved to be a very successful modeling tool for nonlinear systems and especially time series [12]. NARX networks converge faster, are less likely to develop long-term dependencies and typically have better generalization abilities than other networks [12]. The NARX structure considered in this study for simulation can be mathematically represented as:

$$\hat{y}(k) = f\big[F_{OIL}^{in}(k-n_k), \dots, F_{OIL}^{in}(k-n_k-n_b), \; F_{OIL}^{in}(k-n_k), \dots, F_{OIL}^{in}(k-n_k-n_b), T_A(k-n_k), \dots, T_A(k-n_k-n_b), DNI(k-n_k), \dots, DNI(k-n_k-n_b), OM(k-n_k), \dots, OM(k-n_k-n_b)\big] \tag{5}$$

The nonlinear mapping f is generally unknown and can be approximated, for example, by a standard Multilayer Perceptron (MLP) network.

Since in this paper the black box model is intended to be used as simulation model, the true past values of $\hat{y}(k)$ are not available when the model is deployed (differently from predictive models).

Therefore, the resulting architecture is a particular case of NARX network.

2.4. Random forest

Breiman [13] defined a "random forest" as a variant of bagging meta-algorithm. Random forest is a general class of ensemble building methods which use decision trees for regression or classification. To be labeled a "random forest", an ensemble of decision trees should be built by generating independent and identically distributed random vectors and should make use of each vector to model a decision tree. Therefore, a random forest could be built by sampling from the data set or feature set or just varying randomly some of the parameters of the tree. Any combination of these sources of diversity will also lead to a random forest.

2.5. Identification procedure

Data pre-processing is the first step before the identification procedure. In particular, for ARX, data detrend is performed. This data processing operation helps to estimate more accurately linear models and overcome their inability to capture arbitrary differences between input and output signal levels. For NARX, data are normalized in the range [-1; 1] since a sigmoid function is considered in the hidden layer. In order to reduce the overfitting issue, regularization term is considered for both ARX and NARX. For all the three models, the 10-fold cross-validation technique is used. Only for RF modelling, the input operation mode of the plant (OM) is considered as a categorical predictor.

The System Identification Toolbox in Matlab [14] is applied on a training dataset to estimate the unknown parameters for ARX. In the NARX model, instead, the optimal values of the model parameters have been estimated using the Neural Network Toolbox. Finally, RF regression model is built by the Statistics and Machine Learning Toolbox.

A grid search optimization procedure is considered to set the hyperparameters of the three models, in particular, the orders of ARX (i.e, n_a, n_b and n_k), the orders of NARX (i.e, n_b and n_k) and the orders of regression (i.e., n_b and n_k), the leaf size and the number of decision trees of RF model.

After identification, the models are tested by means of the following indicators:

- the RMSE-values on the validation dataset;
- the level of fit (NRMSE) on the whole dataset.

The RMSE (root mean square error) is the objective function to be minimized both for training and validation sets. RMSE is defined as follows:

$$RMSE = \left(\frac{1}{N}\sum_{k=1}^{N} e(k)^2\right)^{1/2} \tag{6}$$

where N is the number of samples and $e(k) = y(k) - \hat{y}(k)$ represents the difference between the variable $\hat{y}(k)$ predicted by the simulation model and the variable $y(k)$ predicted by the white box model. NRMSE values are the normalized root mean square errors and thus they show in percentage the model goodness of fit.

3. Results

The different black box models were first trained and then tested, as described in the previous section. Firstly, the ARX models were considered, because they have a simpler structure. Then the NARX and eventually the RF models, in order to improve the performance in fitting with the white box model.

3.1. ARX model results

The optimum parameters of the ARX model identified are: n_a=4, n_b=4 and n_k=3 for T_{TES}; n_a=1, n_b=9 and n_k=0 for T_{OIL}^{out}; n_a=0, n_b=6 and n_k=0 for P_{LOSS}. The RMSE and NRMSE values are reported in Table 1.

Table 1. ARX results.

Output variable	RMSE	NRMSE
T_{TES}	3.1 (°C)	0.241
T_{OIL}^{out}	8.4 (°C)	0.914
P_{LOSS}	71.4 (kJ/h)	0.362

The NRMSE obtained with the ARX model is not very good, especially for the variable T_{TES}. Looking in detail to the trend of such variable during the year (figure 4a e figure 4b), a different behavior of the storage system in summer and in winter is evident. That was expected, because the micro-solar CHP plant performance is strongly influenced by the solar radiation available. In winter the plant is off for longer periods of time and the LHTESS is partially charged, without reaching the melting condition, and rarely discharged. In summer, instead, the LHTESS works properly and can be fully charged and discharged using the latent heat available.

The ARX model, as here identified, cannot represent such different behaviors by means of a single model. Looking at the predicted and original values of the output variables (figure 4a e figure 4b), the model can mimic the LHTESS temperature much better in summer than in winter. For this reason, a separate identification procedure for the two seasons was performed. The global performance indicators of the two new ARX models are reported in Table 2.

Table 2. ARX results in summer and winter.

Output variable	NRMSE summer	NRMSE winter
T_{TES}	0.455	0.077
T_{OIL}^{out}	0.914	0.884
P_{LOSS}	0.415	0.167

The results show an increased ability, even if still low, of the summer ARX model to predict the output variables trend, while in winter the goodness of fit is still poor.
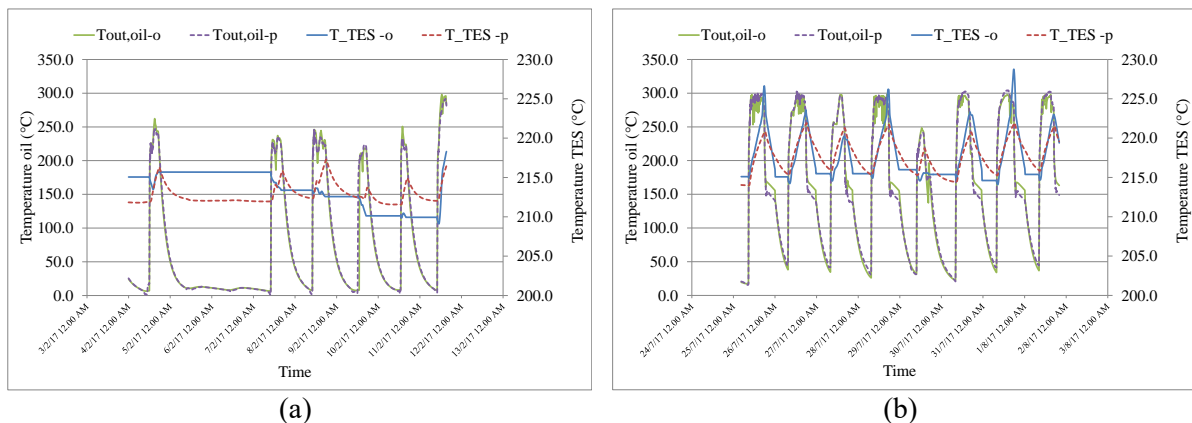

Figure 4. Predicted (p) vs original (o) values of the output variables for the ARX model in (a) winter and in (b) summer.

3.2. NARX model results

Given the unsatisfying results shown in the previous section, another class of black box models was considered. The optimum parameters of the NARX model identified are: n_b=12 and n_k=0.

The RMSE and NRMSE values are reported in Table 3. Again, a single NARX model cannot properly predict well the different LHTESS behavior in the different seasons. Considering the results already obtained for the ARX model, the NARX model has not been furtherly investigated.

Table 3. NARX results.

Output variable	RMSE	NRMSE
T_{TES}	2.8 (°C)	0.303
T_{OIL}^{out}	6.9 (°C)	0.931
P_{LOSS}	60.4 (kJ/h)	0.463

3.3. RF model results

In order to improve the ability to reproduce the behavior of the LHTESS during the whole year, a more complex category of black box models was considered. Indeed the RF models contain internal different models and their outcome is an average of all the included models. The optimum parameters of the RF model identified are: n_b=12 and n_k=0 and it is used 1 leaf size and 20 decision trees. In Table 4 the corresponding RMSE and NRMSE values are reported.

Table 4. RF results.

Output variable	RMSE	NRMSE
T_{TES}	0.7 (°C)	0.904
T_{OIL}^{out}	4.2 (°C)	0.973
P_{LOSS}	15.3 (kJ/h)	0.929

In this case the NRMSE (FIT) obtained is pretty good, especially for T_{OIL}^{out} and P_{LOSS}. Even the prediction of T_{TES} has been greatly improved and can be considered acceptable. However, looking at the RMSE values, it must be highlighted that, even if the absolute value of the RMSE is low, it could have a huge influence. For example, a RMSE of 0.7°C on the T_{TES} is not big, but given that the melting temperature range is 7°C (216-223°C), it could affect the ability to predict the latent heat available. Furthermore, T_{OIL}^{out} has values around 250-300°C, thus a RMSE of 4.2°C is a very small error in prediction, nevertheless the oil mass flow rate is pretty big, then also a small error in this temperature prediction is translated in a consistent mistake in assessing the heat exchanged with the TES. Instead the RMSE on the P_{LOSS} (kJ/h) is really very low, even if the relevance of this output variable is limited. It could also be obtained as result of a calculation, once known the input variables and the other output variables.

In figure 5a and figure 5b the predicted and original output variables are shown for the two seasons. Predicted T_{OIL}^{out} follows pretty good the trend of the original value, while T_{TES} shows, especially in winter, an oscillating trend not visible in the original variable. As already mentioned, in winter there are long periods in which the LHTESS does not exchange energy with the rest of the plant, because there is not a surplus of energy to be stored or recovered. During these periods the TES exchanges heat only with the external environment as thermal losses. Thus, the T_{TES} results highly correlated with the external ambient temperature and this is reflected by the prediction of the black box model. However, the variability of the external ambient temperature is much higher than the actual variability of the temperature of the storage tank.
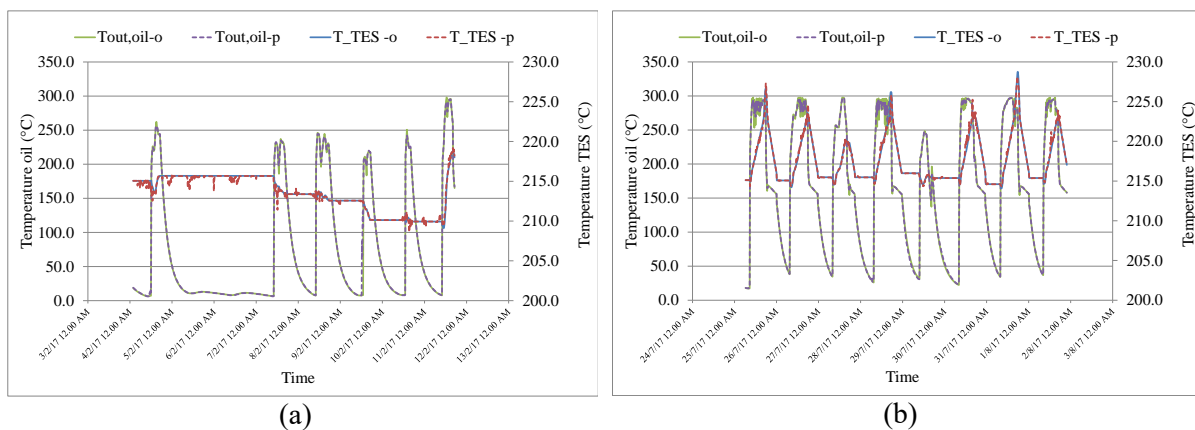

Figure 5. Predicted (p) vs original (o) values of the output variables for the RF model in (a) winter and in (b) summer.

Such aspect could be further improved with an in depth study of the influence of the input data on the output variables, in order to better represent the system behavior during the whole year. In Fig. 6 the influence of each input variable on the output variables is shown. In particular, for any variable, the prediction importance is the increase in prediction error if the values of that variable are permuted across the out-of-bag observations. This measure is computed for every tree, then averaged over the entire ensemble and divided by the standard deviation over the entire ensemble (it is a number >0).
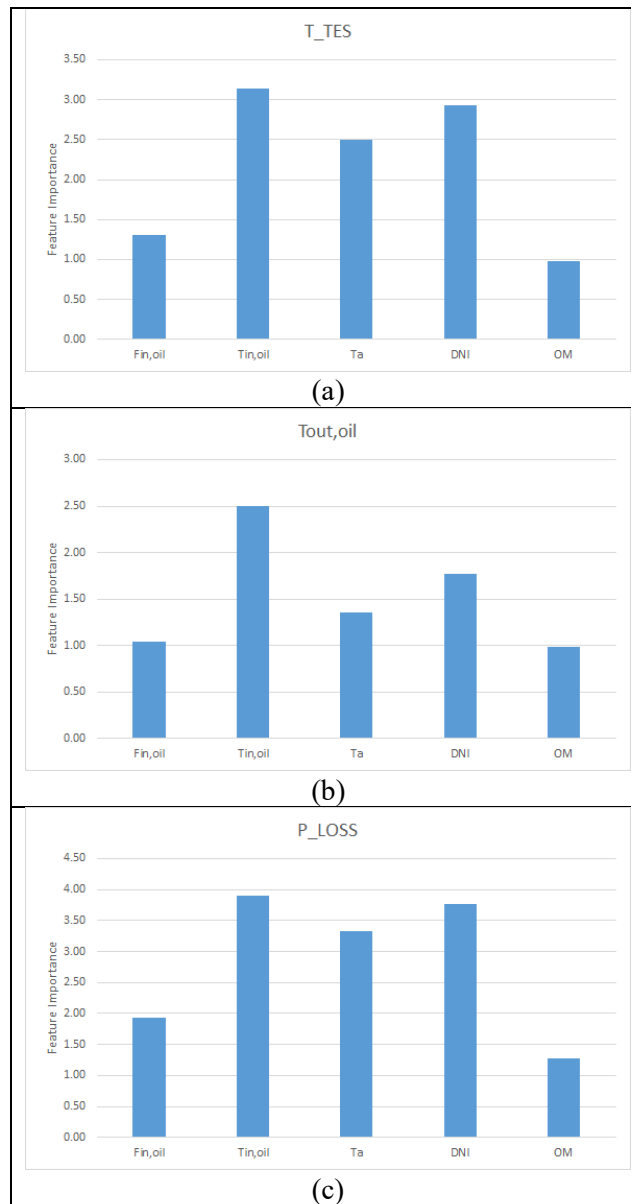
(a)

(b)

(c)

Figure 6. Influence of the input variables on the output variables: a) T_TES, b) Tout,oil, c) Ploss.

It can be observed that T_{OIL}^{in} and DNI are the most influencing variables for all the different outputs. Moreover it is confirmed that the ambient temperature has also a quite important effect on the heat losses and on the TES temperature, as already discussed previously.

4. Conclusions

In this study a first attempt to model a complex Latent Thermal Heat Energy Storage System (LHTESS) coupled with heat pipes by means of black box models is presented. Several configurations of black box models were considered in order to find a good fit between predicted and original values of the output variables of the system. As original values were taken the simulation results of a white box model of the LHTESS placed in a micro-solar CHP plant, obtained with a dynamic simulation tool to represent the system behavior during variable operating conditions.

The analysis performed is intended as a preliminary study to better understand the influence of the

input variables of the system on its outputs. This will simplify the planned future work of training the black box models on real measured data. Main conclusion of this work is that the HP-LHTESS shows a very different behavior with changing the season and it is particularly difficult to predict its behavior during winter, when the system works less hours and cannot be completely charged/discharged for lack of surplus of energy. Thus, a single model for the all year cannot mimic very well the output variables. Therefore, different models identified in different seasons must be used, or more complex models, as the RF model here proposed, need to be considered.

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