



Dynamic programming model for a thermal energy storage-based heat recovery system in a process industry plant[☆]

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ABSTRACT

Heat recovery systems (HRS) exist in conceptual configurations which encompass a set of energy-using processes installed on a particular site, a set of waste heat recovery technologies and all potential recirculation of material and energy streams with the overall aim to generate an overall benefit related to improvement in energy efficiency. A specific example of HRS are those that contain thermal energy storage (TES) components. In the context of the development of computational models, this type of HRS is modelled according to a dynamic simulation and optimisation perspective, owing to the transient state-based nature of these systems. This work presents the development and further analysis of an optimisation model developed according to the dynamic programming (DP) methodology for an HRS set to be implemented in a process industry plant. Such model was developed with the Modelica language, being an integral part of the ThermWatt simulation and optimisation tool. The developed model proved to be useful for the proposed objective of analysing transient state-based heat recovery systems, allowing an accurate modelling of the physical phenomena occurring during the time of operation of these systems. A relative reduction of 20.80% energy-related operational costs has been assessed for the system's optimal configuration, which corresponds to a 0.51 M€/year absolute reduction (from 2.38 M€/year to 1.87 M€/year). This work is set to compensate for a knowledge gap related to the inexistence of studies approaching the use of mathematical programming methods for the dynamic (transient state-oriented) optimisation of thermal energy storage-based heat integration systems.

1. Introduction

The principle of progress towards industrial sustainability is based on the reduction of resource consumption and the environmental impacts associated with the waste produced in plants [1]. In practice, the promotion of industrial sustainability may be performed by improving the overall use of water and energy [2,3], the application of renewable energy resources [4] and the application of waste-to-energy technologies [5].

The concept of circular economy has been emerging to transform waste into potential by-products, promoting reuse, recovery and recycling, in which the life cycles of the production chains are optimised [6]. In the limit, the application of several measures converges on the reuse of resources (either material or energy) within the same industrial site. Waste heat recovery (WHR) systems depend on the application of energy management principles when planning the installation of WHR technologies to recirculate streams with an associated waste heat potential so as to improve energy efficiency and so promote the circular economy associated with industrial systems [7–10]. For additional energy supply,

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| Nomenclature | |
|----------------------|--|
| AF | Air-to-fuel ratio (kg/kg) |
| C_p | Specific Heat Capacity (J/(°C.kg)) |
| d | Infinitesimal variation |
| Elec | Generated electricity (W) |
| h | Specific enthalpy (J/kg) |
| H | Absolute enthalpy (J) |
| Inv | Investment Costs (€) |
| k | Thermal conductivity (W/(m.kg)) |
| M | Mass (kg) |
| OBJ | Objective-function of the dynamic programming problem over unit of time (€/s) |
| OBJEff | Objective-function of the dynamic programming problem (€) |
| PB | Payback time (years) |
| Price | Unitary price (€/J) |
| r | Radius (m) |
| Sav | Economic Savings (€/year) |
| t | Time (s) |
| T | Temperature (°C) |
| <i>Greek letters</i> | |
| ρ | Density (kg/m ³) |
| τ | Temperature constant associated to phase change material microstructure (°C) |
| <i>Subscripts</i> | |
| Air | Air stream |
| Amb Air | Ambient air stream |
| app | Apparent |
| Baseline | Baseline case of a plant (a Water and Energy Integration System has yet to be implemented) |
| C.Air | Combustion Air Stream |
| Cond. | Condensation (phase change range) |
| Eff | Effective |
| Ex | Exhaust Gas Stream |
| Fuel | Inlet Fuel Stream in a Combustion-based process |
| gas | Heat source gas stream |
| in | Inlet |
| int | Internal |
| l | Phase change material liquid phase |
| mixed | Stream which has been mixed with others |
| out | Outlet |
| ORC | Organic Rankine Cycle unit |
| PCM | Phase change material |
| Rec Air | Recirculated hot air stream |
| s | Phase change material solid phase |
| split | Stream that has been divided |
| to –be –mixed | Stream which is set to be mixed with others |
| to –be –splitted | Stream which is set to be divided |
| <i>Superscripts</i> | |
| . | Time-dependent derivative |
| <i>Other symbols</i> | |
| d | Infinitesimal variation |
| exp | Exponential function |
| mean | Mean function |
| <i>Abbreviations</i> | |
| CFD | Computational fluid dynamics |
| DP | Dynamic programming |
| EU | European Union |
| GHG | Greenhouse gases |
| HRS | Heat recovery system |
| NLP | Non-linear programming |
| ORC | Organic Rankine Cycle |
| TES | Thermal energy storage |
| WEIS | Water and Energy Integration Systems |
| WHR | Waste heat recovery |

thermal energy storage (TES) may reveal a particularly attractive set of technologies, considering its potential to surpass limitations of WHR such as significant distance between the heat source and the heat sink, the lack of identification of existing heat sinks, operational disturbances and overall techno-economic viability associated with the implementation of these technologies [11,12].

Industrial sectors such as ceramics, chemicals, and steel remain highly energy-intensive, with significant potential for energy efficiency improvements through waste heat recovery. Recent studies emphasize that approximately 20–50% of industrial energy input is lost as waste heat [13], often at low to medium temperature levels, making its recovery crucial for decarbonization and cost reduction strategies. WHR technologies have evolved from conventional heat exchangers to advanced systems such as heat pipe heat exchangers, which demonstrate high efficiency in harsh industrial environments [14–20]. Parallel to WHR, thermal energy storage systems are increasingly deployed to balance energy supply and demand, stabilize industrial processes, and facilitate renewable integration. TES technologies are categorized into sensible heat storage (e.g., water, molten salts), latent heat storage using phase change materials (PCMs), and thermochemical storage based on reversible reactions [21–24].

In addition to the installation of real-life systems (through the implementation of technology-based energy efficiency improvement measures), the research on the thermal energy storage (TES) area has been subsisting on the development and further use of computational models. The existing studies have approached simulation modelling of

systems integrating TES units [25], the detailed simulation modelling of TES units (namely through the use of computational fluid dynamics (CFD) codes) [26] and parametric design-based optimisation [27]. On the side of process integration studies, there has been an effort to conjugate the commonly implemented graphical methods (namely those based on the implementation of the pinch analysis methodology) with the case of thermal energy storage and time-dependent energy supplies and demands, as well as the most complex existing paradigm of total site integration [28].

The intensive critical analysis of the overall content presented in the aforementioned works converges in the verification of the inexistence of studies oriented to the application of mathematical programming methods (in opposition to graphical methods) for the optimisation of heat recovery systems integrating thermal energy storage (with these systems being conceptualized on a previously adopted heat integration rationale). The transient state nature of these systems justifies the selection of dynamic programming (DP) as the MP methodology. In the case that the main objective for model development is the modelling of physical phenomena only (not being required the minimization of any cost-related function), dynamic simulation shall be the method used to model these types of systems. Such framework has been adopted by several authors, namely those that have been developing these types of computational models using MATLAB, Aspen Plus [29] and GAMS [30].

This work presents the development and further analysis of a dynamic programming (DP) model applied to a transient state-based heat recovery system (HRS) to be implemented in a process industry plant.

The model was developed with the Modelica language, namely using the *Built-in Dynamic Optimization using Annotations* method within OpenModelica. Such a model is an integral part of the ThermWatt simulation and optimisation tool (intellectual property of ISQ – Instituto de Soldadura e Qualidade) [31–44].

The approached DP model has been developed in an effort to expand the scope of previously developed simulation models for the same exact physical system, one encompassing a set of continuous and batch combustion-based processes, a thermal energy storage unit and, electricity generation unit (Organic Rankine cycle) and heat stream (exhaust gas and hot air) recirculation between each one of these unit operations. The DP model was developed owing to the inherent inability of the simulation model to find an optimal point of heat stream allocation, in which the energy-related operational costs of the whole plant are minimized. Such is able to create an integrated dynamic simulation and optimisation model, which has been overall developed to allow the implementation of a specific paradigm related to the conceptualization of highly complex physical systems encompassing a significant number of existing and newly installed unit operations in a site. Such complexity in terms of the quantity of considered operations is also significant of a complexity of considered physical phenomena, with such complexity in terms of overall paradigm having yet to be considered in terms of computational modelling, with the already developed modelling considering the detailed simulation and optimisation of TES units in a more local manner (essentially focused on the TES unit itself, although commonly considering the impact of surrounding unit operations connected to it through stream allocation [30]) or, rather, the optimisation modelling of similar systems not considering the implementation of a TES unit (which is the case of steady state-based heat recovery systems [34]). The approached modelling framework (overall created using the capacities of the ThermWatt computational tool) secures a high level of accuracy in terms of physical phenomena modelling (similar to the one achieved in models considering the simulation and optimisation of TES in a more local manner), while being able to integrate optimised results related to the heat stream allocation (in a similar manner to steady state-

based optimisation models created for standard heat recovery systems).

2. Characterization of the case-study

The conceptualization of the case-study focuses on the analysis of an overall transient mode of operation of the case-study plant, considering the implementation of the dynamic heat recovery system (HRS) configuration. Such a configuration is based on the installation of a phase change material (PCM)-based TES module, which is supplied with all the existing waste heat streams from the plant and from which the stored heat is then distributed to all the energy-using units. This case-study plant is inserted into a ceramic industry plant, constituted by a set of two combustion-based processes operating in a continuous mode (tunnel kilns) and another set of two processes operating in batch production (intermittent kilns).

The sequence of Figs. 1 and 2 presents the superstructure associated with the HRS described, as well as the data related to mass and enthalpy balances for the baseline scenario of the case-study. This superstructure is further characterized considering the following aspects:

- Each one of the two kilns is characterized by having two waste heat streams: exhaust gas and hot air.
- A fraction of the total hot air stream from each of the tunnel kilns is recirculated to the TES unit (instead of the exhaust gas stream).
- During the cooling cycle of the kilns, another fraction of the total hot air streams from each of the tunnel kilns is recirculated to the TES unit (instead of the exhaust gases).
- During the firing cycle of the kilns, the aforementioned quantity of hot air is recirculated to an Organic Rankine cycle (ORC) system (for electricity generation).
- The hot air streams from each of the two tunnel kilns are recirculated to the respective tunnel kiln and to the heat recovery steam generator (HRSG) unit of the ORC.
- The remaining quantities of the hot air streams from each of the two tunnel kilns are mixed and recirculated to compensate for energy

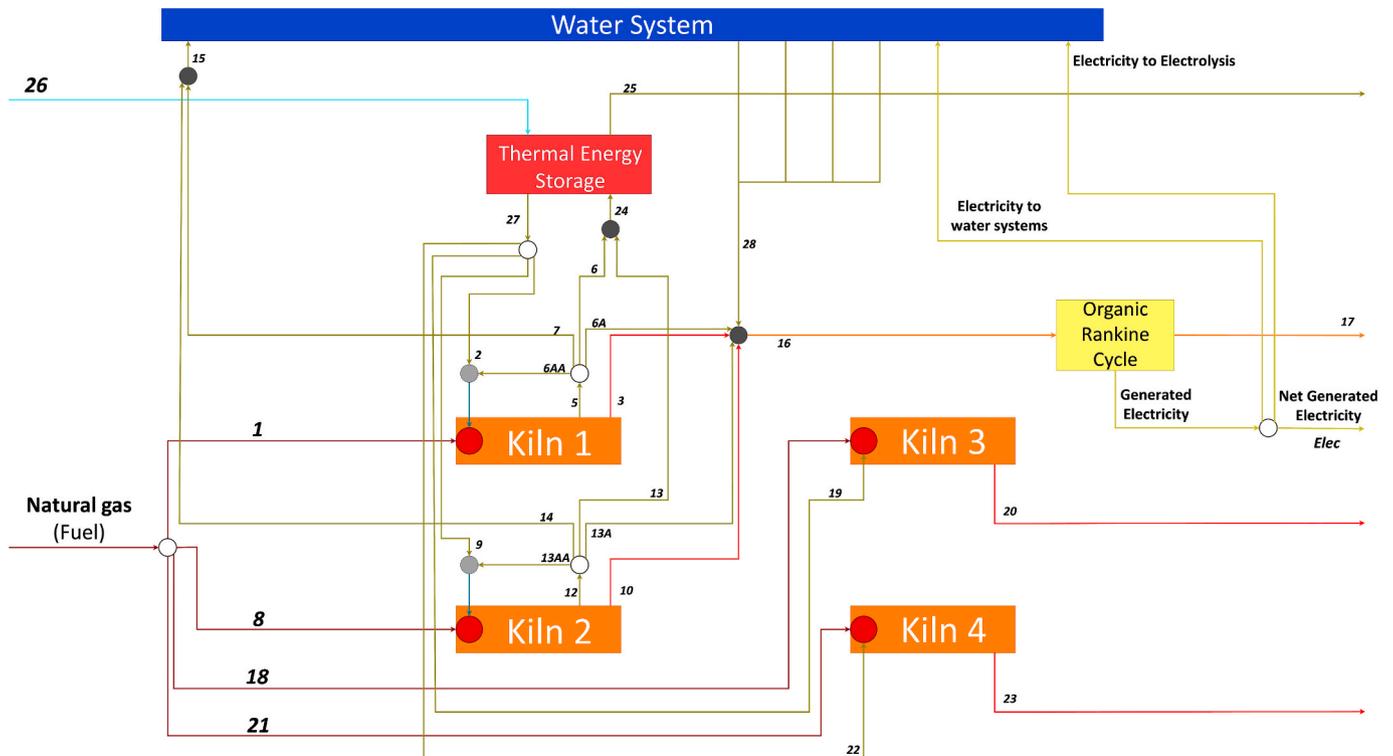
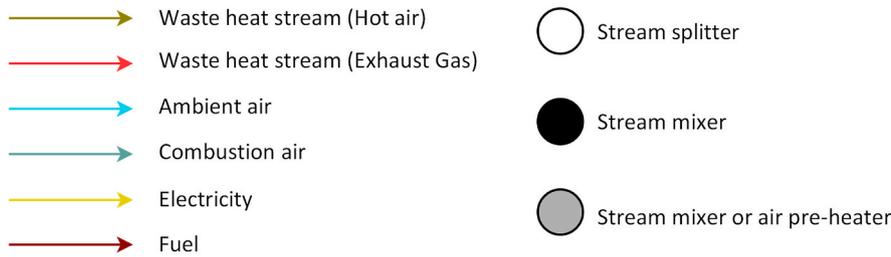


Fig. 1. Superstructure for the heat recovery system (HRS), in which the indexes in *Italic* are referent to either the material streams or specific variables of the optimisation model which have been defined to assist the definition of the decision variables within the model.

Legend



| Intermittent Kilns (Kilns 3 and 4) Data | | |
|---|-------------|------------------|
| Cooling Time | Firing Time | Total Cycle Time |
| 25.5 Hours | 16.5 Hours | 42.0 Hours |

| | Kiln 1 | | Kiln 2 | | Kiln 3 | | Kiln 4 | |
|------------------------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|
| Natural Gas Consumption (kg/cycle) | 5355.00 | | 5044.20 | | 334.29 | | 1266.05 | |
| Stream | Flow rate (kg/h) | Temperature (°C) |
| Inlet Streams | | | | | | | | |
| Natural Gas | 196.5 | 37.0 | 103.5 | 37.0 | 20.26 | 35.0 | 76.73 | 35.0 |
| Combustion Air | 16284.0 | 35.0 | 14351.0 | 35.0 | 7832.74 | 41.5 | 14629.3 | 41.5 |
| Cooling Air | 20711.7 | 35.0 | 23583.1 | 35.0 | | | | |
| Outlet Streams | | | | | | | | |
| Exhaust Gas | 16480.5 | 230.0 | 14454.5 | 159.3 | 7853.0 | 51.0 | 14706.0 | 127.1 |
| Cooling Air (Hot Air) | 20711.7 | 111.5 | 23583.1 | 196.5 | | | | |

Fig. 2. Legend associated to the superstructure for the heat recovery system (HRS) (Fig. 1) and data related to the baseline scenario).

demands associated with energy-using units installed in other parts of the plant (water systems).

- The hot air streams from the water system are further recirculated to be mixed with the conjoined exhaust gas streams, so then the mixed gas stream is recirculated to the ORC.

3. Formulation of the optimisation problem

The solution of the optimisation problem in question is based on the use of the dynamic programming (DP) methodology, which has been selected due to the transient requirements associated with the case-study (a set of variables characterizing the system are associated with appreciable variations during the operational time). The DP methodology has been selected from the set of the remaining optimisation methodologies that have been implemented to solve similar problems, according to a method of elimination:

- Conventional single-objective optimisation methodologies, such as linear programming, non-linear programming and their mixed-integer counterparts, are not applicable, since these are mostly steady state-oriented [34];
- Multi-objective programming (based on the use of genetic algorithms for the solving of optimisation problems) is not applicable, since it is mostly steady state-oriented and the conceptual objective of the work is not to obtain a set of optimal solutions for disaggregated cost minimization objectives [37];
- Model predictive control-based optimisation methodologies (although with proved applicability for transient state-oriented optimisation problems similar to the one approached in this work) have been set aside in favour of DP, owing to this primary applicability for local optimality (instead of global optimality, which is the scope of this work) [45].

The development and running of the developed DP model was proceeded through the use of the version 18.1 of OpenModelica software.

3.1. Definition of decision variables and constraints

In respect of the definition of decision variables, inequality constraints and equality constraints, the following aspects are considered:

- The decision variables are all the mass flow rates, temperatures/specific enthalpies that characterize each of the fuel, air and exhaust gas streams of the system.
- In respect of inequality constraints, the optimisation model in question has been created bearing in the mind the definition of these as the lower and upper bounds for each of the system variables.
- The equality constraints characterizing this model consist of mass balance, enthalpy balance and heat transfer equations that define the variations of each mass flow rate, specific enthalpy and temperature, in addition to the equations characterizing the storage of thermal energy within the PCM-TES unit (which must be elaborated as time-dependent equations, according to the specific requirements of this case study).

3.1.1. Definition of decision variables

In the sequence of Tables 1–6, all the variables which characterize the developed model are presented. The ones which have an associated fixed value (instead of associated start values, lower bounds and upper bounds) are in the context of the developed model considered parameters (which are constant during the 42.0 h simulation time). The numeric indexes associated to each variables in Tables 1, 3 and 4 are the same numeric indexes associated to each material stream presented in Fig. 1. (the indexes are set to allow an association between each variable

Table 1
Characterization of model variables (Mass flow rates, unit of kg/h).

| Parameters Variable | Fixed Value |
|---------------------|--|
| Ṁ 4 | 21622.10 |
| Ṁ 5 | 21622.10 |
| Ṁ 6AA | 5000.00 (Charge phase) 10000.00 (Discharge phase) |
| Ṁ 7 | 6141.24 |
| Ṁ 11 | 16528.40 |
| Ṁ 12 | 16528.40 |
| Ṁ 13AA | 5000.00 (Charge phase) 10000.00 (Discharge phase) |
| Ṁ 14 | 0.00 |
| Ṁ 28 | 6141.24 |

| Control Variables | | | |
|-------------------|-------------|-------------|-------------|
| Variable | Start Value | Lower Bound | Upper Bound |
| Ṁ 6 | 2000.00 | 0.00 | 21622.10 |
| Ṁ 13 | 5000.00 | 0.00 | 16528.40 |

| State Variables | | | |
|-----------------|-------------|-------------|-------------|
| Variable | Start Value | Lower Bound | Upper Bound |
| Ṁ 1 | 127.50 | 0.00 | 127.50 |
| Ṁ 2 | 24952.00 | 0.00 | 24952.00 |
| Ṁ 2A | 24952.00 | 0.00 | 24952.00 |
| Ṁ 3 | 25079.50 | 0.00 | 25079.50 |
| Ṁ 6A | 1000.00 | 0.00 | 21622.10 |
| Ṁ 8 | 120.10 | 0.00 | 120.10 |
| Ṁ 9 | 30736.00 | 0.00 | 30736.00 |
| Ṁ 9A | 30736.00 | 0.00 | 30736.00 |
| Ṁ 10 | 30856.10 | 0.00 | 30856.10 |
| Ṁ 13A | 1000.00 | 0.00 | 16528.40 |
| Ṁ 15 | 30856.10 | 0.00 | 30856.10 |
| Ṁ 16 | 94086.10 | 0.00 | 94086.10 |
| Ṁ 17 | 94086.10 | 0.00 | 94086.10 |
| Ṁ 18 | 20.26 | 0.00 | 20.26 |
| Ṁ 19 | 7832.74 | 0.00 | 7832.74 |
| Ṁ 20 | 7853.00 | 0.00 | 7853.00 |
| Ṁ 21 | 76.73 | 0.00 | 76.73 |
| Ṁ 22 | 14629.30 | 0.00 | 14629.30 |
| Ṁ 23 | 14706.00 | 0.00 | 14706.00 |
| Ṁ 24 | 30856.10 | 0.00 | 30856.10 |
| Ṁ 25 | 30856.10 | 0.00 | 30856.10 |
| Ṁ 26 | 78150.04 | 0.00 | 78150.04 |
| Ṁ 27 | 78150.04 | 0.00 | 78150.04 |

Table 2
Characterization of model variables (Air-to-fuel ratios, unit: kg Air/ kg Fuel).

| Parameters Variable | Significance | Fixed Value |
|---------------------|---|-------------|
| AF1 | Air-to-fuel ration associated to Kiln 1 | 195.70 |
| AF2 | Air-to-fuel ration associated to Kiln 2 | 255.92 |
| AF3 | Air-to-fuel ration associated to Kiln 3 | 386.61 |
| AF4 | Air-to-fuel ration associated to Kiln 4 | 190.66 |

and the stream these are associated to). The tables entries which are filled on correspond to undefined numeric values. In the sequence of tables, the Start values column mostly corresponds to initial guesses (in opposition to fixed initial conditions). Only for the OBJEff variable is defined a fixed start value, since it corresponds to the cumulative total operational costs in respect to the start of the analysis time.

3.1.2. Definition of constraints and state-transition equations

Table 7 presents the equality constraints (governing equations) characterizing the model, which include all the equations delineating

Table 3
Characterization of model variables (Temperatures, unit: °C).

| Parameters Variable | Fixed Value |
|---------------------|-------------|
| T1 | 34.0 |
| T4 | 41.5 |
| T5 | 111.5 |
| T6 | 111.5 |
| T6A | 111.5 |
| T6AA | 111.5 |
| T7 | 111.5 |
| T8 | 34.0 |
| T11 | 41.5 |
| T12 | 196.5 |
| T13 | 196.5 |
| T13A | 196.5 |
| T13AA | 196.5 |
| T14 | 196.5 |
| T18 | 35.0 |
| T20 | 59.1 |
| T21 | 35.0 |
| T23 | 127.1 |
| T26 | 41.5 |
| T28 | 84.53 |

| Control Variables | | | |
|-------------------|-------------|-------------|-------------|
| Variable | Start Value | Lower Bound | Upper Bound |
| T17 | 70.0 | 70.0 | 196.5 |

| State Variables | | | |
|-----------------|-------------|-------------|-------------|
| Variable | Start Value | Lower Bound | Upper Bound |
| T2 | 41.5 | 41.5 | 300.0 |
| T2A | 41.5 | 41.5 | 300.0 |
| T3 | 104.7 | 104.7 | |
| T9 | 41.5 | 41.5 | 300.0 |
| T9A | 41.5 | 41.5 | 300.0 |
| T10 | 84.2 | 84.2 | |
| T15 | 196.5 | 111.5 | 196.5 |
| T16 | 196.5 | 84.2 | 196.5 |
| T19 | 41.5 | 41.5 | 300.0 |
| T22 | 41.5 | 41.5 | 300.0 |
| T24 | 196.5 | 111.5 | 196.5 |
| T25 | 41.5 | 41.5 | 196.5 |
| T27 | 41.5 | 41.5 | 196.5 |

the occurring physical phenomena encompassing mass balance, enthalpy balance and reaction-based equations. The mentioned equations are presented in a more generic form (not being enunciated in the exact same form these are enunciated on the actual Modelica code constituting the optimisation model), to avoid the delineation of the same equation for different cases (such as different stream splitting and mixing phenomena occurrences, which are characterized by the same equations for all cases). Table 8 presents the most fundamental aspects in respect of the definition of inequality/ equality constraints.

3.1.3. Description of the detailed model for PCM-based heat exchanger units

The set of equations presented in Table 7 describing the PCM-based heat exchanger unit fundamentally consist in a reduced model of such unit, delineated for the context of the presented dynamic programming model. This DP model has been developed in its turn to handle the optimisation procedure required to assess a level of minimised energy use in the approached heat recovery system (HRS). In general, such procedure is set to complement the scope of a previously developed simulation model for the same physical system of the HRS, in which all the physical phenomena associated to the system is set to be modelled with the highest possible accuracy. In this sense, it is developed a modelling framework which encompasses a final model allowing a highly accurate modelling of physical phenomena (which is the fundamental aim of the initially developed simulation model), while securing

Table 4
Characterization of model variables (Specific enthalpies, unit: kJ/kg).

| Parameters | |
|------------|-------------|
| Variable | Fixed Value |
| h1 | 0.00 |
| h4 | 309.55 |
| h5 | 384.45 |
| h6 | 384.45 |
| h6A | 384.45 |
| h6AA | 384.45 |
| h7 | 384.45 |
| h8 | 0.00 |
| h11 | 309.55 |
| h12 | 475.40 |
| h13 | 475.40 |
| h13A | 475.40 |
| h13AA | 475.40 |
| h14 | 475.40 |
| h18 | 0.00 |
| h20 | 328.38 |
| h21 | 0.00 |
| h23 | 401.14 |
| h26 | 309.55 |
| h28 | 355.59 |

| State Variables | | | |
|-----------------|-------------|-------------|-------------|
| Variable | Start Value | Lower Bound | Upper Bound |
| h2 | 309.55 | 309.55 | 586.15 |
| h2A | 309.55 | 309.55 | 586.15 |
| h3 | 377.17 | 377.17 | |
| h9 | 309.55 | 309.55 | 586.15 |
| h9A | 309.55 | 309.55 | 586.15 |
| h10 | 355.24 | 355.24 | |
| h15 | 475.40 | 384.45 | 475.40 |
| h16 | 475.40 | 355.24 | 475.40 |
| h17 | 340.05 | 340.05 | 475.40 |
| h19 | 309.55 | 309.55 | 586.15 |
| h22 | 309.55 | 309.55 | 586.15 |
| h24 | 475.40 | 384.45 | 475.40 |
| h25 | 309.55 | 309.55 | 475.40 |
| h27 | 309.55 | 309.55 | 475.40 |

Table 5
Characterization of model variables (Thermal energy storage component).

| Parameters | | | |
|------------|-----------------------------|------|-------------|
| Variable | Significance | Unit | Fixed Value |
| L | Height of the TES unit | m | 10 |
| rint | Internal radius of TES unit | m | 0.10 |
| rext | External radius of TES unit | m | 0.12 |

| State Variables | | | | | |
|---|--|------|-------------|-------------|-------------|
| (Primary ones, in which start values, lower and upper bounds are defined) | | | | | |
| Variable | Significance | Unit | Start Value | Lower Bound | Upper Bound |
| TPCM | PCM Temperature | °C | 41.5 | 41.5 | 196.5 |
| TPCM1 | Temperature at the point more proximate to the heat source | °C | 196.5 | 41.5 | 196.5 |
| TPCMN | Temperature at the point more proximate to the walls of the TES unit | °C | 196.5 | 41.5 | 196.5 |

| State Variables | | |
|---|----------------------------|-----------|
| (Secondary ones, in which start values, lower and upper bounds are not necessary to be defined) | | |
| Variable | Significance | Unit |
| MPCM | PCM Mass | kg |
| CPCM | PCM specific heat capacity | J/(°C.kg) |

Table 6
Characterization of model variables (Energy inputs/ outputs and objective-function variables).

| Parameters | | |
|---------------|------|-------------|
| Variable | Unit | Fixed Value |
| Elec | kW | 0.657 |
| ORCEfficiency | % | 4.22 |

| State Variables | | |
|---|------|-------------|
| (Primary ones, in which start values, lower and upper bounds are defined) | | |
| Variable | Unit | Start Value |
| OBJEff | € | 0.00 |

| State Variables | | |
|---|------|--|
| (Secondary ones, in which start values, lower and upper bounds are not necessary to be defined) | | |
| Variable | Unit | |
| OBJ | €/s | |

the consideration of the operational scenario associated to a minimised level of energy use (which is obtained by the running of the counterpart optimisation model and the subsequent allocation of the numerical results obtained for each corresponding variable to the simulation model).

The system-level simulation model for the HRS includes an equipment-level model for the PCM-based heat exchanger, which corresponds to the detailed model from which the reduced model (created for the context of the DP system-level model) is based on. In Table 9, the generalist governing equations describing the detailed model for the PCM-based heat exchanger unit are presented. The adaptation of the generalist equations to the conditions of the presented case-study (considering the properties assumed for the selected PCM) are presented in Table 10.

3.2. Definition of the Objective-Function

While the decision variables and constraints of the developed optimisation model are formulated considering all the variables that characterize the streams and the mass balance, enthalpy balance and heat transfer equations, the objective-function is formulated on the basis of the minimization of operational costs (the total costs associated with energy use from start to finish of the time of analysis). Such minimization procedure must consider the transient state nature of the occurring phenomena, in which the variables characterizing the optimisation model (and in consequence the energy-related operational costs in a determinate instant of time) present significant variations across the whole analysis time. In this sense, the defined objective-function must be enunciated based on the following procedures typically adopted for dynamic programming:

- Minimization of operational costs for each period of time (Lagrange Term).
- Minimization of operational costs by the final time (Mayer Term).

The adoption of one or the other method leads to similar results, as these are enunciated with the objective of ensuring that the total operational costs by the finishing time (given in absolute € units) are the least possible. In a similar manner to the previously developed models, the following procedure was taken based on the aforementioned reference unitary prices for the industrial sector. The objective-function formulated for the present optimisation problem is presented in Table 11 (in which equation (40) is a form of equation (37) obtained through the application of the premises of equations (38) and (39)). The aforementioned second method (using the Mayer Term) was used for the described purpose (minimization of the total operational costs by the final time of the analysis).

Table 7

Equality constraints of the optimisation model (most general enunciation).

| General Equations | |
|--|---|
| Stream Splitting | $\dot{M}_{\text{to-be-split}} = \sum_{i=1} \dot{M}_{\text{split},i}$ (1) |
| | $h_{\text{to-be-split}} = h_{\text{split},i}$ (2) |
| Stream Mixing | $\sum_{i=1} \dot{M}_{\text{to-be-mixed},i} = \dot{M}_{\text{mixed}}$ (3) |
| | $\sum_{i=1} (\dot{M} \cdot h)_{\text{to-be-mixed},i} = (\dot{M} \cdot h)_{\text{mixed}}$ (4) |
| | $h = 1070.00 \cdot T + 265145.40$ (5) |
| Temperature – Specific Enthalpy relation for Air/ Exhaust Gas | |
| Thermal Process System (Stream Recirculation) | |
| | $\dot{M}_{\text{Fuel,Baseline}} \cdot \text{LHV}_{\text{Fuel}}(T_{\text{Fuel,in}}) = \dot{M}_{\text{Fuel}} \cdot \text{LHV}_{\text{Fuel}}(T_{\text{Fuel,in}}) + \dot{M}_{\text{C,Air}} \cdot (h_{\text{C,Air}} - h_{\text{C,Air,Baseline}})$ (6) |
| | $\dot{M}_{\text{C,Air}} = \dot{M}_{\text{Rec,Air}} + \dot{M}_{\text{Amb,Air}}$ (7) |
| | $\dot{M}_{\text{C,Air}} \cdot h_{\text{C,Air}} = \dot{M}_{\text{Rec,Air}} \cdot h_{\text{Rec,Air}} + \dot{M}_{\text{Amb,Air}} \cdot h_{\text{Amb,Air}}$ (8) |
| | $\dot{M}_{\text{Fuel}} + \dot{M}_{\text{C,Air}} = \dot{M}_{\text{Ex}}$ (9) |
| | $\dot{M}_{\text{Fuel}} \cdot \text{AF} = \dot{M}_{\text{Comb,Air}}$ (10) |
| | $\dot{M}_{\text{gas,in,ORC}} \cdot (h_{\text{gas,in,ORC}} - h_{\text{gas,out,ORC}}) \cdot 0.0422 = \text{Elec} \bullet 3600$ (11) |
| Thermal Energy Storage-Related | |
| Charge Phase | |
| | $\frac{dT_{\text{PCM}}}{dt} = \frac{0.15}{890 \cdot C_{\text{PCM}}} \frac{1}{(r_{\text{ext}} + r_{\text{int}}) \cdot 0.5} \left(\frac{(T_{\text{PCM,N}} - T_{\text{PCM,1}})}{r_{\text{ext}} - r_{\text{int}}} + \frac{(T_{\text{PCM,N}} - 2 \cdot T_{\text{PCM}} + T_{\text{PCM,1}})}{(r_{\text{ext}} - r_{\text{int}})^2} \right)$ (12) |
| Discharge Phase | $\frac{dT_{\text{PCM}}}{dt} = \frac{0.15}{890 \cdot C_{\text{PCM}}} \frac{1}{(r_{\text{ext}} + r_{\text{int}}) \cdot 0.5} \left(\frac{(T_{\text{PCM,1}} - T_{\text{PCM,N}})}{r_{\text{ext}} - r_{\text{int}}} + \frac{(T_{\text{PCM,1}} - 2 \cdot T_{\text{PCM}} + T_{\text{PCM,N}})}{(r_{\text{ext}} - r_{\text{int}})^2} \right)$ (13) |
| | $C_{\text{PCM}} = \frac{225000}{(2 \cdot 3.1416)^{0.5} \cdot 0.1626} \exp\left(\frac{-(T_{\text{PCM}} - 72)^2}{2 \cdot 0.1626^2}\right) + 2200$ (14) |

Table 8

Relevant aspects for the definition of inequality and equality constraints.

| Inequality Constraints | | |
|--|-------------------|---|
| (Relevant aspects for the definition) | | |
| <ul style="list-style-type: none"> The generated electricity was defined as the output from the ORC already discounting electricity consumption in the ORC pump but not the electricity that is used for the operation of the MED unit, so a lower limit has been defined representing the latter (0.657 kW); The initial value for the PCM temperature has been defined as the temperature of the inlet ambient air in the kilns (41.5 °C). | | |
| Equality Constraints | | |
| (Characterization of considered constants) | | |
| Constant | Unit | Characterization |
| 0.0422 | | Thermal-to-electric conversion efficiency associated with the Organic Rankine cycle (ORC) |
| 3600 | kJ/kWh | Factor of conversion of kWh to kJ energy units |
| 0.15 | W/(m.°C) | Thermal conductivity of the PCM considered |
| 890 | kg/m ³ | Density of the PCM considered |
| 225000 | J/kg | Latent enthalpy associated with the melting/ solidification of PCM (as required as a parameter in the apparent specific heat capacity equation) |
| 3.1416 | | Approximation of pi |
| 0.1626 | °C | Temperature constant for the PCM microstructure |
| 72 | °C | Lower bound for the temperature range of the melting/ solidification phase of the PCM |
| 2200 | J/(°C.kg) | Specific heat capacity for the solid phase of the PCM |

3.3. Formal formulation of the optimisation problem

The formulation of the approached optimisation problem in formal terms is presented in equation (42).

$$\begin{aligned} \text{Min. } Z &= \left(\int_{t_0}^{t_f} L(x(t), u(t), t) dt \right), L(x(t), u(t), t) \\ &= \left(23.66 \cdot 0.0453 \cdot \frac{1}{3600} \cdot \dot{M}_{\text{Fuel}}(t) - 0.1459 \cdot \frac{1}{3600} \cdot \text{Elec}_{\text{Eff}}(t) \right) \end{aligned}$$

$$\text{s.t. : } 0 = f(x(t), \dot{x}(t), u(t), t)$$

$$0 \leq g(x(t), u(t), t) \quad (42)$$

Attending to the specific notation used in equation (42), it is to the following association to the sequence of tables presented in section 3.1:

- The $u(t)$ terms correspond to the vector of variables identified as **Control Variables** in the sequence of Tables 1 – 6, which are only three variables in this case (\dot{M} 6, \dot{M} 13 and T_{17});
- The $x(t)$ terms correspond to the vector of variables identified as **State Variables** in the sequence of Tables 1 – 6;
- The $\dot{x}(t)$ terms correspond to the vector of variables which result as time derivatives from a set of **State Variables** identified in the sequence of Tables 1 – 6, which in this case it is only the $\frac{dT_{\text{PCM}}}{dt}$ term delineated in equation (12) on Table 7;
- The $f(t)$ terms correspond to the sequence of equality constraints presented in Table 7;
- The $g(t)$ terms correspond to the considered inequality constraints, which may be formulated in the following general forms (considering the formal notation of state variables):
 - o $x(t) - LB \geq 0$ in the case of lower bounds (LB);
 - o $UB - x(t) \geq 0$ in the case of upper bounds (UB).

3.4. Model validation

The validation procedure shall subsist on the comparison of modelling results with corresponding theoretical data. In the scope of the present work, both the model for the PCM-based heat exchanger unit and the model for the Organic Rankine cycle (ORC) unit are set to be validated. As mentioned in section 3.1.3, the set of variables and equations describing the physical phenomena within each one of these units subsist in reduced models obtained from adaptation of counterpart detailed models (encompassed in system-level simulation models for the same heat recovery systems considered in the dynamic programming model developed in this work). Since the optimisation results are set to be ultimately integrated in a final model (from which the modelling results are set to be ultimately analysed and assessed), the approached validation procedure has been performed by taking as a basis the detailed models from each one of these units. For the purpose of the model validation procedure, a set of test-models for each one of the units of interest (the PCM-TES unit and the ORC) have been created, with the aim to allow the comparison of simulated results with pre-defined theoretical results.

Table 9
Generalist governing equations describing the detailed PCM-based heat exchanger unit model.

| | | |
|---|--|------|
| PCM Side (General) | $\frac{k_{ij}}{\rho_{ij} \cdot C_{p,ij}} \cdot \left(\frac{1}{r_{ij}} \left(\frac{T_{ij+1} - T_{ij-1}}{r_{ij+1} - r_{ij-1}} \right) + \left(\frac{T_{ij+1} - 2 \cdot T_{ij} + T_{ij-1}}{(r_{ij+1} - r_{ij-1})^2} \right) \right) = \frac{dT}{dt_{ij}}$ | (15) |
| Boundary Conditions (Charge Phase) | $T_{i,1} = \text{mean}(T_{gas_i}, T_{gas_{i+1}})$ | (16) |
| Boundary Conditions (Discharge Phase) | $T_{i,N} = \text{mean}(T_{gas_i}, T_{gas_{i+1}})$ | (17) |
| PCM Side (Solid Phase) | $C_{p,app,ij} = C_{p,s}$ | (18) |
| | $k_{ij} = k_s$ | (19) |
| | $\rho_{ij} = \rho_s$ | (20) |
| PCM Side (Phase Change) | $C_{p,app,ij} = \frac{\Delta h_{Cond}}{(2 \cdot \pi)^{0.5} \cdot \tau} \exp\left(\frac{-(T_{ij} - T_s)^2}{2 \cdot \tau^2}\right) + C_{p,s} + (C_{p,l} - C_{p,s}) \cdot 0.5 \cdot \left(1 + \left(\frac{-1 + \frac{2}{1 + \exp\left(-2.5 \cdot \left(\frac{T_{ij} - T_s}{\sqrt{2} \cdot \tau}\right)\right)}}{1 + \exp\left(-2.5 \cdot \left(\frac{T_{ij} - T_s}{\sqrt{2} \cdot \tau}\right)\right)} \right) \right)$ | (21) |
| | $k_{ij} = k_s + (k_l - k_s) \cdot 0.5 \cdot \left(1 + \left(\frac{-1 + \frac{2}{1 + \exp\left(-2.5 \cdot \left(\frac{T_{ij} - T_s}{\sqrt{2} \cdot \tau}\right)\right)}}{1 + \exp\left(-2.5 \cdot \left(\frac{T_{ij} - T_s}{\sqrt{2} \cdot \tau}\right)\right)} \right) \right)$ | (22) |
| | $\rho_{ij} = \rho_s + (\rho_l - \rho_s) \cdot 0.5 \cdot \left(1 + \left(\frac{-1 + \frac{2}{1 + \exp\left(-2.5 \cdot \left(\frac{T_{ij} - T_s}{\sqrt{2} \cdot \tau}\right)\right)}}{1 + \exp\left(-2.5 \cdot \left(\frac{T_{ij} - T_s}{\sqrt{2} \cdot \tau}\right)\right)} \right) \right)$ | (23) |
| PCM Side (Liquid Phase) | $C_{p,app,ij} = C_{p,l}$ | (24) |
| | $k_{ij} = k_l$ | (25) |
| | $\rho_{ij} = \rho_l$ | (26) |
| Heat Source/ Sink Side | $\dot{M}_{gas_i} = \dot{M}_{gas_{i+1}}$ | (27) |
| | $q_{Gas_i} = \dot{M}_{gas_i} \cdot (h_{gas_i} - h_{gas_{i+1}})$ | (28) |

Table 10
Governing equations describing the detailed PCM-based heat exchanger unit model (adapted for the presented case-study).

| | | |
|---|---|------|
| PCM Side (General) | $\frac{k_{ij}}{\rho_{ij} \cdot C_{p,ij}} \cdot \left(\frac{1}{r_{ij}} \left(\frac{T_{ij+1} - T_{ij-1}}{r_{ij+1} - r_{ij-1}} \right) + \left(\frac{T_{ij+1} - 2 \cdot T_{ij} + T_{ij-1}}{(r_{ij+1} - r_{ij-1})^2} \right) \right) = \frac{dT}{dt_{ij}}$ | (29) |
| Boundary Conditions (Charge Phase) | $T_{i,1} = \text{mean}(T_{gas_i}, T_{gas_{i+1}})$ | (30) |
| Boundary Conditions (Discharge Phase) | $T_{i,N} = \text{mean}(T_{gas_i}, T_{gas_{i+1}})$ | (31) |
| PCM Side (Solid Phase) | $C_{p,app,ij} = 2200$ | (32) |
| PCM Side (Phase Change) | $C_{p,app,ij} = \frac{225000}{(2 \cdot 3.1416)^{0.5} \cdot 0.1626} \exp\left(\frac{-(T_{ij} - 72)^2}{2 \cdot 0.1626^2}\right) + 2200$ | (33) |
| PCM Side (Liquid Phase) | $C_{p,app,ij} = 2200$ | (34) |
| Heat Source/ Sink Side | $\dot{M}_{gas_i} = \dot{M}_{gas_{i+1}}$ | (35) |
| | $q_{Gas_i} = \dot{M}_{gas_i} \cdot (h_{Gas_i} - h_{Gas_{i+1}})$ | (36) |

Table 11
Enunciation of the objective-function.

| | | |
|---------------------------|---|------|
| Objective-function | $OBJ = \left((23.66(\text{€}/\text{GJ}) \cdot 0.0453(\text{GJ}/\text{kg}) \cdot \dot{M}_{Fuel}(\text{kg}/\text{h}) - 0.1459(\text{€}/\text{kWh}) \cdot \text{Elec}_{Eff}(\text{kWh}/\text{h})) \cdot \frac{1}{3600}(\text{h}/\text{s}) \right) (\text{€}/\text{s})$ | (37) |
| | $OBJ(\text{€}/\text{s}) = \left(\frac{d}{dt}(\text{OBJEff}(\text{€})) \right) (\text{€}/\text{s})$ | (38) |
| | $\text{OBJEff}(t = 0 \text{ s}) = 0 \text{ €}$ | (39) |
| | $\text{OBJEff}(\text{€}) = \left(\int_{t=0s}^{t=151200s} \left((23.66(\text{€}/\text{GJ}) \cdot 0.0453(\text{GJ}/\text{kg}) \cdot \dot{M}_{Fuel}(\text{kg}/\text{h}) - 0.1459(\text{€}/\text{kWh}) \cdot \text{Elec}_{Eff}(\text{kWh}/\text{h})) \cdot \frac{1}{3600}(\text{h}/\text{s}) \right) dt \right) (\text{€})$ | (40) |
| Objective-function | $\min(\text{OBJEff}(t = 151200 \text{ s})) (\text{€})$ | (41) |

3.4.1. Validation of the PCM-based heat exchanger model

The following variables were set as key variables to be analysed in the validation procedure:

- Temperature of PCM (along with time) for the enthalpy charge (supply of the heat source stream);
- Temperature of PCM (along with time) for the enthalpy discharge (supply of heat sink stream).

For the purpose of the validation of two different phenomena

associated to thermal energy storage (enthalpy charge and discharge), two different simulations were proceeded using the same test model:

- One for the charge phase (attribution of values for the heat source stream);
- Other for the discharge phase (attribution of values for the heat sink stream).

The obtained relative deviations associated to two simulations are presented in Table 12. The theoretical and simulation time-varying

plots for the PCM temperature during the charge phase are presented in Fig. 3. In Table 13, the comparison of real and simulated values in terms of the determination of relative deviation to the PCM-based heat exchanger model is presented.

As may be verified by the analysis of Fig. 3– a), the profiles corresponding to literature and simulation results effectively for the enthalpy charge phase generally present the same tendency in terms of temperature variation. Nonetheless, it is possible to observe slight differences in terms of temperature variation in determinate sets of simulation time intervals, which may be effectively verified by two intersections points between both temperature profiles. Such deviation is more pronounced on the simulation points in which the temperature is more proximate to the phase change interval (41 – 55 °C). In this prospect, such occurrence may be attributed to the use of different methods for the computation of the PCM temperature between the corresponding literature model and the model developed for this work.

In relation to the temperature profiles obtained for the enthalpy discharge phase, it is possible to appoint similar verifications for this simulation based on the analysis of Fig. 3 – b). Two intersections points between the literature and simulations temperature profiles are visible and the most significant deviations are obtained for simulation points in which the temperature is more proximate to the phase change interval.

Taking into account the obtained mean deviation values between the temperature profiles of literature and the performed simulations (which in terms of accuracy assessment may be considered acceptable values), it may be affirmed that the literature and simulation temperature profiles for both simulations are consistent and the model is valid, and thus set to be integrated in system-level simulation.

3.4.2. Validation of the Organic Rankine cycle (ORC) model

The Organic Rankine Cycle (ORC) model is roughly a system-level model considering the assembly of several component models. For the effects of the performance of the validation procedure, the ORC model will be assessed as an integrate (the system-level model as a whole and not each one of the components). Such procedure is taken since this model is also set to be included in the integrate within the system-level models of each one of the case-studies. The following variables were set as key variables to be analysed in the validation procedure:

- Temperature of the water stream at the inlet of the condenser;
- Temperature of the water stream at the outlet of the condenser;
- Power consumption associated to the main cycle pump;
- Generated electricity (in the generator connected to the turbine).

A test model was developed for the purpose of the validation of the developed ORC model. In Table 14, the comparison of real and simulated values in terms of the determination of relative deviation to the ORC model is presented.

As may be verified by the analysis of Table 14, the obtained deviation values are considerably low. All the key parameters (in the exception of the Temperature of the Water Stream at the Outlet of the Condenser) present deviation lower than 1%, which are highly acceptable. As for the parameter identified as an exception, such considerably higher deviation may be attributed to the determination of the heat duty to be inputted to the cooling tower. Such heat duty value corresponds to the

Table 12
Setup values for stream parameters.

| Phase | Stream | Mass Flow Rate (kg/h) | Inlet Temperature (°C) | Initial PCM Temperature (°C) |
|-----------|--------------------|-----------------------|------------------------|------------------------------|
| Charge | Heat Source Stream | 10.80 | 90.00 | 35.00 |
| Discharge | Heat Sink Stream | 10.80 | 30.00 | 60.00 |

total enthalpy allocated from the organic fluid stream circulating in the main cycle to the water stream within the cooling water cycle, for the purpose of maintaining the enthalpy balance within the water cycle assuming the inexistence of heat losses. In its turn, this heat duty is influenced by the condensation enthalpy associated to the organic fluid (which in turn depends on the specific enthalpies of saturated liquid and saturated steam, considered as constants within the definition of the medium package) and the enthalpy associated to the temperature decrease from the inlet temperature to the boiling point temperature (52.00 °C). While the vaporization enthalpy is considered as a constant by model definition, the second term depends on the outlet temperature from the regenerator. In this sense, the verified difference in relation to the heat duty (and, as such, the water temperature) may be attributed either to a difference in terms of the considered vaporization enthalpy or the definition of the values attributed to the parameters associated to the regenerator that permit the output of a temperature of the corresponding hot stream (the organic fluid in the gas phase) of 70.40 °C. Taking into account these considerations, and at the light of the obtained simulated value, such deviation may be considered overall acceptable.

Taking into account the presented results, the ORC model may be considered valid and as such apt to be used in system-level models.

4. Optimisation results

The results obtained by running the dynamic optimisation model must be analysed considering the variation of each variable of interest vary with time. For the approached case, the variables of interest to be analysed are the mass flow rates and temperatures/ specific enthalpies that characterize each of the system streams (in this case these are only gas streams), as well as the temperature of the PCM within the TES unit (PCM-based heat exchanger) must also be analysed.

4.1. Sensitivity analysis

The developed DP model has been submitted to a sensitivity analysis, with the objective to assess the robustness of the model in obtaining optimal results. For the performance of this sensitivity analysis, and one-at-a-time (OAT) procedure has been used. This OAT procedure is performed in a sequential manner, in which the performed variations on the model parameters (designated as adjustments) are set to supplant the previous set of results obtained by the running of the optimisation models or not attending to a determinate criterion (namely more favourable results in terms of the minimization of a relevant parcel of energy use or the minimization of total operational costs).

The handling of this procedure was based on the variation of the following categories of parameters (designated as adjustments):

- The start values for the mass flow rate of the hot air allocated from the kilns to the TES unit;
- The mass flow rate of the hot air recirculated as preheated combustion air in each of the kilns;
- The thermal-to-electric conversion efficiency associated with the ORC.

While the described sensitivity analysis has been performed with the primary aim to evaluate the robustness of the developed dynamic programming model, the afore described sequential approach has been adopted to ensure that the results obtained from the running of the optimisation model are the ones corresponding to a minimum level of fuel consumption in the four approached kilns and a maximum level of net electricity generation. As such, two different sets of optimisation results are set to be primarily considered: the results before sensitivity analysis and the results after sensitivity analysis. The last results are the ones set to be allocated to the counterpart simulation model to integrate the final model (primarily those associated to stream allocation, this is, mass flow rate-based variables), as mentioned in sections 3.1.3 and 3.4.

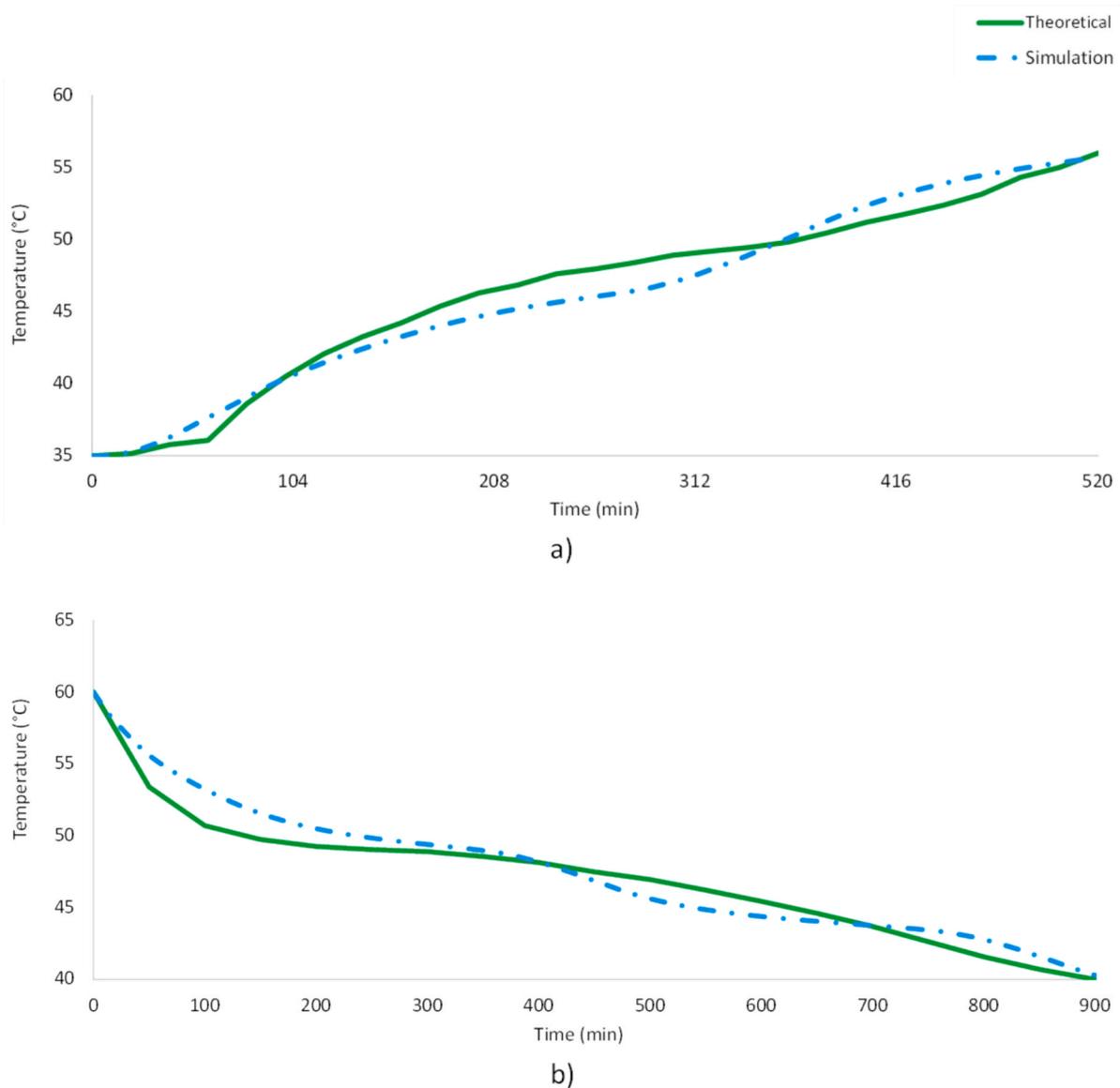


Fig. 3. Comparison of profiles for the inside PCM temperature between literature and simulation for a) the enthalpy charge phase, b) enthalpy discharge phase.

Table 13
Relative deviation obtained for the Charge and Discharge phase models.

| Phase | Relative Deviation |
|-----------|--------------------|
| Charge | 2.16% |
| Discharge | 2.12% |

Table 14
Determination of the deviation associated to key variables characterizing the ORC model.

| Variable | Real Value | Simulated Value | Relative Deviation |
|---|------------|-----------------|--------------------|
| Temperature of the Water Stream at the Inlet of the Condenser (°C) | 44.00 | 43.97 | 0.07% |
| Temperature of the Water Stream at the Outlet of the Condenser (°C) | 54.00 | 55.08 | 2.00% |
| Power Consumption associated to the main cycle pump (kW) | 16.00 | 15.85 | 0.94% |
| Generated Electricity (kW) | 99.80 | 98.97 | 0.83% |

In respect to the selected categories of parameters to constitute the set of adjustments considered in this work, it is to note that only the first category (start values for hot air mass flow rates) is the one set to serve for the performance of a more formal sensitivity analysis, in which it is performed the evaluation of the impact of the variation of model inputs on the uncertainty relative to outputs (and such evaluation is set to in its turn contribute to the assessment of the robustness of the model). The two other categories of parameters, while associated to a determinate input–output uncertainty, serve essentially to perform a more manual tuning of the model. In respect to each one of the mentioned two categories:

- The mass flow rates of the hot air recirculated as preheated combustion air in each of the kilns are set to be varied to verify that total operational costs are reduced by the increase of hot air allocation to the tunnel kilns (kilns 1 and 2), which in its turn cause the reduction of fuel consumption on these kilns. In the case this occurrence is verified, the results obtained by adjustment are considered, instead of the results before the adjustment. Such variation has been performed primarily to compensate for the option taken in model development to define these mass flow rates as parameters instead of

variables (an option which in its turn had to be taken to make possible that the number of variables in the model was equal to the number of states);

- The thermal-to-electric conversion efficiency associated with the ORC is set to be varied to verify the appreciable impact on energy use-related variables which are in principle not directly impacted by such variation (fuel consumption in kilns), and also to ensure that the net electricity generation in the final model is higher than the one obtained by the optimisation model (so to ensure that the final set of results correspond to the one with the highest possible minimization of energy use-related operational costs).

The performed variations on the model parameters and the respective results are presented in Table 15 and Table 16, respectively. The sequence associated to the performed adjustments (including the sequential supplantation of sets of optimisation results) is pictorially presented in Fig. 4.

In respect to formal sensitivity analysis-related adjustments, it is possible to perform the following affirmations:

- In respect to the adjustments performed to the start values for the mass flow rate of hot air recirculated as combustion air in kiln 1 (those within the overall adjustment 1), it is possible to verify that significant relative variations in relation to the initially considered value (either significant decreases or increases) do not have a considerable impact on the final results, based on the analysis of the considered energy-related indicators (fuel consumption and net electricity generation) and total operational costs;
- In respect to the adjustments performed to the start values for the mass flow rate of hot air recirculated as combustion air in kiln 2 (those within the overall adjustment 2), it is possible to verify the inexistence of significant variations for decreases in relation to the initially considered values (negative relative variations, as it is the case of adjustments 2.1 and 2.2);
- For the case of increases in relation to the initially considered values (positive relative variations, as it is the case of adjustments 2.3), it is possible to verify slight decreases of fuel consumption for all the kilns in relation to the initial optimisation values and the other sets of results obtained by the performance of adjustments, as well as the decrease of net electricity generation, for a relatively low relative variation of 2.00%. The combination of these two occurrences results in the relative decrease of total operational costs, which is significant that the effect of the decrease of fuel consumption is more prevalent in relation to the effect of the decrease of net electricity generation;
- By comparing the results obtained in adjustment 2.3 with subsequent adjustments based on this same adjustment, namely adjustments 3, it is possible to verify that the fuel consumptions for the kilns other than kiln 1 (which is the one to which the adjustment is set to decrease fuel consumption) are maintained in similar levels in relation to initial optimisation values and adjustments 1, 2.1 and 2.2. The net electricity generation is considerably decreased, which may be attributed to the allocation of a relative higher quantity of hot air to cause fuel savings in kiln 1 instead to production of electricity in the ORC;
- The verification of the maintenance of the same levels of fuel consumption in kilns 2, 3 and 4 for the same start value for the variable \dot{M}_{13} in adjustment 3 allows the interpretation of the results obtained in adjustment 2.3 as a punctual disparity of the final obtained results, rather than an occurrence that significantly impacts the verification of the robustness of the developed model;
- Considering all the aforementioned affirmations performed in the context of the formal sensitivity analysis, it is possible to affirm that the developed dynamic programming model is robust, and it is able to attain a considerable global optimum for the design configuration

Table 15
Characterization of each adjustment.

| Formal Sensitivity Analysis Adjustments | | Characterization | Variation from Initially Defined Values | Previous Results |
|---|----------------|--|---|----------------------------|
| Adjustment | Adjustment | | | |
| Adjustment 1 | Adjustment 1.1 | Start value for the mass flow rate of the hot air stream allocated from kiln 1 to the TES Unit (\dot{M}_6 , as delineated in Table 1) is varied to 500.00 kg/h. | - 75.00% | Initial Optimised Scenario |
| | Adjustment 1.2 | Start value for the mass flow rate of the hot air stream allocated from kiln 1 to the TES Unit (\dot{M}_6 , as delineated in Table 1) is varied to 1000.00 kg/h. | - 50.00% | Initial Optimised Scenario |
| | Adjustment 1.3 | Start value for the mass flow rate of the hot air stream allocated from kiln 1 to the TES Unit (\dot{M}_6 , as delineated in Table 1) is varied to 3000.00 kg/h. | 50.00% | Initial Optimised Scenario |
| Adjustment 2 | Adjustment 2.1 | Start value for the mass flow rate of the hot air stream allocated from kiln 2 to the TES Unit (\dot{M}_{13} , as delineated in Table 1) is varied to 4500.00 kg/h. | - 10.00% | Adjustment 1.2 |
| | Adjustment 2.2 | Start value for the mass flow rate of the hot air stream allocated from kiln 2 to the TES Unit (\dot{M}_{13} , as delineated in Table 1) is varied to 4800.00 kg/h. | - 4.00% | Adjustment 1.2 |
| | Adjustment 2.3 | Start value for the mass flow rate of the hot air stream allocated from kiln 2 to the TES Unit (\dot{M}_{13} , as delineated in Table 1) is varied to 5100.00 kg/h. | 2.00% | Adjustment 1.2 |
| Manual Tuning Adjustments | | Characterization | Previous Results | |
| Adjustment | Adjustment | | Previous Results | |
| Adjustment 3 | Adjustment 3 | Start value for the mass flow rate of the hot air stream allocated from kiln 1 as combustion air (\dot{M}_{6AA} , as delineated in Table 1) is varied from 5000 kg/h (charge phase) and 10000 kg/h (discharge phase) to 12000 kg/h. | Adjustment 2.3 | |
| Adjustment 4 | Adjustment 4 | Start value for the mass flow rate of the hot air stream allocated | Adjustment 3 | |

(continued on next page)

Table 15 (continued)

| Formal Sensitivity Analysis Adjustments | | | |
|---|--|---|------------------|
| Adjustment | Characterization | Variation from Initially Defined Values | Previous Results |
| Adjustment 5 | from kiln 2 as combustion air (M13 AA, as delineated in Table 1) is varied from 5000 kg/h (charge phase) and 10000 kg/h (discharge phase) to 10000 kg/h. | | Adjustment 4 |
| Adjustment 6 | Value for the thermal-to-electric efficiency associated to the ORC system (ORCEfficiency, as delineated in Table 6) is varied from 4.22% to 1.50%. | | Adjustment 4 |

of the model (before the performance of manual tuning-related adjustments).

In respect to manual tuning-related adjustments (only), it is possible to perform the following affirmations:

- In relation to the adjustment of stream parameters (adjustments 3 and 4), it is verified that a further re-assessment of the initially defined values may be performed so as to obtain larger operational cost reductions. The most significant benefit with these two adjustments is effectively the reduction of the natural gas consumption of the kilns operating in continuous mode (kilns 1 and 2), which overall causes the decrease in total operational costs;
- On the other hand, the natural gas consumption of the intermittent kilns (kilns 3 and 14) increases from adjustment 2 to 3 and 3 to 4 (which is expected due to the decrease in the availability of hot air to be supplied to the PCM-TES unit);
- The value obtained for the net generated electricity at the end of the analysis (42 h) has been affected differently, with the adjustment of the mass flow rate of the hot air recirculated from kiln 1 (adjustment 3) producing a lower level of net generated electricity and the one for the hot air from kiln 2 (adjustment 4) producing a higher level. This higher level of net generated electricity may be attributed to a more effective allocation of the hot air to the ORC system in adjustment 4;
- In relation to the adjustments related to thermal-to-electric energy conversion efficiency of the ORC system (adjustment 5 and 6), it is verified that only slight variations occur for natural gas consumption, with the net generated electricity being the energy use-related indicator with the highest variation (in this case, decrease and increase for adjustments 5 and 6, respectively). As such, it may be affirmed that adjustments performed for the ORC thermal-to-electric conversion efficiency essentially cause a corresponding variation in the net generated electricity, not affecting the remaining indicators;
- Obtaining such levels for each of the referred indicators may be attributed to similar levels of allocation of hot air at all times, that is, the solution converges to similar mass flow rates for each of the hot air streams from the kilns to the TES unit in adjustments 4, 5 and 6.

In the light of the observations presented, the configuration obtained by adjustment 5 is set as the one to be considered for further integration steps within the simulation model. Adjustment 5 is the one which is a compromise between the highest possible reduction of total operational costs and the assurance of obtaining the most coherent results associated with electricity generation, in which the thermal-to-electric energy conversion efficiency is considerably decreased so as to ensure that the

Table 16
Results obtained for each adjustment.

| Indicator | Initial Optimisation Results | Adjustment 1.1 | Adjustment 1.2 | Adjustment 1.3 | Adjustment 2.1 | Adjustment 2.2 | Adjustment 2.3 | Adjustment 3 | Adjustment 4 | Adjustment 5 | Adjustment 6 |
|---|------------------------------|----------------|----------------|----------------|----------------|----------------|----------------|--------------|--------------|--------------|--------------|
| System | | | | | | | | | | | |
| Natural Gas Flow Rate (kg/cycle) | Kiln 1 4839.79 | 4827.98 | 4825.89 | 4831.57 | 4832.29 | 4835.68 | 4765.10 | 4491.19 | 4493.45 | 4480.88 | 4491.75 |
| | Kiln 2 3941.36 | 3930.55 | 3928.58 | 3933.68 | 3934.52 | 3937.53 | 3872.90 | 3936.21 | 3470.81 | 3456.20 | 3469.04 |
| | Kiln 3 319.59 | 312.91 | 311.64 | 314.70 | 315.39 | 317.17 | 277.15 | 316.43 | 317.67 | 308.91 | 316.82 |
| | Kiln 4 1234.03 | 1219.19 | 1216.57 | 1223.71 | 1224.60 | 1228.87 | 1140.22 | 1226.92 | 1230.19 | 1210.15 | 1227.81 |
| Net Generated Electricity (kWh/cycle) | 1588.61 | 1508.02 | 1608.87 | 1564.15 | 1594.15 | 1606.85 | 1378.23 | 852.03 | 1378.23 | 470.47 | 1655.85 |
| Overall Total Operational Cost (k€/cycle) | 10.80 | 10.76 | 10.74 | 10.77 | 10.77 | 10.78 | 10.53 | 10.52 | 9.95 | 10.02 | 9.90 |
| Total Operational Cost (M€/year) | 2.01 | 2.00 | 2.00 | 2.01 | 2.01 | 2.01 | 1.96 | 1.96 | 1.85 | 1.87 | 1.84 |

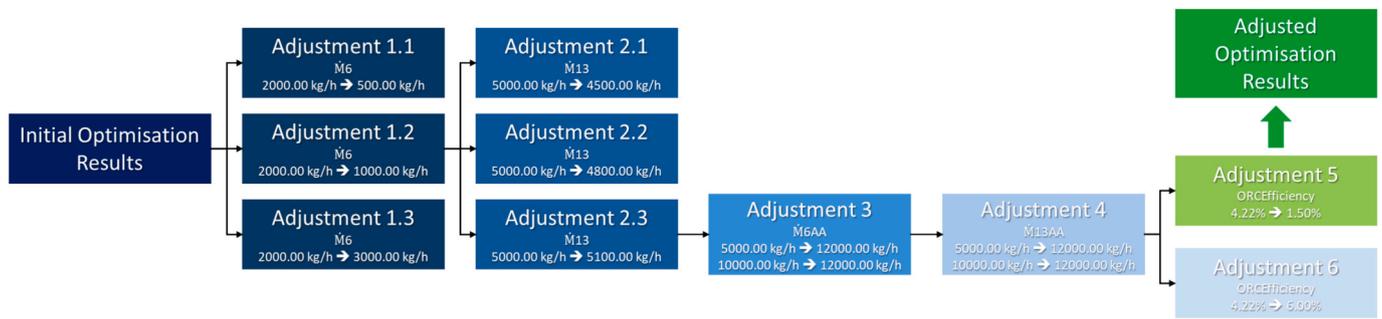


Fig. 4. Sequence of adjustments for the sensitivity analysis process (from initial to adjusted optimisation results).

definitive solution is the one associated with the minimum level of total operational costs.

4.2. Final optimisation results

The results generated by the modelling framework and optimisation procedure adopted in the present work must be analysed not only in terms of its technical implications (in the context of the occurrence of the physical phenomena and the optimisation process), but also in terms of the economic favourability associated to the Engineering projects of the conceptualized heat recovery systems. While the more technical-oriented results have been possible to be obtained by the presented overall framework, the more economic-oriented results must be completed with a brief post-processing procedure, with the aim to proceed with the determination of indicators related to economic favourability. In the context of the present work, such economic favourability may be evaluated through the determination of the payback time, as enunciated in equation (43), in which *Inv* corresponds to the total investment cost (summation of equipment costs and maintenance costs) estimated for an Engineering project and *Sav* corresponds to the net economic benefit generated by the project (which in this case corresponds to savings in energy-related total operational costs).

$$PB \text{ (Years)} = \frac{Inv \text{ (€)}}{Sav \text{ (€/year)}} \quad (43)$$

The conceptual objective of this work has been directed to the minimization of costs related to energy use in the overall approached ceramic plant (this is, total energy-related operational costs), since the primary aim of the study is oriented to the promotion of the energy efficiency improvement benefit brought by the implementation of the heat recovery system. In this sense, the objective-function delineated in the approached optimisation procedure also focus on energy-related costs minimization, while investment costs related to the Engineering project are set to serve for the aforementioned post-processing procedure. This post-processing procedure is performed with the aim to furtherly allow a comparison of the results obtained in this work with other results obtained in similar works, through the assessment of aggregated indicators, as well as acceptable levels of economic favourability delineated for energy technologies-based projects in European industry (a reasonable 2 – 3 years is considered for the payback time for a project to be favourable [3]). The investment cost parcels for the approached Engineering project have been estimated based on acquisition cost for each piece of equipment included in each considered system making part of the overall heat recovery system (the PCM-TES and the Organic Rankine cycle). In line with focus of the present work being energy-related costs minimization, the investment cost parcels are only briefly presented, with the aim to justify the determination of the payback time indicator. The extensive determination of investment cost parcels had already been performed in a previous related work by the authors approaching the same ceramic industry case-study [42].

In Table 17, it is presented the comparison of results between the

baseline and optimised scenarios (with the optimised scenario corresponding to the adjustment 5). The optimisation results (corresponding to the initial set of optimisation results and the final set of results obtained by the integration of a set of results generated from the running of DP model considering adjustment 5 into the counterpart simulation model) in respect of specific system variables are presented in the sequence of Figs. 5–7.

5. Discussion

The results obtained from the whole optimisation process performed for the case-study approached on this work may be analysed at light of its adequacy with expected real-life observations and through its comparison with results obtained from similar case-studies (namely those present in already published literature).

Table 17
Comparison between the Baseline and Optimised scenarios.

| Indicator | | Baseline | Optimised |
|--|---------------------------------------|--------------------|--------------------------|
| Natural Gas Consumption (kg/cycle) | Kiln 1 | 5355.00 | 4530.38 |
| | Kiln 2 | 5044.20 | 3529.69 |
| | Kiln 3 | 334.29 | 318.18 |
| | Kiln 4 | 1266.05 | 1230.65 |
| | Net Generated Electricity (kWh/cycle) | | |
| Savings in Total Operational Costs | | | |
| Indicator | | Baseline | Optimised |
| Total Operational Costs (k€/cycle) | | 12.80 | 10.14 |
| Total Operational Costs (M€/year) | | 2.38 | 1.89 |
| Breakdown on Economic Savings | | | |
| Indicator | | Savings (k€/cycle) | Share over Total Savings |
| Natural Gas Consumption | Kiln 1 | 0.88 | 33.04% |
| | Kiln 2 | 1.62 | 60.67% |
| | Kiln 3 | 0.02 | 0.65% |
| | Kiln 4 | 0.04 | 1.42% |
| | Net Generated Electricity | 0.11 | 4.23% |
| Total Economic Savings | | | |
| 0.50 M€/year reduction (20.80% relative reduction) | | | |
| Economic Viability Assessment | | | |
| Equipment Costs (k€) | | 467.83 | |
| Maintenance Costs (k€) | | 820.53 | |
| Total Investments Costs (k€) | | 1288.37 | |
| Payback Time (Years) | | 2.60 | |

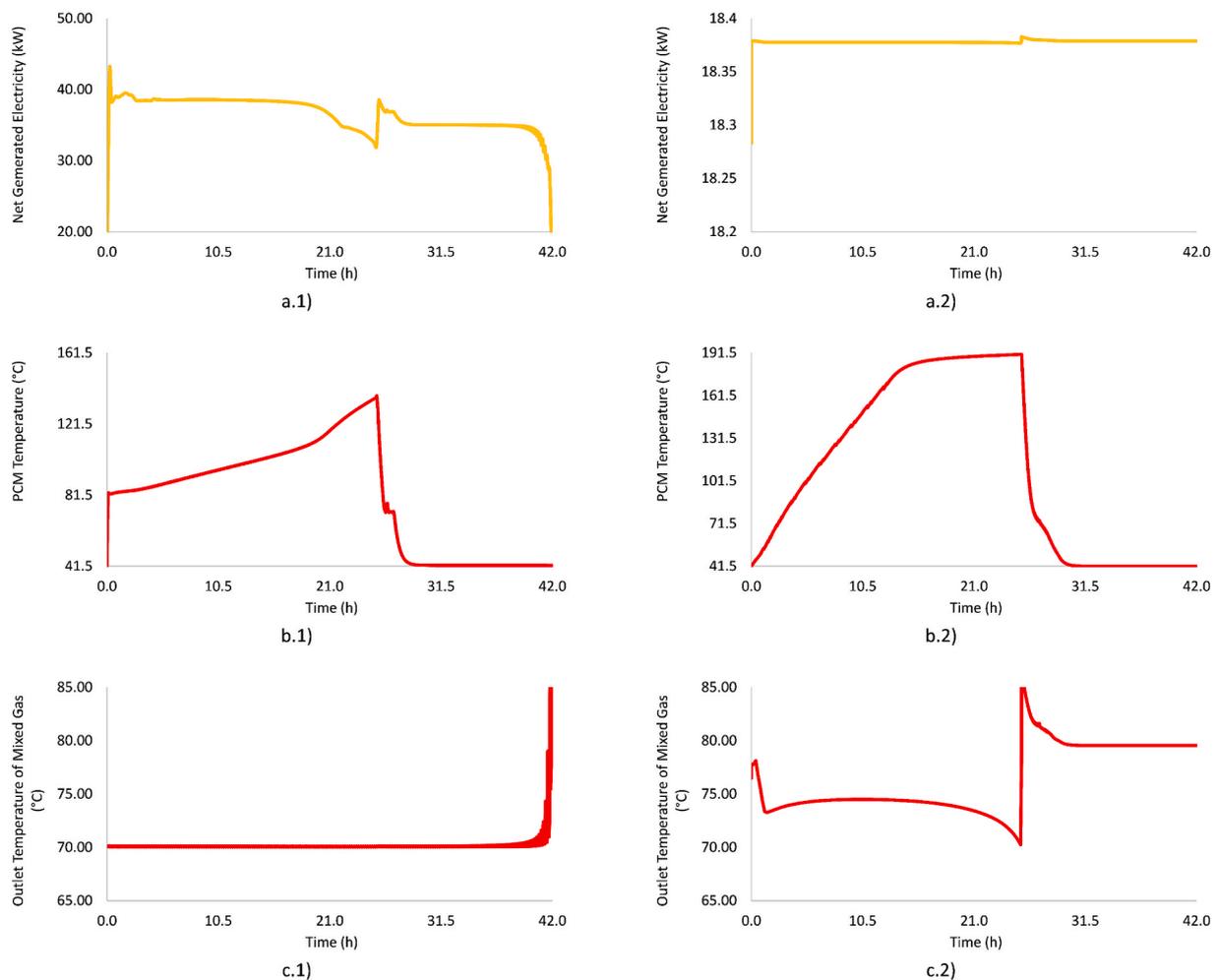


Fig. 5. Optimisation results against time for a) Generated electricity, b) Temperature of the PCM inside the PCM-based heat exchanger, c) Temperature of the mixed gas at the outlet of the HRSG unit included in the ORC system (1 – Initial Optimisation Results, 2 – Final Results).

5.1. Analysis of optimisation results

From the results presented in Table 17, the following deductions may be made:

- The solution of the optimisation problem converges to a point in which the total operational costs (the summation of each of the energy-related costs) are considerably lower than the corresponding baseline value and the value obtained for the previously elaborated scenario;
- For all the combustion-based processes (kilns), the natural gas consumption is significantly lower than the corresponding values for the baseline scenario;
- A significant quantity of electricity is also generated (as may be verified by the results obtained for net generated electricity).

In light of these verifications, it may be considered that solving the optimisation problem has been successful for achieving the objective of assessing potential energy use-related improvements.

The analysis of the transient results for the system variables (presented in Figs. 5 – 7) may be conveniently seen by dividing it into two parts:

- Analysis of the results during the charge phase (first 25.5 h of analysed time);
- Analysis during the discharge phase (the remaining 16.5 h).

Table 18 presents a detailed analysis of the results obtained by the running the developed optimisation model, considering the most fundamental aspects.

5.2. Comparison with literature results

The results obtained by the whole optimisation procedure taken in this work may be compared to results present in literature. The literature works which may more conveniently serve to perform such comparison process would be research works approaching the application of computational models to assist the conceptualization of heat recovery systems (HRS). It is to note, however, that the research topic inherent to the present work is relatively new. The HRS concept approached in this worked is based on a specific application of the Water and Energy Integration Systems (WEIS) conceived developed by the authors for a physical system including combustion-based processes only (in opposition to a system including these processes and also water-using processes). Although simulation models have been developed for similar unit operations (namely thermal energy storage units) and similar dynamic programming models have been developed, the computational modelling framework is also considerably new, and the specific methodology adopted in the context of this work is proper of that same framework. In this sense, the only sets of works that would be in a valid manner used as a basis of comparison in respect to the present work would be the ones approaching the computational model-assisted implementation of HRS in process industry plants.

In this prospect, it is possible to perform a comparison between the

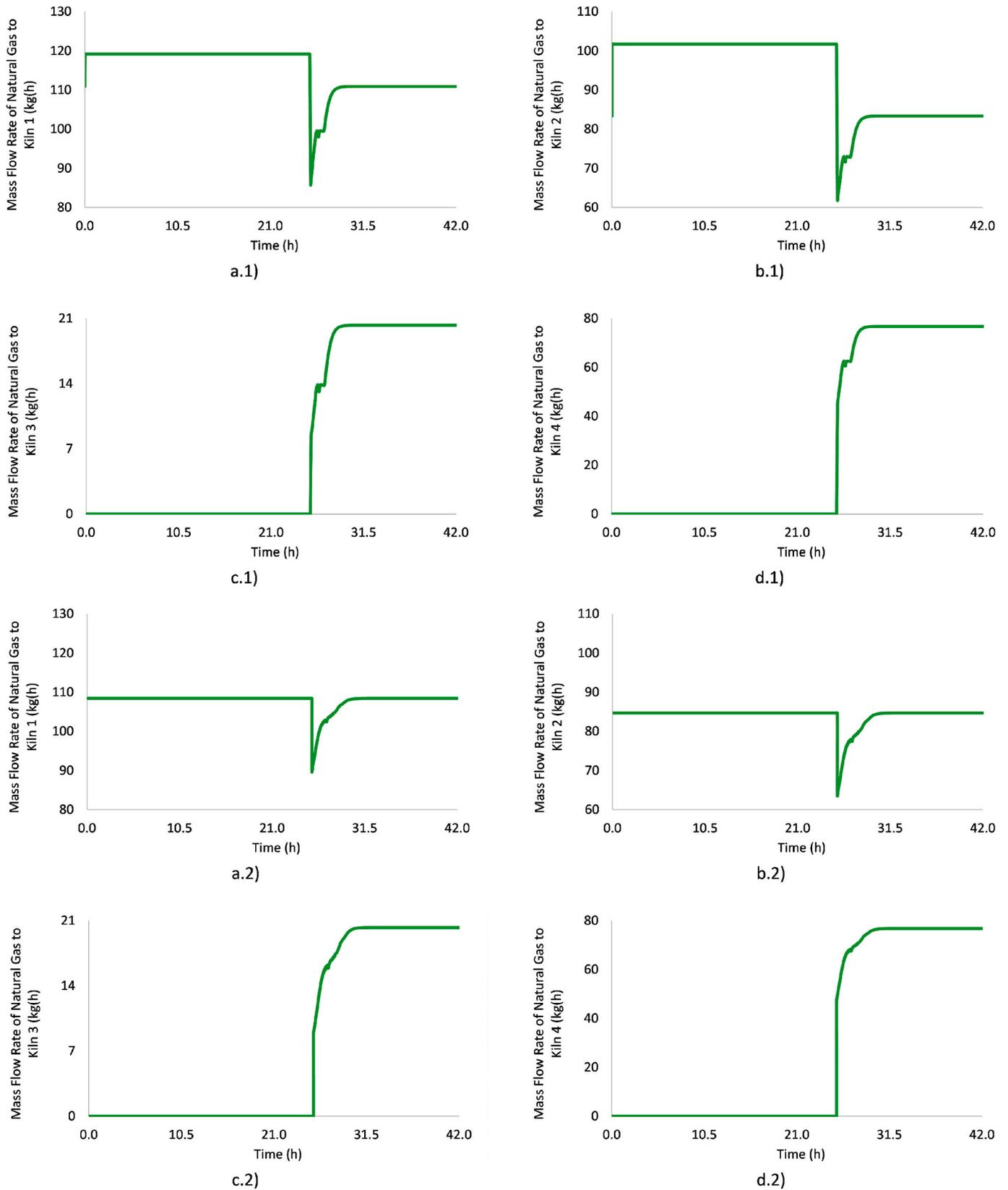


Fig. 6. Results for the natural gas mass flow rate of a) Kiln 1, b) Kiln 2, c) Kiln 3 and d) Kiln 4 (1 – Initial Optimisation Results, 2 – Final Results).

results obtained for specific aggregated indicators which have been conveniently and simultaneously determined in the context of the studies developed for the presented work and a previous work by the authors [40]. In this previous work, a similar ceramic industry has been

analysed and an HRS has been proposed and virtually implemented. Since the ceramic plant approached in this work only included continuous combustion-based processes, it was not necessary to adopt a dynamic optimisation perspective, and only a non-linear programming

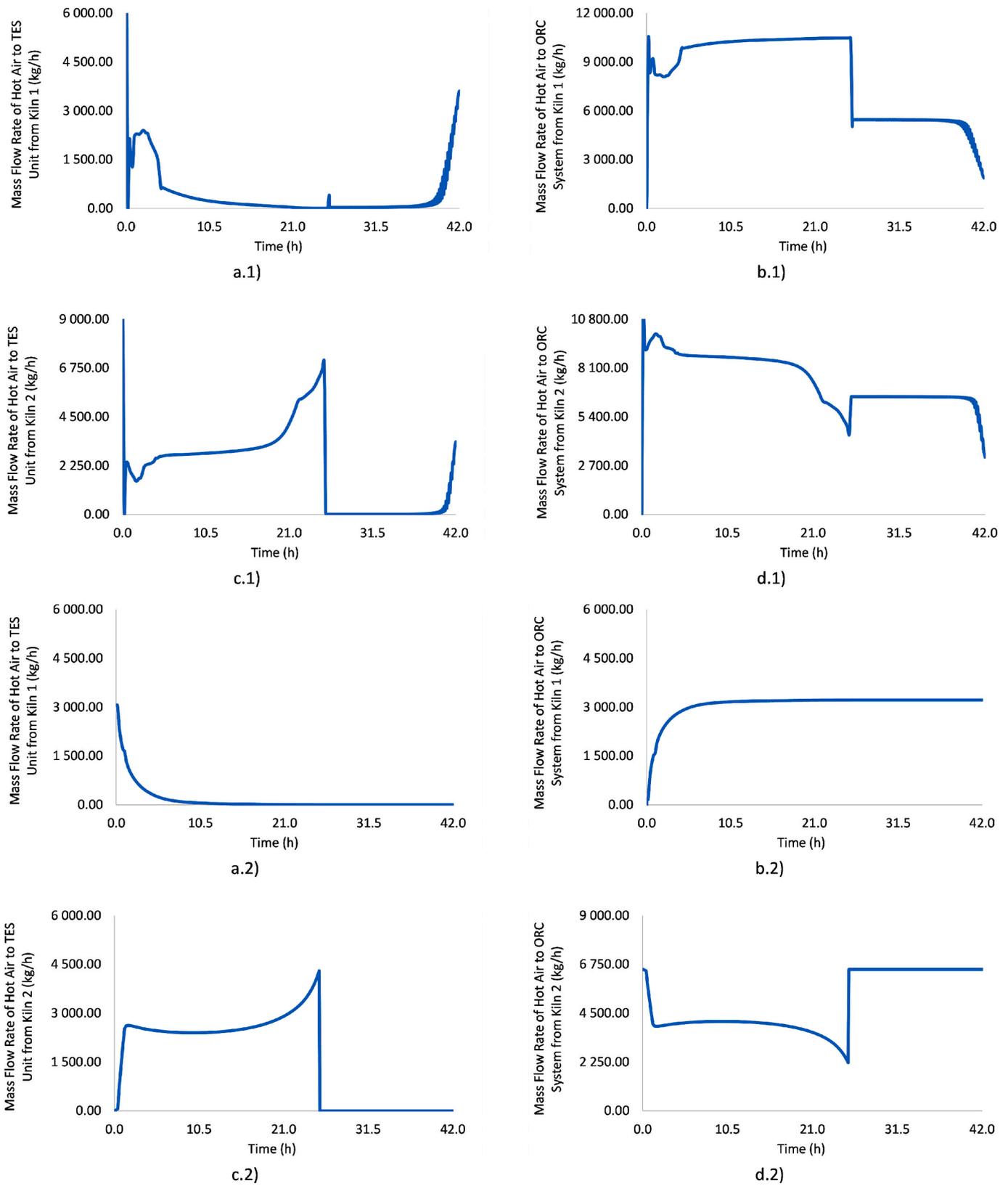


Fig. 7. Results for hot air mass flow rate: a) Kiln 1 to TES Unit, b) Kiln 1 to ORC, c) Kiln 2 to TES Unit, d) Kiln 2 to ORC (1 – Initial Optimisation Results, 2 – Final Results).

(NLP) methodology has been adopted to perform the necessary optimisation procedure. In Table 19, the results for aggregated indicators for both case-studies (the one approached in this work and the literature one) are presented.

As may be verified by the analysis of Table 19, the optimisation procedure performed for the case-study approached in this work allows the obtention of economic savings comparable to the ones obtained for the reference literature work. The absolute savings are comparable in

Table 18
Analysis of Optimisation Results.

| Charge Phase | |
|--------------|--|
| | <ul style="list-style-type: none"> It is possible to verify by analysing Fig. 6 that the mass flow rate of natural gas at the inlet of each kiln is constant throughout all the time in question, as the temperature of combustion air at the inlet of each kiln is set to the value corresponding to the scenario. For kilns 3 and 4, the natural gas flow rate is zero since these are intermittent kilns that do not operate while being charged; From an analysis of Fig. 7 – a.1) and c.1), it is possible to verify a slight increase of the quantity of hot air allocated from kiln 1 to the TES unit followed by two periods of gradual decrease and a gradual increase of the quantity of hot air from kiln 2. Such behaviour may be attributed to an adopted tendency of the OpenModelica optimization solver to converge to a point at which the stored enthalpy within the PCM-TES unit is increased (which may be observed by the increase of the PCM temperature in Figs. 5 – b.1)), which may be achieved through the supply of the hot air stream with a higher temperature (in this case the one from kiln 2) in higher quantities; The verified decrease of hot air supply to the PCM-TES unit from kiln 1 at a determinate point in time is an occurrence that is more in line with the real-life expected occurrence, in opposition to the initial increase of hot air supply until that point. The hot air stream from kiln 2 is the one with the highest temperature (196.5 °C, in opposition to the lower temperature of 111.5 °C for the hot air stream from kiln 1). The inclination of the supply of hot air from kiln 2 instead of kiln 1 would, in this sense, allow that the thermal equilibrium in PCM-TES unit would be achieved at a higher temperature, and as such the total stored enthalpy at the end of the charge time would be higher. In this sense, it shall be expected that in a system with the configuration as the one described that the mass flow rate of hot air from kiln 1 decreases with time until it reaches near-null values (in the case that it initially presents a considerable value, such as this one) and that the supply of hot air from kiln 2 increases with time; In respect to the achievement of thermal equilibrium in the PCM-TES unit, it is possible to verify by the analysis of Figs. 5 – b.1) and b.2) that the highest temperature possible to be achieved by heat transfer between the heat source (hot air) and the storage material (PCM) is only at the latest stages of the total 25.5-hours charge phase. Such is more noticeable in Figs. 5 – b.2) (which presents the results obtained by the running of the final model), in which the PCM temperature corresponding to thermal equilibrium (which is also the highest possible temperature to be achieved in the performance of the whole stream allocation process, namely the temperature of the hot air from kiln 2, 196.5 °C) is only achieved in a stage close to the end of the 25.5-hours charge phase; The aforementioned verification is in line with the expected behaviour of a system with the described configuration. The supply of hot air to PCM-TES unit shall be performed in such a manner so to ensure that the PCM temperature is the highest possible at the end of the charge phase. Nonetheless, the achievement of this temperature before the end of the charge phase would not be desirable, since the achievement of that temperature level at an earlier time instant is significant that a significant allocation of hot air has been performed to the TES unit instead of the ORC unit, thus decreasing the relative net electricity generation. The achievement of the highest possible PCM temperature at the latest stages of the charge time is significant that the net electricity generation is the highest possible during the charge phase, without compromising the total quantity of net electricity generation in the discharge phase from that point on. Such occurrence allows that net electricity generation is the highest possible during the whole 42.0 cycle time, without compromising the achievement of the achievement of the lowest possible fuel consumption in the kilns (and, as such, allows the achievement of the lowest possible total operational costs); In relation to the generated electricity, it is possible to observe in Figs. 5 – a.1) a relative stagnation for the first hours of the analysis (roughly the first 19 h), with a gradual decrease from that point to the end of the charge phase. The first moment (of relative stagnation) may be interpreted as assuming an equilibrium between the hot air supplied from kiln 1 (which is |

Table 18 (continued)

| | |
|-----------------|---|
| | <ul style="list-style-type: none"> gradually increasing) and kiln 2 (which is decreasing). The second period (of gradual decrease) may be attributed to the verifiable decrease of the quantity of hot air from kiln 2 to the ORC system from 19 h onwards (which is directed to the TES unit instead); The temperature of the mixed gas at the outlet of the ORC is roughly maintained at 70.0 °C (the defined lower limit), which may be attributed to the convergence of the solver for the maximization of generated electricity for the whole period of the analysis. |
| Discharge Phase | <ul style="list-style-type: none"> The mass flow rate of the hot air streams allocated to the TES unit in the last hours of the analysed time present higher than zero values, which is not supposed to be verified (since the mentioned analysed time corresponds to the discharge phase); By the same set of reasons associated with the previous point, the mass flow rate of the hot air streams allocated to the ORC system present considerably low values (for the same time interval); In a further analysis attributed to the same set of reasons associated with the previous point, the temperature of the mixed gas at the outlet of the ORC presents an exacerbated increase from 37 h to the end of the discharge phase; It is possible to verify that the mass flow rate of the natural gas in each kiln is effectively lower than the corresponding baseline. In the simulation, the natural gas flow rate to kiln 1 reaches a level above 90.0 kg/h for the optimised scenario, but it decreases to a much lower value during the first part of the discharge phase. This is expected due to the relatively superior temperature of the combustion air that is preheated through the withdrawal of enthalpy from the TES unit; The mass flow rates of the hot air streams allocated to the TES unit take approximately null values, which is an expected result. Since the discharge phase subsists on the withdrawal of enthalpy from the TES unit, the total allocation of waste heat streams to this unit is supposed to be null, so to ensure that the withdrawal of enthalpy is performed as fast and as efficient as possible. |
| Overall | <ul style="list-style-type: none"> In general, the optimiser allows that the recirculation of the total quantity of hot air (combination of the hot air streams from both kilns 1 and 2) is shifted to the TES unit during charging (in order to allow that the highest possible energy storage during the charge phase) and to the ORC unit during discharging (in order to allow the highest net electricity generation during discharge phase, in the absence of another requirement to be fulfilled by stream allocation); Such observation is in line with the expected behaviour of a real-life installation for the proposed heat recovery system. During discharge phase, heat stream recirculation is only inclined to the ORC unit, since that same stream recirculation procedure allows the highest net electricity generation, which in its turn allows the highest possible minimization of total energy-related economic costs. However, during charge phase, another requirement exists in addition to the electricity generation in the ORC, which is the supply of thermal energy to be stored in the PCM-based heat exchanger. In this prospect, stream recirculation must be oriented to both the TES unit and the ORC unit during charge phase, favouring the requirement of energy storage on the TES unit (which is only set to occur during charge phase); The aforementioned arrangement of stream recirculation along time is set to produce the highest possible minimization of fuel consumption on the kilns (by the allocation with the highest possible enthalpy to the TES unit curing charge phase) and the maximization of net electricity generation (with the highest possible allocation of heat streams to the ORC unit during charge phase, without compromising the requirement brought by the implementation of the TES unit, and the total inclination of stream recirculation to the ORC unit during the discharge phase). The combination of these two occurrences causes the highest possible minimization of total operational costs at the end of the analysis time (42.0 h). |

Table 19
Comparison between obtained and literature results.

| Indicator | Approached Case-study | Literature Case-study |
|------------------------------|-----------------------|-----------------------|
| Savings (M€/year) | 0.50 | 0.67 |
| Relative Savings | 20.80% | 28.70% |
| Total Investments Costs (k€) | 1288.37 | 388.48 |
| Payback Time (Years) | 2.60 | 0.58 |

terms of order of magnitude, and relative savings are also relatively close. The total investment costs are significantly higher for the approached case-study, which may be attributed to the additional implementation of the PCM-TES unit in relation to the literature case-study (which is a unit associated to significant acquisition and maintenance costs). Such increase of total investment costs is also significant of a relative superior payback time for the approached case-study, although not sufficient for the involved Engineering project for the heat recovery system to not become economically unfavourable (the payback time is still below the reasonable maximum limit of 3 years for which a project of this type is considered economically favourable). In this prospect, it may be affirmed that although it has not been possible with the adopted optimisation framework to surpass relative savings results in relation to the optimisation frameworks adopted in the context of similar case-study (this is mostly related to the operational conditions of each case-study in particular, rather than the developed optimisation models), it is, however, possible to obtain similarly economically favourable Engineering projects for heat recovery systems including thermal energy storage units.

6. Conclusions

This work considers aspects related to the development and further utilization of a dynamic programming (DP) model for a heat recovery system (HRS) to be implemented in a process industry plant. The requirement for the development of such a model appeared due to the necessity to create a modelling methodological framework for optimising systems in the perspective of a transient state (in which a set of variables characterizing the overall system display significant variations during the operational time).

With respect to the adopted optimisation procedure and modelling framework:

- In general, the developed model may be considered robust with respect to the defined objective, taking into account that the adjustments performed in the context of a more formal sensitivity analysis demonstrate in general that the model is relatively insensitive to these perturbations;
- The solution of the optimisation problem converges to a point at which energy-related operational costs are considerably lower than the corresponding baseline values (for all sets of optimisation results, including initial optimisation results and final results, as may be verified in Table 17 and the sequence of Figs. 5 – 7);
- Nonetheless, although the model is able to produce optimisation results that may be integrated with a counterpart simulation model, only such an integration is able for the final results to be used for further post-processing assessment (as may be verified in the sequence of Figs. 5 – 7), since obtaining the most accurate results for energy savings (as well as the indicators of payback time and absolute emission reductions) are essential for the determination of the economic and environmental viability associated with the HRS engineering projects
- The results obtained by the implementation of the presented modelling framework and optimisation procedure are considered favourable in comparison to results for similar works in literature

(namely those approaching the implementation of an optimisation procedure to a steady state-based heat recovery system).

In this prospect, the optimisation methodology adopted in this work had allowed the obtention of a robust dynamic programming (DP) model. The results obtained by the running of this model being set to complement a validated modelling framework encompassing the highest possible level of accuracy of physical phenomena representation and the consideration of a configuration in which total operational costs are reduced to the highest possible level of minimization. Such favourable situation is furtherly with a proved economic favourability associated to the inherent Engineering project of the referred systems.

6.1. Limitations of the current research

The overall modelling framework and adopted optimisation procedure are associated to the following limitations:

- The planning of the heat recovery system (HRS) is only possible to be performed taking as a starting point a configuration in which waste heat streams (in this case, hot air) are already recirculated attending to a pre-defined configuration, namely in terms of fixed values associated to the mass flow rates of the recirculated streams (as may be verified in Fig. 1, it is only planned the recirculation of hot air as combustion air within the same kilns, and these are associated to fixed allocations along time). Such is attributed to limitations in terms of the development of the DP model, in which the number of state variables must equal the number of states (which would not be possible in an arrangement in which the aforementioned mass flow rates are variables instead of parameters);
- The incompatibility between the solvers within OpenModelica used in context of simulation models (the DASSL solver is the one that is commonly used) and the ones used in the context of DP model (the internal *optimization* solver). Such makes impossible to run an optimisation model for the type of physical systems approached in this work simultaneous with a counterpart simulation model (encompassing the same physical system, being characterized by the same set of variables and governing equations), or instead the allowance of the implementation of an optimisation procedure over the layer of a simulation model (including the minimization of a defined objective-function by directly controlling inputs on the simulation model);
- Furthermore, an alternative for the aforementioned limitation would be an application programming interface (API) in which a set of results from a Modelica-based DP model would be allocated to the counterpart Modelica-based simulation model (similar to the OpenModelica Python API implemented for the passage of results from a steady state-based optimisation model developed with the Python language and a Modelica-based simulation model). Nonetheless, such alternative does not also exist at the time of the elaboration of the present work.

6.2. Future work

In a future work perspective, the following aspects may be exploited:

- The development of a new modelling paradigm (which may be adapted to any case with a similar overall setup as this one), in which a non-linear programming (NLP) methodology is firstly implemented (for the obtention of the optimal point for stream recirculation within the continuous combustion-based processes of the plant), and then a dynamic programming (DP) model is build over the heat recovery system configuration obtained after the running of the NLP model (which is in practice performed to allow the integration of the paradigm of thermal energy storage on a heat recovery system which has already considered an optimum stream allocation to allow an even further minimization of energy-related operational costs);

- For a reason of improved automation in terms of the integration of optimisation results from the DP model to a counterpart simulation model, the development of an application programming interface (API) (similar to OpenModelica Python) would be beneficial, allowing the allocation of results between two Modelica models developed for different purposes (in this case, dynamic optimisation and dynamic simulation).

CRedit authorship contribution statement

Miguel Castro Oliveira: Writing – original draft, Software, Methodology, Investigation, Conceptualization. **Bertrand Delpech:** Writing – review & editing, Writing – original draft. **Abdulrahman Alhajri:** Writing – review & editing, Writing – original draft. **Hussam Jouhara:** Writing – review & editing, Writing – original draft. **Luca Montorsi:** Writing – review & editing, Writing – original draft. **Rui M. Filipe:** Writing – review & editing, Writing – original draft. **Henrique A. Matos:** Writing – review & editing, Writing – original draft.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: M. Castro Oliveira, Simulation and Optimisation of Water and Energy Integration Systems (WEIS): An Innovative Approach for Process Industries, 2023. <https://scholar.tecnico.ulisboa.pt/records/KwfdB28dqObhPEiL7RtB3VJ6YxvixXFEhWnt..>

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Data availability

No data was used for the research described in the article.

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