

1 Article

2 Price and carbon-based energy flexibility of residential 3 heating and cooling loads using model predictive control

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10 **Declarations of interest:** None.

11 **Abstract:** Model predictive controllers (MPC) have shown great potential for activating the energy
12 flexibility of thermal loads, especially in buildings equipped with heat pump systems. In this work,
13 an MPC controller is developed and tested within a co-simulation framework which couples an
14 optimization software with a dynamic building simulation tool. The development phase is
15 described in detail, in particular the methods to obtain simplified models to be used by the
16 controller. The building envelope and the heat pump performance (based on experimental data)
17 were thus modelled, both in heating and cooling seasons. Three different objective functions of the
18 MPC are tested on a study case consisting of a Spanish residential building: promising results are
19 obtained when the controller aims at minimizing operational costs (savings of 13 to 29%) or CO₂
20 marginal emissions (savings of 19 to 29%). The development efforts, the required tuning and
21 sensitivity of the MPC algorithm parameters, the adaptations needed between the cooling and
22 heating operations are also discussed and put into perspective with the obtained benefits in terms
23 of savings, comfort and load-shifting.

24 **Keywords:** model predictive control; energy flexibility; carbon footprint minimization; variable
25 speed heat pump; heating and cooling loads; co-simulation; HVAC control; heat pump control.
26

27 1. Introduction

28 The latest report of the Intergovernmental Panel on Climate Change (IPCC) establishes clearly
29 that the Earth has already warmed on average by 1°C compared to pre-industrial levels, and that
30 global warming will certainly reach at least 1.5°C by 2030 due to manmade activities [1]. To avoid
31 going beyond 1.5°C and the catastrophic consequences related to such an important climate change,
32 the IPCC calls among other recommendations for a deep and fast decarbonization of our energy
33 systems. The introduction of a large share of renewable sources of energy has therefore become an
34 absolute and urgent necessity. However, this transition might provoke challenges and instability in
35 the electricity grids, if non-dispatchable sources such as solar and wind become predominant. Some
36 regions already experience the effects of a high penetration of renewable energy sources (RES): in
37 California or Germany for example, where the share of solar energy is high, prices can become
38 negative at times of high production. In such cases, curtailment of the RES constitutes an easy
39 solution, but basically consist in wasting free available energy, like these days of December 2012
40 where 300 MW of wind power were curtailed in Germany [2].

41 This situation calls for better solutions, and notably for an increase in the flexibility of the
42 demand side. The momentum towards a more flexible electricity system based on RES is increasing
43 [3] and it has definitely become a “hot topic”, given the large amount of literature recently published
44 on the matter [2]. Through an increased flexibility, energy systems could have inherent capabilities

45 to accommodate a larger share of variable RES without requiring massive new investments. In
46 particular, treating thermal and electrical systems as a whole could offer major new opportunities [2].
47 Along this line, enhancing the flexibility of buildings energy use has concentrated an important
48 amount of research [4]. Buildings possess an inherent thermal mass which can be regarded as a
49 storage means and activated by appropriate control strategies [5]. Additional storage options such as
50 water tanks or embedded phase-change materials can also be valued for that purpose [6]. Heating,
51 Ventilation and Air Conditioning (HVAC) systems operate inherently shiftable loads which can
52 contribute to the energy flexibility of a building, and heat pumps in particular show a promising
53 potential as a means to couple the electrical grids with thermal storages and to provide demand-side
54 management [7].

55 To unlock the flexibility potential of heat pumps in buildings, smart controls are required, which
56 can take the form of simple rule-based controls or model predictive controls (MPC) [8]. In the present
57 work, the focus lies on indirect control, i.e. strategies that provide an incentive signal such as a
58 variable electricity price, and then let the end users (or a controller for them) decide whether to react
59 or not. MPC has been extensively studied in recent years for such control strategies in building
60 climate control [9]–[11]. However, it has still not been widely applied in the control of real buildings,
61 and many aspects require further investigations. For these reasons, the authors are presenting in this
62 study the development and testing of an MPC controller for enhancing the energy flexibility of
63 residential buildings equipped with heat pumps in Spain. Identifying the current lacks in this field
64 of investigation, the motivations behind this research can be summarized with the following points:
65

- 66 • The formulation of the Optimal Control Problem (OCP) in MPC has already been discussed
67 in previous literature [12], in particular the linear modelling of variable speed heat pump
68 (VSHP) performance. However, such formulations only resorted to linear programming
69 (without integer variables), and thus could not reproduce the switching of the heat pump
70 between different modes (like space heating/cooling on one hand and production of
71 Domestic Hot Water (DHW) on the other hand), nor the switching off of the heat pump below
72 certain load level. In the present work, the authors propose a different OCP including integer
73 variables, which increases the complexity of the MPC, but enables to reproduce a more
74 realistic behavior of the systems. It also corresponds to the commands that can be sent to
75 control a real heat pump, which brings this research one step closer to an implementation
76 with real systems. Furthermore, the modelling of the heat pump performance is here realized
77 with experimental data instead of more commonly used manufacturer's data, which are often
78 incomplete and display the performance of the heat pump in ideal conditions.
- 79 • In a previous literature review [8], it was noted that the great majority of published research
80 on the present topic used **economic optimization**, which means these controllers receive a
81 variable price signal and intend to minimize the corresponding energy costs. It was
82 suggested that other objective functions could be studied, since the ultimate goal is actually
83 to reduce the carbon footprint of our energy use. In this regard, the grid carbon intensity has
84 been used in recent research as an alternative input signal for MPC in HVAC control [13],
85 [14]. In the present work, the authors propose to use a model of the *marginal* CO₂ emissions
86 [15], instead of the average emissions of the electrical grid. The marginal emissions consider
87 the merit order in which the production plants are activated in a given grid, and thus the
88 emissions savings are meant to be calculated more accurately. For instance, if a demand-side
89 management action triggers a reduction of the energy use, this will not affect a base plant
90 like nuclear, which is too slow to start and stop for balancing the grid. Instead, this variation
91 will be compensated for example by a gas turbine, and therefore the resulting marginal
92 emissions saved will be greater. The Marginal Emissions Factor (MEF) will thus be used in
93 this study, as it represents a novel and more appropriate input signal for reducing the CO₂
94 emissions in an MPC framework.
- 95 • MPC has shown great potential in prior research for managing HVAC systems in buildings,
96 and increase their demand-side flexibility. However, the development costs of such

97 technology remain high [16]: it was found for example that the creation of suitable control
98 models account for 50 to 80% of the development costs [17]. Furthermore, the computation
99 efforts also remain high in certain MPC configurations. These obstacles notably explain the
100 still low market penetration of MPC controllers despite their repeatedly proven performance
101 in building climate control. The development efforts of the MPC will therefore be explained
102 and analyzed in details in this study.

- 103 • To the knowledge of the authors, an MPC framework enhancing the flexibility of both
104 heating and cooling loads in different seasons has seldom been studied. The present article
105 will relate the adaptations needed to apply MPC in the same building in summer and winter,
106 with the same reversible heat pump that can provide space heating or cooling. In particular,
107 the adaptations needed in the models (building envelope, heat pump performance) and the
108 MPC formulation will be discussed.
- 109 • Finally, a co-simulation platform for testing MPC configurations will be presented. In this
110 case, TRNSYS is used as a dynamic simulation software to emulate the behavior of a virtual
111 building in details. MATLAB is used as the optimization software in which the MPC
112 controller is implemented. Coupling these two powerful tools enables to benefit from the
113 very accurate simulation results of TRNSYS, while overcoming its limitations, since it cannot
114 integrate predictive controllers directly [18]. The overall co-simulation framework will here
115 be used to test different MPC configurations, and could be reused **as a benchmark** for later
116 studies, notably to perform sensitivity analysis on the multiple parameters of the MPC
117 controller, or with different building typologies, for example including on-site RES
118 production.

119
120 The article is structured as follows: firstly, the methods section introduce the development and
121 implementation process of the MPC controller. The overall co-simulation framework is laid out to set
122 the context of the work. The study case and the building model identification process are then
123 described: this work focuses on residential building in the Mediterranean area, therefore this
124 typology is modelled. The performance of a VSHP is also modelled based on experimental data
125 obtained in a laboratory setup. The whole MPC algorithm is then detailed, focusing on the different
126 objective functions tested: minimization of delivered thermal energy, of the electricity costs or the
127 CO₂ marginal emissions due to the heat pump operation. Simulations of three days duration were
128 carried out in this framework, with different MPC configurations, both in heating and cooling mode:
129 they are reported in the results section. The analysis focuses on the following aspects: energy
130 flexibility, levels of thermal and electrical energy, efficiency of the systems, monetary costs, CO₂
131 marginal emissions and comfort of the occupants. Finally, the benefits and drawbacks of MPC are
132 discussed, in particular the development efforts required by such technology, its high sensitivity to
133 certain parameters and the confirmed benefits it can provide. Conclusions are drawn in the final
134 chapter.

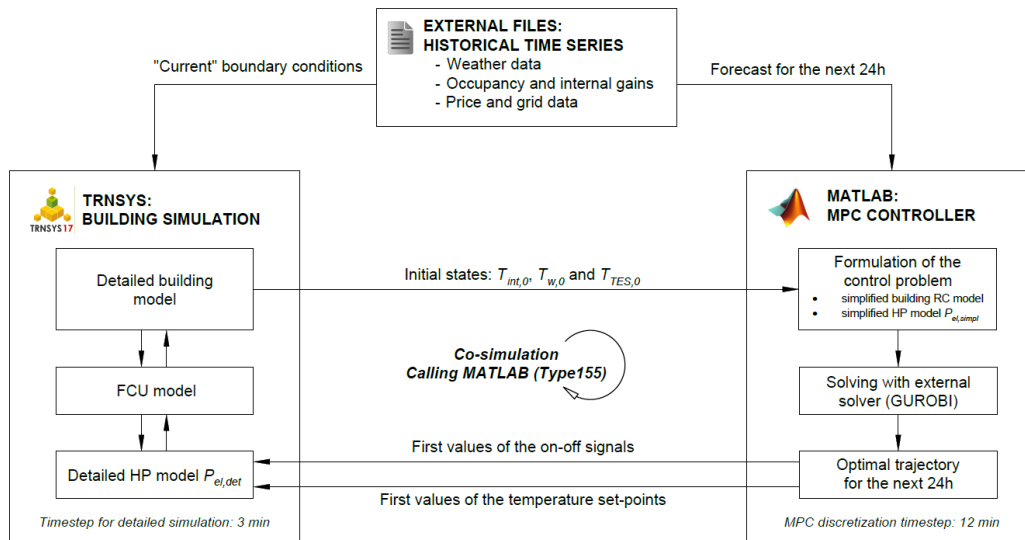
135 2. Methods: implementation of a Model Predictive Control framework

136 2.1. Co-simulation framework with MATLAB and TRNSYS

137 To test different configurations, a co-simulation framework has been implemented. In this
138 scheme, the detailed model in TRNSYS serves as the “real building”, in other words it constitutes a
139 virtual plant with which the control strategies can be tested. TRNSYS does not contain suitable tools
140 for optimization, therefore the MPC calculation must be externalized in another software, MATLAB
141 in the present case. For clarity, the term “detailed” generally refers to the TRNSYS framework, while
142 the term “simplified” refers to the MPC framework (the models and time steps of these two
143 frameworks are notably distinct). The scheme of the co-simulation and the exchange of variables is
144 presented in Figure 1. The TRNSYS simulation runs using the necessary inputs (weather, occupancy
145 grid etc...) from external files. When the MPC controller in MATLAB is called, it is provided with the

146 necessary input (the initial values of the states and the forecasts for the next 24h taken from the same
147 files).

148 In MATLAB, the control problem is formulated with the YALMIP tool [19] and solved with
149 GUROBI [20]. To limit the computation efforts, the MPC controller requires simplified or low order
150 models of the building envelope and the heat pump performance: these are detailed respectively in
151 sections 2.2 and 2.3. From the optimal control trajectory calculated over the horizon of the next 24
152 hours, only the first values are sent to TRNSYS, before a new computation of the MPC is carried out
153 and new values are obtained. In practice, the Type155 of TRNSYS enables to establish the connection
154 between both software.



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Figure 1. Co-simulation scheme between TRNSYS and MATLAB.

157 2.2. Building modelling

158 2.2.1. Study case and detailed model

159 The present study focuses on the Mediterranean climate and the typical residential buildings
160 constructed in this zone. They present the characteristics of having relatively balanced heating and
161 cooling loads in winter and summer. Therefore such buildings can be used for demand response in
162 both seasons. However, despite the great amount of literature on MPC and building energy flexibility
163 published in the recent years, few studies have focused on cooling applications, and even less on
164 study cases that make use of flexibility in both seasons [8]. Given this state of the art, the authors have
165 deemed worthy to investigate in more details the potential of energy flexibility of Mediterranean
166 buildings.

167 A typical block of flats of the region of Catalonia in Spain was chosen as a case study. In
168 particular, one flat situated on the first floor is studied in details. The apartment, where lives a family
169 of four, comprises 4 bedrooms, a living room, kitchen and bathroom for a total surface of 110 m². The
170 external walls contain 12 cm of insulation which represents a high insulation level for the Spanish
171 climate. The HVAC systems comprise an air-to-water heat pump which provides heating or cooling
172 to the Fan-Coil Units (FCU) situated in the rooms. The heat pump also contains an integrated 200
173 liters tank for storing DHW. The apartment is simulated in TRNSYS, with a detailed model that was
174 previously validated with experimental metered data [21], [22]. This detailed model runs with a time
175 step of 3 minutes, enabling to capture short-term variations with sufficient accuracy.

176 2.2.2. Reduced order simplified RC model: structure and variables

177 For reasons of computation effort, simplified and linear models are necessary in the MPC
178 framework to predict the dynamic behavior of the building [23]. A state-space model of the building
179 study case was thus developed and identified through grey-box modelling techniques. The structure

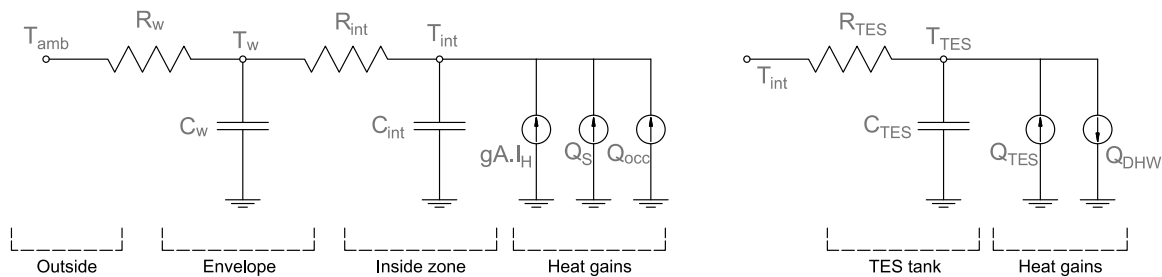
180 represented in Figure 2 was chosen, with three temperature states $\mathbf{x} = [T_{int} \ T_w \ T_{TES}]^T$: the indoor
 181 temperature, an intermediate temperature at the inside surface of the walls, and the average water
 182 tank temperature. It should be emphasized that such simplified models are developed only for
 183 control purposes, and not for matching exactly with the real building structure, therefore the level of
 184 details is kept to a minimum.

185 The first state T_{int} lumps all the rooms of the apartment into one single operative temperature
 186 state, which is sufficient for MPC applications as shown for example in [24]. Its associated capacity
 187 C_{int} mostly represents the heat capacity of the air, furniture and internal partitions present within
 188 the entire inside zone, and considered as a single body [25], [26]. Lumping these elements of different
 189 thermal capacities into the single parameter C_{int} represents an important simplification, however the
 190 purpose of the simplified model is only to provide a general prediction of the building dynamics for
 191 the controller, and in this scope such assumption is valid, even if the physical phenomena are not
 192 represented in the most accurate manner. External heat inputs enter the building at the level of the
 193 state T_{int} : the heat naturally emitted by the occupants and the equipment Q_{occ} , the heat gains due to
 194 the ground horizontal solar irradiation I_H (buffered by the aperture area coefficient gA) and the heat
 195 Q_S provided by the FCU and heat pump system (negative in case of cooling).

196 The second state T_w represents an intermediate temperature at the surface of the external walls,
 197 and its associated capacity C_w covers the heat capacity of the massive walls. T_w is linked with the
 198 outside temperature T_{amb} through the resistance of the walls R_w . The different dynamics of the two
 199 states are therefore both captured by this type of model. A first order model lumping all the thermal
 200 capacitance into a single parameter would not have been able to capture both the fast dynamics of
 201 the indoor zone and the slower dynamics of the massive structural elements. On the other hand, a
 202 third order model with an additional capacity accounting for internal walls and/or furniture could
 203 represent an alternative modelling approach, but adding unknown parameters increases the
 204 complexity of the obtained model and of the identification process. The second order modelling
 205 approach presented here is thus considered sufficient for MPC applications [26], and was used in
 206 many previous works as shown in the introductory review of [27].

207 Moreover, the DHW tank constitutes an additional state T_{TES} , which represents the average
 208 water temperature of the tank under a fully mixed tank assumption. The capacity C_{TES} covers the
 209 heat capacity of the 200 liters of water and the resistance R_{TES} takes into account the insulation of
 210 the tank. The DHW tank is charged through the heat Q_{TES} (positive term) coming from the heat
 211 pump circuit, and discharged with the heat tapped by the occupants Q_{DHW} (negative term, which
 212 follows the deterministic tapping program L from the standard [28]).

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Figure 2. Representation of the simplified RC model.

216 To conform to the state-space model format, the model takes the form of Eq.(1), which stems
 217 from writing the differential equations ruling the heat transfers of every state. For clarity, the matrix
 218 \mathbf{B} is separated into \mathbf{B}_u which corresponds to the controllable inputs $\mathbf{u} = [Q_S \ Q_{TES}]^T$, and \mathbf{B}_e which
 219 corresponds to the exogenous, non-controllable inputs $\mathbf{e} = [T_{amb} \ I_H \ Q_{occ} \ Q_{DHW}]^T$. The considered
 220 relevant outputs are $\mathbf{y} = [T_{int} \ T_{TES}]^T$. The continuous time model is discretized using a 12 minutes
 221 sampling time for use into the discrete MPC scheme.

222

$$\begin{cases} \dot{x} = A \cdot x + B_u \cdot u + B_e \cdot e \\ \dot{y} = C \cdot x \end{cases} \quad (1)$$

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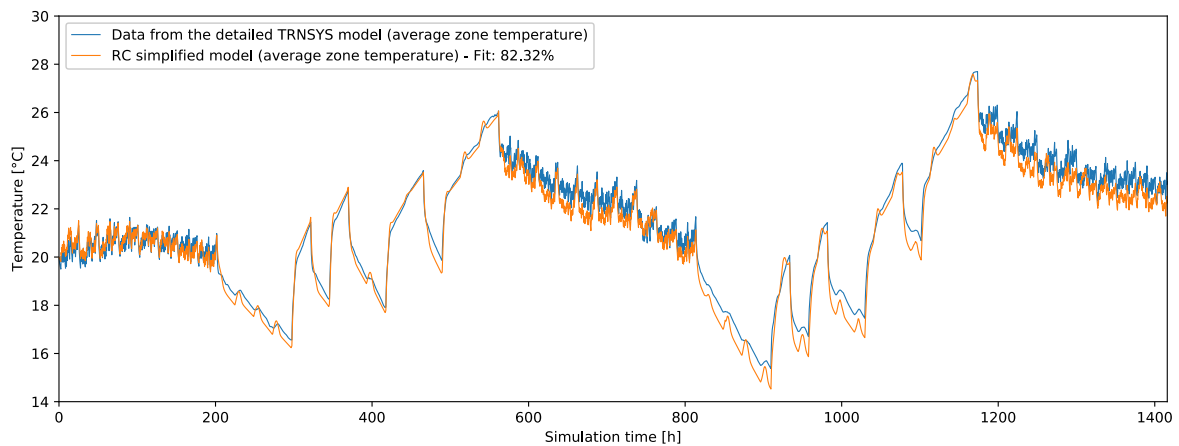
With:

$$A = \begin{bmatrix} -\frac{1}{R_{int}C_{int}} & \frac{1}{R_{int}C_{int}} & 0 \\ \frac{1}{R_{int}C_w} & -\frac{1}{R_wC_w} - \frac{1}{R_{int}C_w} & 0 \\ \frac{1}{R_{TES}C_{TES}} & 0 & -\frac{1}{R_{TES}C_{TES}} \end{bmatrix}, \quad B_u = \begin{bmatrix} \frac{1}{C_{int}} & 0 \\ 0 & 0 \\ 0 & \frac{1}{C_{TES}} \end{bmatrix},$$

$$B_e = \begin{bmatrix} 0 & \frac{gA}{C_{int}} & \frac{1}{C_{int}} & 0 \\ \frac{1}{R_wC_w} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{C_{TES}} \end{bmatrix} \quad \text{and} \quad C = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

228 2.2.3. Reduced order simplified RC model: identification process

229 The building part of this RC model was identified with data generated by the detailed model
230 created and previously validated in TRNSYS [21]. The parameters to be identified were R_{int} , C_{int} ,
231 R_w , C_w and gA (R_{TES} and C_{TES} were assumed based on manufacturer datasheets). The inputs were
232 the outdoor temperature T_{amb} , the ground horizontal solar irradiation I_H and the total heat provided
233 to the indoor zone $Q_{occ} + Q_S$. In order to have enough dynamic content in the generated data, the
234 building model was excited following a Pseudo Random Binary Signal (PRBS) of the heating Q_S ,
235 similarly to the methodology described in [29] and the guidelines of the IEA EBC Annex 68 [30]. The
236 PRBS contains on-off cycles at different frequencies so that both the fast and slow responses of the
237 building are captured in the data, making the identification of the parameters easier and more
238 reliable. Finally, the observation measurements consisted of the temperatures of the states T_{int} and
239 T_w . The model identification was realized with the system identification toolbox of MATLAB [31]
240 ("greyest" method which uses Gauss Newton least square search), and the data generated covered
241 1400 hours, with time steps of 3 minutes. The results for heating season are presented in Figure 3 and
242 Table 1 (first row). The obtained fit reached 82.3%, which is satisfactory considering the low order of
243 the simplified model.
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Figure 3. Representation of the data (generated by a detailed model in TRNSYS) and the fitted RC model in heating mode.

248 The RC model preserves a certain structure which can be interpreted physically, therefore the
249 resistance and capacity values can be compared to an order of magnitude expected for these
250 parameters. Since a lot of smaller parameters are lumped into a limited number of R and C values (4
251 in this case), it can still result a difficult task to find suitable comparisons. Furthermore, the virtual
252 intermediate state T_w can "move" within the thickness of the wall, which would modify the balance

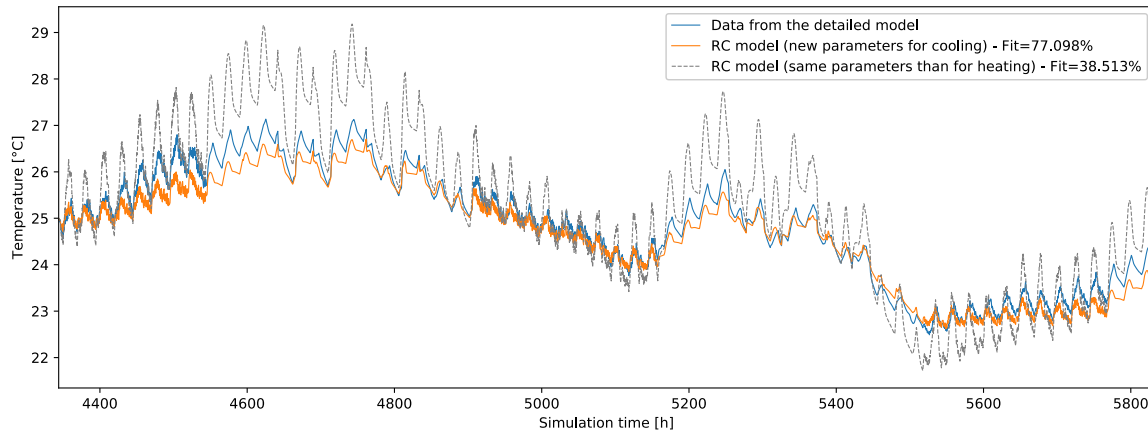
253 between the inside zone values (indexed int) and the wall values (indexed w). However, the overall
 254 resistance $R_{int} + R_w$ and the overall capacity $C_{int} + C_w$ should remain approximately at the same
 255 level. In the present case, the RC model gives $R_{int} + R_w = 10.1 K/kW$. When considering the
 256 resistance of the materials in all individual layers of the external walls, a parallel calculation gives
 257 $R_{eq} = 11.5 K/kW$, which is relatively close. For the capacities, we obtain $C_{int} + C_w = 26.0 kWh/K$.
 258 Summing all the capacities of the materials in the building gives $C_{eq} = 41 kWh/K$. However, only a
 259 part of the external walls mass is activated by the heating of the room (mostly until the insulation
 260 layer), the most external layers not being affected by a change of the indoor air temperature [25]. This
 261 concept is known as the effective capacity C_{eff} , and is calculated as a portion of C_{eq} . The ratio can
 262 vary in a great range and is not known precisely; values ranging from 1/2 to 1/3 are for example
 263 mentioned in [32]. Applying this rule to the present case $C_{eff} = 1/3 \cdot C_{eq} = 13.7 kWh/K$, which
 264 should be compared to $26.0 kWh/K$. A discrepancy is observed, in fact the ratio in the present case
 265 is closer to 2/3: $C_{int} + C_w = 0.63 \cdot C_{eq}$. Since there does not exist any agreement in the literature about
 266 the calculation of the effective capacity, it is preferred to keep the values originating from the model
 267 identification process, given that they offer a good fit with the data, **and that the primary goal of the**
 268 **model consists in predicting well rather than being physically meaningful.** Furthermore, the balance
 269 between the wall and the inside zone values is conserved with the obtained values of R and C: R_w
 270 and C_w are much greater than R_{int} and C_{int} respectively, which is expected since the massive walls
 271 have a higher resistance and capacity than the air of the inside zone.

272 **Table 1.** Parameters of the RC model for heating and cooling.

Coefficient	R_{int}	R_w	R_{TES}	C_{int}	C_w	C_{TES}	gA
Unit	K/kW	K/kW	K/kW	kWh/K	kWh/K	kWh/K	m ²
Value (heating)	1.089	9.013	601	1.771	24.22	0.29	1.948
Value (cooling)	0.286	9.404	601	1.771	45.648	0.29	1.558

273
 274 Theoretically, the values of resistances and capacities obtained in the heating case should also
 275 be valid for the cooling case, since they are intrinsic parameters of the building. However, they are
 276 subject to changes, for instance the thermal resistance or capacity of a material depend on its
 277 temperature, therefore the situation varies with the different boundary conditions in winter and
 278 summer. This is especially true for the aperture area gA , which represents the proportion of the
 279 outside solar irradiation entering the building, since the sun angle changes significantly between
 280 seasons. It can be observed in Figure 4 that keeping the same parameters results in a poor model fit
 281 (38.5%) and the apparition of temperature peaks in the cooling season. For this reason, the model
 282 identification process is repeated in the cooling mode; **this illustrates the limits of using simplified**
 283 **models.** The methodology remains the same however: the building is virtually excited with a PRBS
 284 signal on the cooling parameter Q_s , which is negative in this case. The parameters obtained for the
 285 heating case are used as initial values of this identification process.

286 The obtained values of the parameters for cooling are presented in the second row of Table 1.
 287 The simulation results of this model are compared in Figure 4 with the original TRNSYS model and
 288 with the simulation results the heating RC model would have given in the cooling scenario. The total
 289 resistance of the model $R_{int} + R_w = 9.69 K/kW$ stays stable compared to the heating case
 290 ($10.1 K/kW$), although the internal resistance has decreased. On the other hand, the total capacity
 291 increases to $C_{int} + C_w = 47.4 kWh/K$ (compared to $26.0 kWh/K$ in heating). One possible
 292 explanation resides in the fact that in reality, the solar irradiation also hits the wall directly (and thus
 293 affects the intermediate state T_w), and this phenomenon has greater amplitude in summer. Since this
 294 is not represented in the chosen RC model, the parameter estimation process instead decreased the
 295 resistance R_{int} between the two states, so that the external input I_H also affects the state T_w in a
 296 more direct manner. As a compensation for this reduced resistance, the capacity state C_w is increased
 297 to act as a buffer. Moreover, the aperture area gA has decreased in the cooling model, since the sun
 298 angle is higher and thus direct irradiation do not penetrate as deep into the building as in the heating
 299 case.



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Figure 4. Two different fittings of the RC model for cooling.

302 The parameter estimation process enabled to emphasize that simplified models for MPC
303 applications in heating and cooling mode should be differentiated. In fact, the RC model simply is a
304 linearization of a detailed model (or a real building) around an operation point; and since this
305 operation point changes significantly between winter and summer, it is preferable to adapt the model
306 as well. In the present case, the RC model was obtained from data created by another, more detailed
307 model, but the identification process would be similar with monitoring data recorded from a real
308 building, although some challenges would arise **with the uncertainties of the input data**, or if the wall
309 temperature measurement is needed.

310 2.3. Modelling of heat pump performance from experimental static tests data

311 When the MPC controller considers the electricity use of the system (see later section 2.5), a
312 model of its performance needs to be provided within its objective function, in order to pass from the
313 thermal energy (determined by the MPC algorithm) to the corresponding consumption of the heat
314 pump. This performance evaluation most often takes the form of a Coefficient of Performance (COP),
315 where $COP = Q/P_{el}$, **the ratio between the thermal power Q and electrical power P_{el}** . The COP of a
316 VSHP depends on various parameters among which the supply temperature T_{sup} , the ambient
317 temperature T_{amb} , the frequency of the compressor f , the part-load ratio PLR , the absolute value of
318 the thermal power Q , the temperature difference between water supply and return ΔT [12], [33],
319 [34]. Some of these parameters are strongly correlated (e.g. the heat pump will work at lower
320 frequency if the part-load ratio is lower), therefore selecting a subset of these parameters will be
321 sufficient to obtain a reliable model of the heat pump performance.
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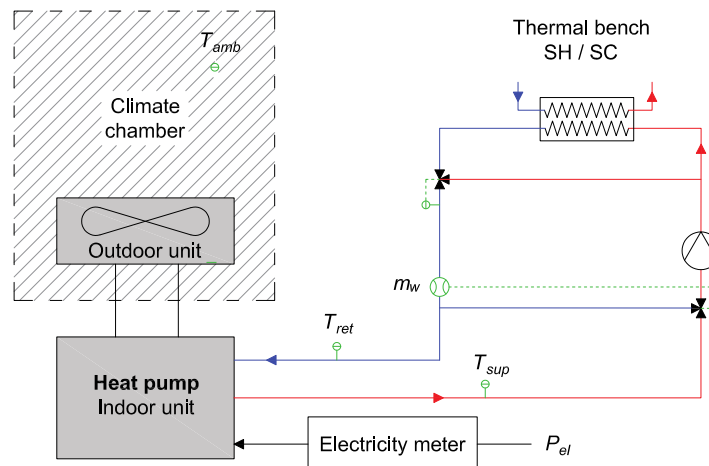


Figure 5. Experimental setup for the measurement of the static tests points.

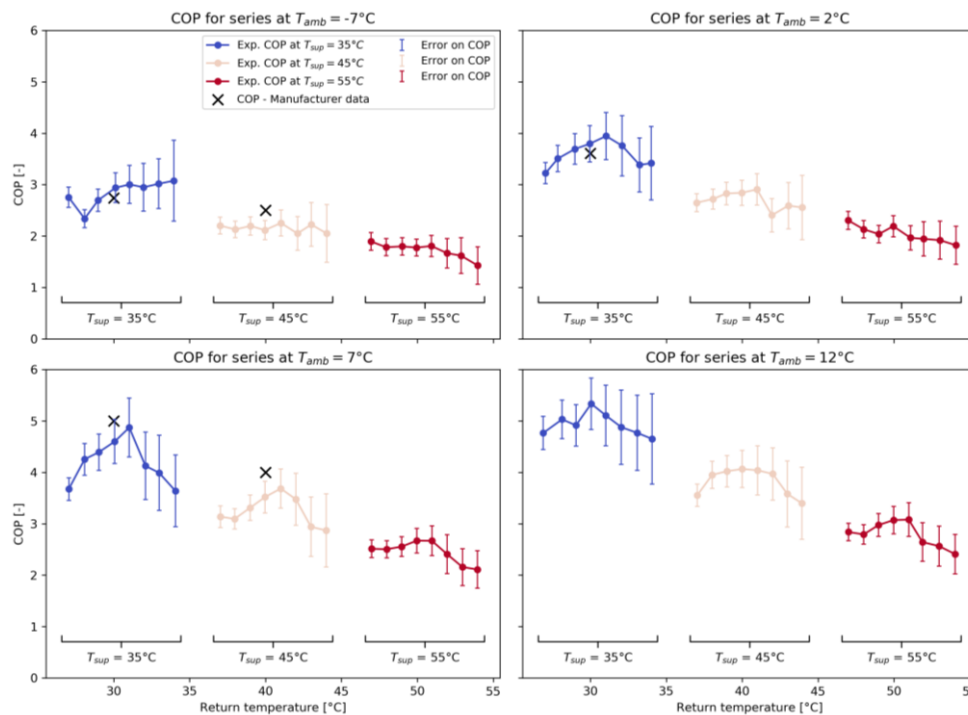
325 Static tests were realized in an experimental setup to obtain data of the selected equipment, as
 326 shown in Figure 5. The device tested in the laboratory is a Hitachi Yutaki reversible air-to-water
 327 VSHP of nominal heating power 10 kW. The outdoor unit of the heat pump was placed in a climate
 328 chamber where the air temperature can be controlled in a range of -30°C to 40°C . The water circuit
 329 was connected to a thermal bench emulating the load, whether in heating or cooling mode.

330 2.3.1. Heating static tests

331 The following parameters were changed in their respective ranges for the static tests in heating
 332 mode: $T_{amb} \in \{-7^{\circ}\text{C}; 2^{\circ}\text{C}; 7^{\circ}\text{C}; 12^{\circ}\text{C}\}$, $T_{sup} \in \{35^{\circ}\text{C}; 45^{\circ}\text{C}; 55^{\circ}\text{C}\}$ and $\Delta T \in [1^{\circ}\text{C}, 8^{\circ}\text{C}]$. The ranges of
 333 T_{amb} and T_{sup} correspond to the standard test conditions found in standard EN 14511-2 [35],
 334 enabling to compare with the manufacturer's data.

335 For each experimental point, at least 30 minutes of data were recorded in steady state, after
 336 leaving 20 minutes of transition between one point and the next one. The measured parameters (T_{sup} ,
 337 T_{ret} , \dot{m}_w , P_{el} , f , T_{amb}) were averaged over the measuring period. It was ensured that no defrost
 338 operation occurred during the measuring period, to avoid distorted measurements. The experimental
 339 points are presented in Figure 6. It is observed that at low load ($\Delta T \leq 3^{\circ}\text{C}$), the heat pump is not able
 340 to modulate and exhibits an on-off cycling behavior that induces a low COP. At high load ($\Delta T \geq 6^{\circ}\text{C}$)
 341 in some cases, the heat pump cannot reach the desired set-point despite the compressor running at
 342 full speed, and a low COP is also observed. The imperfect control of the air temperature in the climate
 343 chamber (standard deviation up to 2°C in some cases) also explains some of the observed deviations
 344 from the desired set-points. In the laboratory, the temperatures are measured with PT100 sensors that
 345 have a precision of $\pm 0.25\text{ K}$ (thus for the temperature difference in the water loop, the precision is ± 0.5
 346 K). The induction flow meter for the measurement of the water flow has a high precision of ± 0.2 to
 347 0.5% , which makes it negligible, and the power measurement has a precision of $\pm 1\%$.

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349

350 **Figure 6.** COP experimental points measured in the heating static tests, represented in function of
 351 T_{sup} , T_{ret} and T_{amb} . The manufacturer data (x markers) from the catalogue are also represented for
 352 comparison.

353 Two different models of the heat pump must be developed for the co-simulation framework: a
 354 detailed one to be used in TRNSYS (subscripted *det*), and a more simplified one for the MPC
 355 controller (subscripted *simpl*), as explained in section 2.1 and shown in Figure 1. Since the heat pump

356 cannot be controlled directly by deciding the frequency of the compressor (it is a ‘hidden’ internal
357 parameter), this variable was discarded for fitting the models.

358 For the simplified model, only terms of T_{amb} and T_{sup} are chosen as inputs, as shown in Eq.(2).
359

$$P_{el,simpl} = \left[\frac{1}{COP}(T_{sup}, T_{amb}) \right] \cdot Q = [a_0 + a_1 T_{sup} + a_2 T_{amb} + a_3 T_{amb}^2 + a_4 T_{sup} T_{amb}] \cdot Q \quad (2)$$

360

361 Since the only quantity that is of interest for the MPC objective is the inverse of the COP (later
362 multiplied by the thermal power Q to obtain the electrical power P_{el}), it is this amount which is
363 modelled. Furthermore, $1/COP$ presents a more linear behavior than the COP itself; a linear model
364 can then be retrieved more easily. The least square method was employed to fit the models on the
365 experimental data, and thus find the optimal values of the coefficients a_i which are presented in
366 Table 2. The series of experimental points with $T_{amb} = -7^\circ\text{C}$ was discarded to fit the model, since
367 such low temperatures never occur in the considered climate for the dynamic simulations in which
368 this model will be used. The model is therefore fitted around the operating conditions in which the
369 heat pump is supposed to function, i.e. it was realized on 72 points. The obtained RMSE was 0.18 kW
370 for the $P_{el,simpl}$ model (NRMSE = 6.4%). On Figure 7, the measured experimental data points are
371 compared with the COP model of Eq.(2). The model does not offer a perfect representation of the
372 data, however this result is considered sufficient given the restrictions of the linear model and the
373 later use of this model. A similar model obtained from the literature [12] was also plotted on Figure
374 7 for comparison: a clear offset is visible since the heat pump presented in that study is a different
375 model, but the same trend is conserved.

376 In previous literature [12], Verhelst et al. already discussed the formulation of the optimal
377 control problem in terms of COP. They found that modelling the heat pump performance in function
378 of (T_{sup}, T_{amb}) seems to perform almost as good as if the frequency of the compressor was
379 additionally taken into account. However, in the present work, Eq.(2) would become non-linear if
380 T_{sup} was kept as a variable in function of Q , and thus it would not be solvable in the current
381 configuration. For this reason, it is chosen to consider constant supply temperatures when accounting
382 for the heat pump performance. However, since the heat pump operates in two distinct modes (for
383 space heating or DHW production), two different supply temperatures are assigned, which still
384 enables to consider different efficiencies at two operating points. $T_{sup,SH,0} = 35^\circ\text{C}$ since the heat
385 pump operates at lower supply temperature in space heating, and $T_{sup,TES,0} = 55^\circ\text{C}$ since the DHW
386 must always be produced at high temperatures to keep the TES tank hot enough and avoid
387 propagation of legionella. As a summary, in the MPC controller the electricity use of the heat pump
388 for heating can be written as in Eq. (3):
389

$$P_{el,simpl,tot} = \left[\frac{1}{COP}(T_{sup,SH,0}, T_{amb}) \right] Q_{SH} + \left[\frac{1}{COP}(T_{sup,TES,0}, T_{amb}) \right] Q_{TES} \quad (3)$$

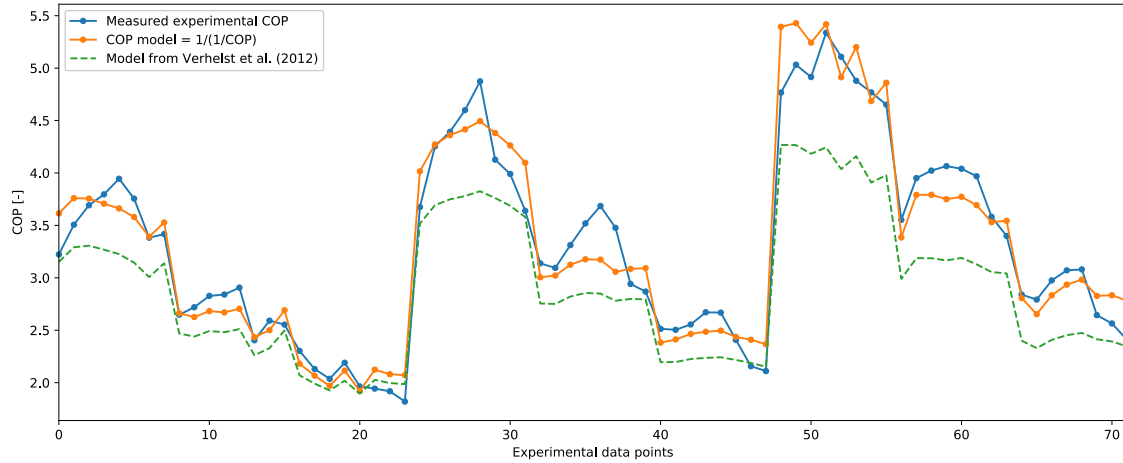
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391 Considering Eq.(3) in its objective function, the MPC algorithm will determine the optimal
392 values of Q_S and Q_{TES} over the prediction horizon. However, an additional equation is needed to
393 obtain the actual values of T_{sup} , which is the actual variable sent to the “real” building (TRNSYS
394 model). This equation represents the heat transfer between the water circuit of the heat pump and its
395 load. For SH, it corresponds to the emitters which in this case are Fan Coil Units (FCU), and Eq. (4) is
396 used. The coefficient M_S depends on the mass flow rate of the water circuit, the efficiency of the FCU
397 and their ventilation rate. A regression on TRNSYS simulation data led to identify the coefficient
398 $M_S = 0.222 \text{ kW/K}$. In the case of DHW, Eq. (5) is used and it corresponds to the tank charging. The
399 coefficient $M_{TES} = 2.32 \text{ kW/K}$ is obtained considering the water flow rate and a fully efficient heat
400 transfer between the two water circuits.
401

$$Q_S = M_S(T_{sup,S} - T_{int}) \quad (4)$$

$$Q_{TES} = M_{TES}(T_{sup,TES} - T_{TES}) \quad (5)$$

402



403

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405

Figure 7. Comparison of the fitted simplified COP model with the experimental data and another model from the literature [12] (in heating mode).

406

Table 2. Obtained coefficients of the heat pump performance models in heating mode.

Simple model – Heating mode							
Coefficient	a_0	a_1	a_2	a_3	a_4		
Value	-0.09792	0.01056	0.00252	-0.00013	-0.00024		
Detailed model – Heating mode							
Coefficient	b_0	b_1	b_2	b_3	b_4	b_5	b_6
Value	-1.3128	0.00076	0.00786	0.6488	0.2678	-0.0381	0.2831

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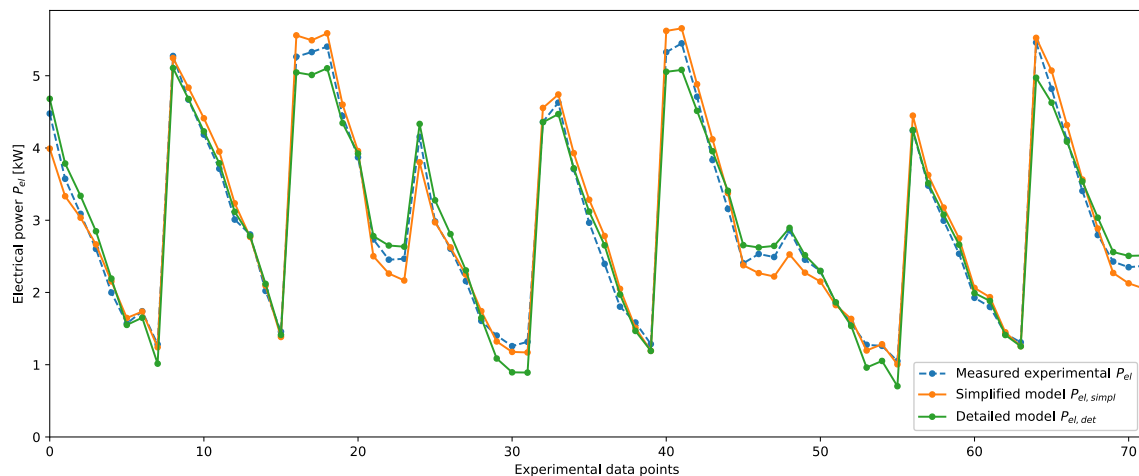
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416

For the detailed model, there are no constraints of linearity like in the MPC simplified model, therefore it contains squared and bilinear terms. The fit is realized on the same data and with the same technique. The part-load ratio term is $PLR = Q/Q_{max}$, with $Q_{max} = 10 \text{ kW}$ chosen as the constant nominal capacity, since this capacity is always guaranteed independently of the operating conditions. The resulting equation is presented in Eq. (6) and the obtained coefficients b_i in Table 2. For the detailed $P_{el,det}$ model, RMSE = 0.121 kW and NRMSE = 5.46%, thus the improvement is relatively minor. This can be observed in Figure 8, where both the detailed and simplified models of P_{el} are represented against the corresponding experimental data. Small discrepancies are observed at the extreme low and high values of P_{el} .

$$P_{el,det} = b_0 + b_1 T_{sup}^2 + b_2 T_{amb} + b_3 PLR + b_4 Q + b_5 T_{amb} Q + b_6 PLR T_{amb} \quad (6)$$

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Figure 8. Comparison of the detailed and simplified P_{el} models with the experimental data (in heating mode).

421 2.3.2. Cooling static tests

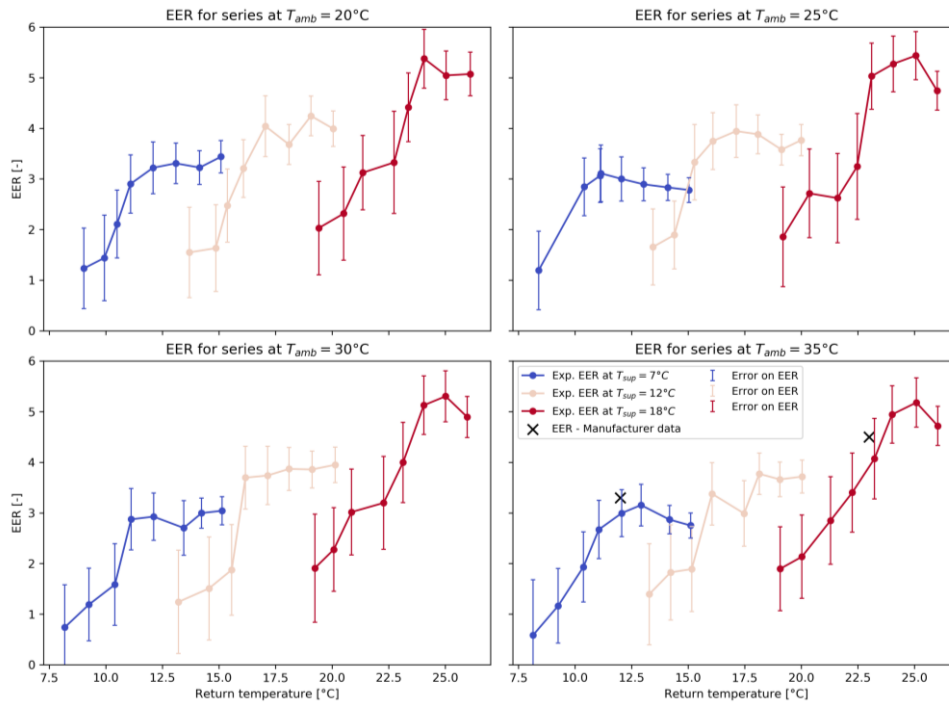
422 A similar methodology was adopted for the cooling mode of the heat pump. In that case, the
 423 parameters for the experimental static tests were varied in the following ranges: $T_{amb} \in$
 424 $\{20^\circ\text{C}; 25^\circ\text{C}; 30^\circ\text{C}; 35^\circ\text{C}\}$, $T_{sup} \in \{7^\circ\text{C}; 12^\circ\text{C}; 18^\circ\text{C}\}$ and $\Delta T \in [-8^\circ\text{C}, -1^\circ\text{C}]$. The results of the data
 425 points in terms of EER (equivalent of COP for cooling) are represented in Figure 9. Contrary to the
 426 heating tests, it appears that the efficiency of the heat pump in cooling mode does not depend much
 427 on the outdoor temperature T_{amb} . Furthermore, a certain load ($|\Delta T| \geq 3^\circ\text{C}$) is required for the heat
 428 pump to function at a higher efficiency, otherwise it will exhibit an on and off behavior, which
 429 produces start-up losses and deteriorates the overall EER.

430 The same methodology than in heating mode was applied to obtain a model of the quantity
 431 $1/\text{EER}$. However, the fit obtained was not satisfactory, hence the electricity use P_{el} of the heat pump
 432 in cooling mode was directly modelled instead. The simpler model to be used by the MPC controller
 433 is presented in Eq. (7), while the more detailed formulation for the TRNSYS simulation is presented
 434 in Eq. (8). In these equations, Q_{SC} is the thermal cooling power (counted positive).

$$P_{el,simpl} = c_0 + c_1 T_{amb} + c_2 T_{sup,SC} + c_3 Q_{SC} \quad (7)$$

$$P_{el,det} = d_0 + d_1 T_{amb} + d_2 T_{sup,SC} + d_3 Q_{SC} b_0 + d_4 PLR + d_5 T_{sup,SC} Q_{SC}^2 + d_6 PLR Q_{SC}^2 \quad (8)$$

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Figure 9. EER experimental points measured in the cooling static tests, represented in function of T_{sup} , T_{ret} and T_{amb} . The manufacturer data (x markers) from the catalogue are also represented for comparison.

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The points chosen for the model identification are only the points with $|\Delta T| \leq 5^\circ\text{C}$. The heat pump model is not suited for higher values of $|\Delta T|$ (it does not reach the desired set-point temperature in these cases), and furthermore, such high loads are not expected in the dynamic simulations in which the model will be used. The model fitting is thus realized on 60 points. After the least square method is applied, an RMSE value of 0.097 kW is obtained (NRMSE: 7.46%) for the simpler model. For the more detailed model, RMSE = 0.078 kW (NRMSE: 6.0%), therefore the gain in precision is relatively small. The optimal c_i and d_i coefficients are presented in Table 3. It can be noted that the coefficients c_1 and d_1 , associated with the ambient temperature, are the lowest coefficients, confirming that this input parameter has little influence on the heat pump performance. The comparison between the models and the data points is presented in Figure 10. The simplified

451 model is considered satisfactory given its simplicity and despite the fact that the spikes of electricity
 452 consumption are not always captured, whereas the detailed model performs better at these points, as
 453 seen in Figure 10.

454 It should be noted that this model is only valid when the heat pump is turned on (approximately
 455 for values of $Q_{SC} \geq 2 \text{ kW}$). To obtain $P_{el,simpl} = 0 \text{ kW}$ when $Q_{SC} = 0 \text{ kW}$, the coefficients c_0 , c_1 and
 456 c_2 must be multiplied by the on-off signal δ_S (see in section 2.5). To summarize, the simplified
 457 electricity use of the heat pump in cooling mode for the MPC is formulated in Eq.(9).
 458

$$P_{el,simpl,tot} = [(c_0 + c_1 T_{amb}(k) + c_2 T_{sup,SC}) \cdot \delta_S(k) + c_3 Q_{SC}(k)] + \left[\frac{1}{COP} (T_{sup, TES}, T_{amb}) \right] Q_{TES} \quad (9)$$

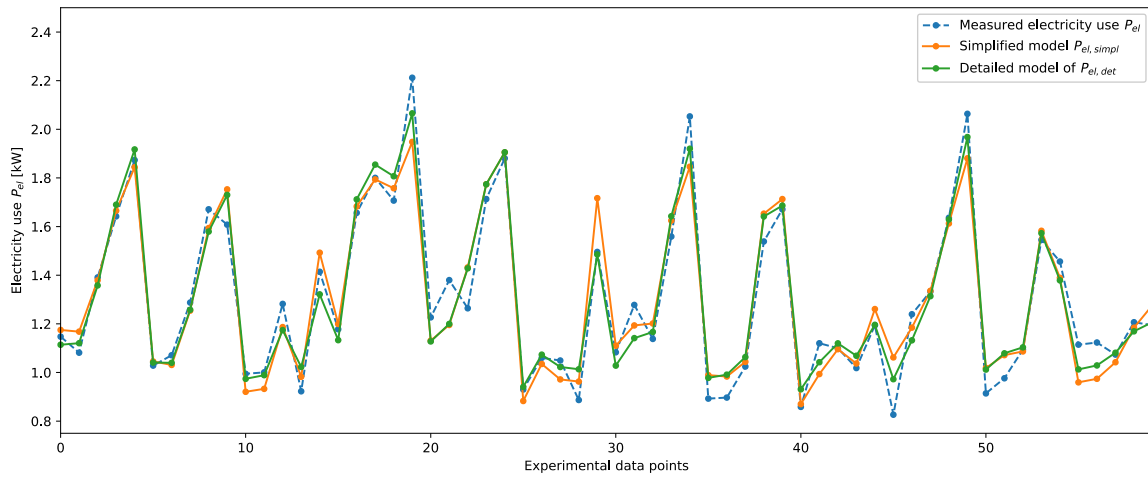
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Table 3. Obtained coefficients of the P_{el} models in cooling mode.

Simple model – Cooling mode							
Coefficient	c_0	c_1	c_2	c_3			
Value	1.2313	0.0008	-0.0343	0.1486			
Detailed model – Cooling mode							
Coefficient	d_0	d_1	d_2	d_3	d_4	d_5	d_6
Value	1.0355	0.0007	-0.021	0.1902	-0.0527	-0.0009	0.0073

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Figure 10. Comparison of the fitted P_{el} models with the experimental data points.

464

2.4. Model Predictive Control algorithm

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The overall MPC control algorithm was developed to manage the heating and cooling of the building, and to exploit the flexibility of those flexible heat pump loads. The mathematical formulation of this problem is presented in Algorithm 1. The model was already described in section 2.2; the constraints and the objective function are clarified in the following subsections.

Algorithm 1 – Model Predictive Controller

Objective:

$$\min_{u, \delta} J = [\alpha_\varepsilon J_\varepsilon + \alpha_{\Delta u} J_{\Delta u} + (1 - \alpha_\varepsilon - \alpha_{\Delta u}) J_{obj}]$$

Subject to:

$$\forall k \in \llbracket 1, N \rrbracket$$

Model:

$$\begin{cases} \mathbf{x}(k+1) = \mathbf{A} \cdot \mathbf{x}(k) + \mathbf{B}_u \cdot \mathbf{u}(k) + \mathbf{B}_e \cdot \mathbf{e}(k) \\ \mathbf{y}(k+1) = \mathbf{C} \cdot \mathbf{x}(k) \end{cases}$$

Constraints on the inputs:

$$\begin{cases} \delta_S(k) \cdot \underline{Q_S} \leq Q_S(k) \leq \delta_S(k) \cdot \overline{Q_S} \\ \delta_{TES}(k) \cdot \underline{Q_{TES}} \leq Q_{TES}(k) \leq \delta_{TES}(k) \cdot \overline{Q_{TES}} \\ \delta_S(k) + \delta_{TES}(k) \leq 1 \end{cases}$$

Constraints on the outputs:

$$\begin{cases} \underline{T_{int}}(k) - \varepsilon(k) \leq T_{int}(k) \quad (\text{heating}) \\ \overline{T_{int}}(k) \leq T_{int}(k) + \varepsilon(k) \quad (\text{cooling}) \\ \underline{T_{TES}} - \varepsilon(k) \leq T_{TES}(k) \quad (\varepsilon \geq 0) \end{cases}$$

470 2.4.1. Constraints on the inputs

471 Continuous variables (i.e. the thermal powers Q_S and Q_{TES} delivered respectively to the
472 building and the tank) were chosen as the inputs controllable by the MPC, to avoid including the heat
473 emitter within the model. In order to switch from the space heating/cooling to the DHW production
474 mode, it is however necessary to introduce the binary variables δ_S and δ_{TES} . They equal 1 when their
475 respective mode is activated, 0 otherwise. The heat pump can only operate in one mode at a time, so
476 the binary variables are constrained by $\delta_S(k) + \delta_{TES}(k) \leq 1$. Introducing binary variables transforms
477 the nature of the control problem, and thus the MPC must resort to Mixed Integer Linear
478 Programming (MILP) instead of simpler Linear Programming (LP) to solve it [36].

479 Such binary variables also enable to limit the heating power Q in a certain range $[Q; \overline{Q}]$ when
480 the heat pump is turned on. With only the continuous variables Q_S and Q_{TES} , the MPC could have
481 decided to provide very low values of the heating power Q , without turning it off. In reality, a heat
482 pump system has a minimum power below which it cannot operate; for instance with the considered
483 equipment, the frequency of the compressor cannot drop below 31 Hz, if the load is still too low for
484 that frequency the heat pump would switch off. The binary variables and the ranges of heating power
485 enable to reproduce this behavior. The chosen ranges correspond to the manufacturers specifications
486 and the range of operation observed in static tests: $[Q_{SC}; \overline{Q_{SC}}] = [-8 \text{ kW}; -2.5 \text{ kW}]$ in cooling
487 mode, $[Q_{SH}; \overline{Q_{SH}}] = [3 \text{ kW}; 10 \text{ kW}]$ in heating mode, and $[Q_{TES}; \overline{Q_{TES}}] = [10 \text{ kW}; 10 \text{ kW}]$ in DHW
488 production mode (DHW is always produced at full load of the heat pump).

489 2.4.2. Constraints on the outputs

490 For comfort reasons, additional constraints are set to the two outputs of the MPC controller. The
491 internal zone temperature T_{int} must stay above the boundary $\underline{T_{int}} = 20^\circ\text{C}$ in winter or below $\overline{T_{int}} =$
492 26°C in summer. These constraints are relaxed with the slack variable ε : in this way, small excursions
493 outside the hard constraints are permitted at a certain cost (see also next section 2.4.3). Regarding the
494 tank storing DHW, its temperature T_{TES} must stay above $\underline{T_{TES}} = 50^\circ\text{C}$ to avoid the spread of
495 legionella. In fact, an additional anti-legionella protection (rising the temperature of the tank to 70°C
496 for 10 minutes) is normally activated every week for more safety, but this feature is not studied in the
497 present work since the considered simulations only last 3 days and the anti-legionella setting make
498 use of an additional electrical resistance to reach 70°C , not the heat pump itself.

499 2.4.3. Objectives of the MPC

500 As seen in Algorithm 1, the MPC algorithm intends to minimize a certain objective over the
501 prediction horizon. In the present case, the objective comprises in fact three aspects, weighted by the
502 corresponding coefficients α :

- 503 • maintaining the comfort level with the objective J_ε , as shown in Eq. (10). In fact, it consists in
504 limiting the discomfort, or in other words, avoid the excursions outside the defined
505 temperature boundaries. ε is a slack variable that enables to soften the constraints on the
506 output temperatures. In principle $\varepsilon = 0$, but exceptionally, the temperature is allowed to
507 trespass the boundaries ($\varepsilon > 0$); the cost of this constraint violation is reflected in the objective

508 J_ε , as shown in Eq. (10). As another advantage, this formulation avoids infeasibility of the
 509 MPC in the case where the initial states are found outside the boundaries (which typically
 510 happens at start-up for instance, or due to discrepancies of the model when operating close
 511 to the boundaries).

$$J_\varepsilon = \sum_{k=1}^N \varepsilon(k) \quad (10)$$

512 • smoothing the control actions to avoid too frequent on-off switching with the objective $J_{\Delta u}$,
 513 as shown in Eq. (11).

$$J_{\Delta u} = \sum_{k=2}^N \|u(k) - u(k-1)\|_1 \quad (11)$$

514 • an actual objective J_{obj} which can be the minimization of the thermal energy delivered to
 515 the building J_{en} , the minimization of the cost of the electricity used by the heat pump for
 516 delivering this energy J_{cost} , or the minimization of the CO₂ emissions related to this
 517 electricity use J_{CO_2} . The formulation of these objectives is detailed in the next section 2.5.

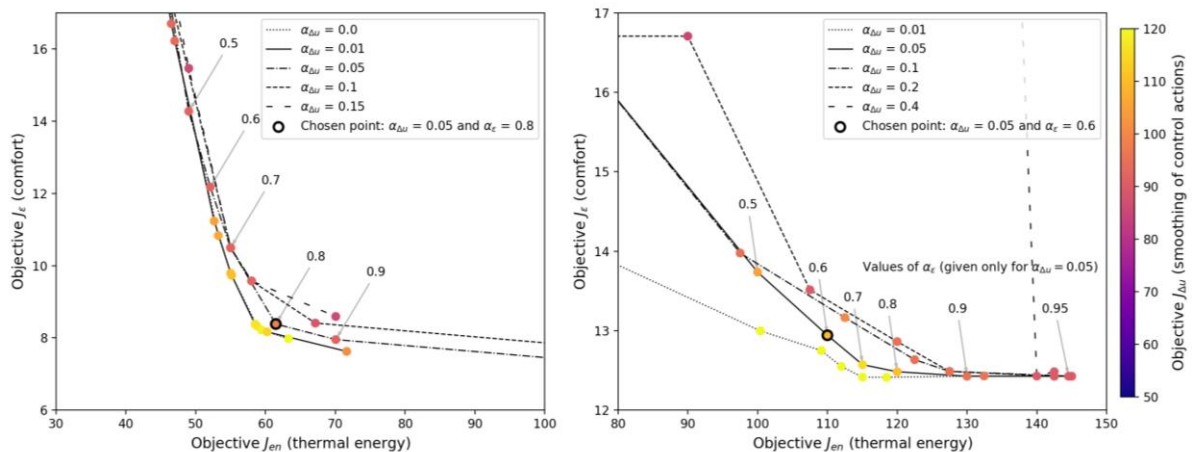
518 2.5. Tested MPC configurations

519 2.5.1. Thermal energy minimization (MPC ThEnergy)

520 In this configuration, the quantity minimized by the MPC over the control horizon is the thermal
 521 energy delivered to the building (in addition to the smoothing and discomfort terms), hence without
 522 taking into account the variable efficiency of the heat pump system. The mathematical formulation
 523 with $J_{obj} = J_{en}$ is written in Eq. (12):

$$J_{en} = \sum_{k=1}^N \|u(k)\|_1 = \sum_{k=1}^N [Q_S(k) + Q_{TES}(k)] \quad (12)$$

524 In the overall objective of the MPC, J_{en} is combined with two other objectives (comfort and
 525 smoothing of the control). To determine the weighting coefficients α between these different
 526 quantities, Pareto fronts are plotted, where several values of the coefficients are tested on simulations.
 527 The results are plotted separating the different components of the objective function, as can be seen
 528 in Figure 11. In this graph, the J_ε objective is represented on the y-axis, J_{en} on the x-axis, and $J_{\Delta u}$
 529 through color mapping of the points. The different lines correspond to different values of $\alpha_{\Delta u}$, while
 530 the different points of a line correspond to different values of α_ε .
 531



532

533 **Figure 11.** Pareto fronts for the J_{en} objective, in the heating (left) and cooling (right) modes.

534 To choose appropriate values of the weighting coefficients, one must remain in the right
 535 horizontal part of the lines, where the discomfort J_ε is at its minimum. At the same time, it is
 536 preferable to minimize the thermal energy J_{en} , therefore to stay as much on the left of the graph as

537 possible. Furthermore, one must also avoid unreasonably high computation times and high values of
 538 $J_{\Delta u}$ (yellow colors on the present graph), even though this is the least relevant parameter (with time
 539 steps of 12 minutes, a cyclic on-off behavior would not cause many problems). As a compromise
 540 between all these considerations, the values chosen are $\alpha_{\Delta u} = 0.05$ and $\alpha_{\varepsilon} = 0.8$ for the J_{en} objective
 541 in heating mode; $\alpha_{\Delta u} = 0.05$ and $\alpha_{\varepsilon} = 0.6$ in cooling mode. The same approach is repeated for every
 542 MPC configuration.

543 2.5.2. Cost minimization (MPC Cost)

544 In this configuration, the cost of the electricity used by the heat pump is minimized by the MPC.
 545 This configuration presents an increased complexity, since the electricity use is introduced in the
 546 equation (and not only the delivered heat as previously), and therefore the heat transmission by the
 547 emitter and the performance of the heat pump must both be taken into account into the objective
 548 function. For this purpose, the simplified models detailed in section 2.3 are utilized.

549 The electricity used by the heat pump is then multiplied at every time step by a time-varying
 550 cost of electricity E_{el} (in €/MWh, changing every hour), normalized by $E_{el,max}$. In the present case,
 551 the voluntary price for small consumers (PVPC in Spanish) is used: it is an available tariff for
 552 consumers of less than 10 kW contracted power in Spain, which historical data and forecasts are
 553 public [37]. Introducing such a penalty helps the decision-making process of the MPC since it already
 554 predefines favorable or non-favorable periods for when to operate the systems. It should be noted
 555 that the other costs of the building (notably related to the energy use of the FCU fans) are not included
 556 in the cost objective J_{cost} , since they would not influence the calculation of the optimal MPC plan
 557 (constant energy use when the FCU are on). The formulation with $J_{obj} = J_{cost}$ differs in heating (Eq.
 558 (13)) and in cooling (Eq.(14)). The Pareto fronts for J_{cost} are presented in Figure 12. In this
 559 configuration, the chosen values are $\alpha_{\Delta u} = 0.01$ and $\alpha_{\varepsilon} = 0.15$ for cooling, $\alpha_{\Delta u} = 0.01$ and $\alpha_{\varepsilon} = 0.5$
 560 for heating.
 561

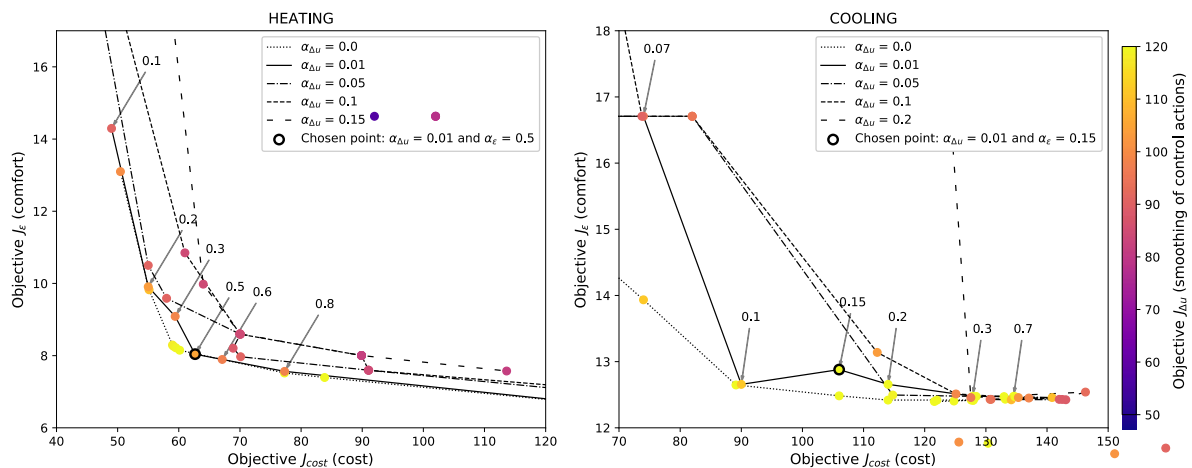
$$J_{cost} = \sum_{k=1}^N [P_{el,SH}(k) + P_{el,TES}(k)] \cdot \frac{E_{el}(k)}{E_{el,max}} \quad (13)$$

$$= \sum_{k=1}^N \left[\frac{1}{COP} (T_{sup,S}, T_{amb}(k)) \cdot Q_S(k) + \frac{1}{COP} (T_{sup,TES}, T_{amb}(k)) \cdot Q_{TES}(k) \right] \cdot \frac{E_{el}(k)}{E_{el,max}} \quad (14)$$

$$J_{cost} = \sum_{k=1}^N [P_{el,SC}(k) + P_{el,TES}(k)] \cdot \frac{E_{el}(k)}{E_{el,max}}$$

$$= \sum_{k=1}^N \left[(c_0 + c_1 T_{amb}(k) + c_2 T_{sup,SC}) \cdot \delta_S(k) + c_3 Q_S(k) + \frac{1}{COP} (T_{sup,TES}, T_{amb}(k)) \cdot Q_{TES} \right] \cdot \frac{E_{el}(k)}{E_{el,max}}$$

562



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Figure 12. Pareto fronts for the J_{cost} objective, in the heating (left) and cooling (right) modes.

565 2.5.3. CO₂ emissions minimization (MPC CO₂)

566 This formulation resembles the previous J_{cost} , except that the monetary cost E_{el} is replaced by
 567 a cost in terms of CO₂ emissions E_{CO_2} (in kgCO₂/kWh). For E_{CO_2} , the marginal emissions factor
 568 (MEF) is used. This parameter estimates the emissions savings that can be realized from a change in
 569 the load (i.e. a demand response action), given the state of the electrical grid. It differs from the
 570 average emissions factor since it considers the supposed merit order in which the different sources
 571 of electricity generation are activated. The MEF is computed for every hour according to the model
 572 and calculations described in [15]. The formulation with $J_{obj} = J_{CO_2}$ is presented in Eq. (15) (heating)
 573 and Eq. (16) (cooling). The Pareto curves for J_{CO_2} are plotted on Figure 13. In this configuration, the
 574 chosen values are $\alpha_{\Delta u} = 0.05$ and $\alpha_\varepsilon = 0.15$ for heating, $\alpha_{\Delta u} = 0.01$ and $\alpha_\varepsilon = 0.15$ for cooling.
 575

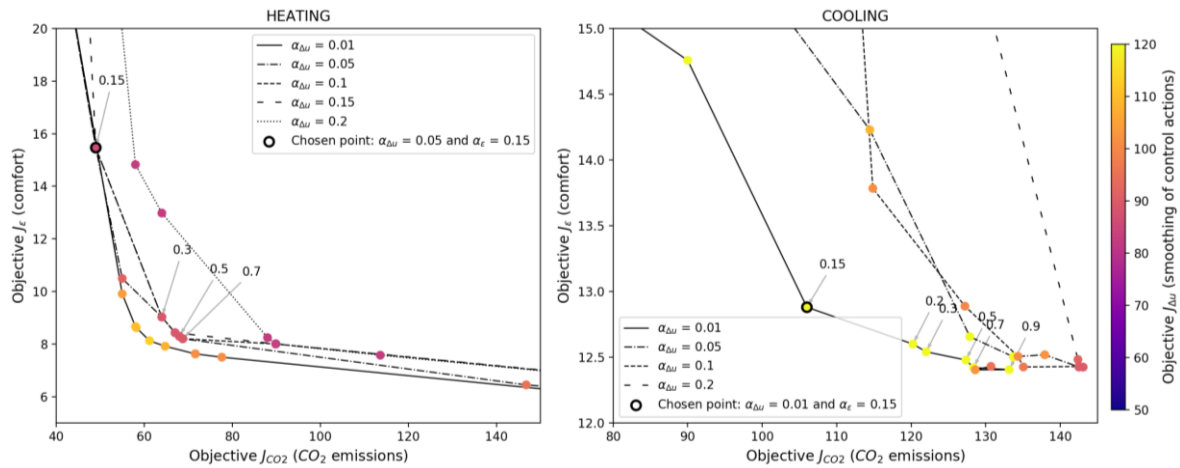
$$J_{CO_2} = \sum_{k=1}^N [P_{el,SH}(k) + P_{el,TES}(k)] \cdot \frac{E_{CO_2}(k)}{E_{CO_2,max}} \quad (15)$$

$$= \sum_{k=1}^N \left[\frac{1}{COP}(T_{sup,S}, T_{amb}(k)) \cdot Q_S(k) + \frac{1}{COP}(T_{sup,TES}, T_{amb}(k)) \cdot Q_{TES}(k) \right] \cdot \frac{E_{CO_2}(k)}{E_{CO_2,max}}$$

$$J_{CO_2} = \sum_{k=1}^N [P_{el,SC}(k) + P_{el,TES}(k)] \cdot \frac{E_{CO_2}(k)}{E_{CO_2,max}} \quad (16)$$

$$= \sum_{k=1}^N \left[(c_0 + c_1 T_{amb}(k) + c_2 T_{sup,SC}) \cdot \delta_S(k) + c_3 Q_S(k) + \frac{1}{COP}(T_{sup,TES}, T_{amb}(k)) \cdot Q_{TES} \right] \cdot \frac{E_{CO_2}(k)}{E_{CO_2,max}}$$

576



577

578

Figure 13. Pareto fronts for the J_{CO_2} objective, in the heating (left) and cooling (right) modes.

579 2.5.4. Other parameters

580

Table 4. Summary of the utilized weighting coefficients.

Mode	Heating			Cooling			
	Objective	J_{en}	J_{cost}	J_{CO_2}	J_{en}	J_{cost}	J_{CO_2}
Value of α_ε		0.8	0.5	0.15	0.6	0.15	0.15
Value of $\alpha_{\Delta u}$		0.05	0.01	0.05	0.05	0.01	0.01
Value of $\alpha_{obj} = (1 - \alpha_\varepsilon - \alpha_{\Delta u})$		0.15	0.49	0.8	0.35	0.84	0.84

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All the weighting coefficients are summarized in Table 4, and it can be seen that the values differ between heating and cooling, similarly than for the low order RC models. Among the other parameters intervening in the MPC configuration, the time horizon was chosen as 24 hours ahead, i.e. $N = 120$ time steps of 12 minutes. Choosing this value for the prediction horizon enables to capture the daily patterns occurring in the occupancy, weather and grid status evolutions. It was

587 shown in [17] that 24h is the most common prediction horizon for MPC in buildings; longer horizons
588 might be better suited if the time constant of the building is large (e.g. TABS applications), but are
589 not necessary otherwise. The discretization time step for the MPC is chosen as 12 minutes: in this
590 way, the heat pump must stay ON or OFF for at least this duration, reflecting the minimum up or
591 down time usually set in the internal controller of a heat pump. Oscillations at a too high frequency
592 would in fact damage the machine in the long term. Furthermore, a time step of 12 minutes captures
593 the dynamics of the building with sufficient accuracy and represents a satisfactory trade-off. In the
594 detailed TRNSYS simulation on the other hand, a finer resolution of 3 minutes is chosen, so as to
595 better observe the intrasampling behavior of the systems within one control action.

596 2.5.5. Boundary conditions and scenarios tested

597 All the tested scenarios consist of 3 days in the winter (24 to 26th of February 2018) and summer
598 season (8 to 10th of July 2016). These periods were chosen because they present the following
599 characteristics: high heating/cooling load, variety of weather conditions (cloudy and sunny days
600 among the three days), sufficient variations in the input signals (especially the emissions signal). The
601 occupancy patterns show some level of stochasticity between the different days (as shown later in
602 sections 3.1 and 3.2), therefore it is considered that simulations of three days are sufficient for the
603 scope of the present work.

604 The weather parameters necessary for the simulations were retrieved from a weather station
605 located in Tarragona, Spain: ambient temperature, relative humidity, solar irradiation, wind direction
606 and velocity. The price of electricity was retrieved from the Spanish Distribution System Operator
607 website [37], and the CO₂ marginal emissions factor was calculated from data also originating from
608 the same source. It should be noted that in the present work, the forecasts used by the MPC are
609 perfect, meaning that the actual measured parameters are used as the prediction of the future.

610 3. Results

611 3.1. Heating cases

612 The boundary conditions and the reference case for heating are presented in Figure 14. In that
613 reference case, the heat pump operation is managed by a simple thermostat controlling the zone
614 temperature T_{int} . The set-point in winter is 21°C with a symmetric deadband of $\pm 1^\circ\text{C}$, which means
615 the lower temperature bound is 20°C, as for the MPC cases. In the following sections, the MPC
616 strategies are analyzed under the angles of the selected KPIs.

617 It can firstly be observed in Figure 14 why the MEF CO₂ signal is preferred to the average EF: it
618 follows the same trend, but it varies with larger amplitude, which represents an advantage for
619 facilitating the optimization calculation of the MPC. The price signal displays a clear day-night
620 pattern, with high price during the peak hours of the grid (afternoons) and low price at night. The
621 price and CO₂ MEF signals show in general an opposite behavior, the peaks of the first one coinciding
622 with the valleys of the other and vice versa. In the reference case, the heating loads predominate at
623 night when the outdoor temperature is coldest, which constitutes a favorable situation with regards
624 to the price signal, less so for the CO₂ MEF signal. Over the three winter days of that case, the heat
625 pump uses 32.6 kWh of electricity which correspond to a cost of 3.26 € and average emissions of 8.99
626 kgCO₂.

627 In the top two graphs of Figure 14, the high and low penalty periods are highlighted by different
628 background colors, whether the considered penalty signal is the price or the CO₂ emissions. The low
629 and high thresholds of the two signals are defined by the 40th and 60th percentiles of the data for the
630 next day define respectively, as studied in the parametric analysis of [39].

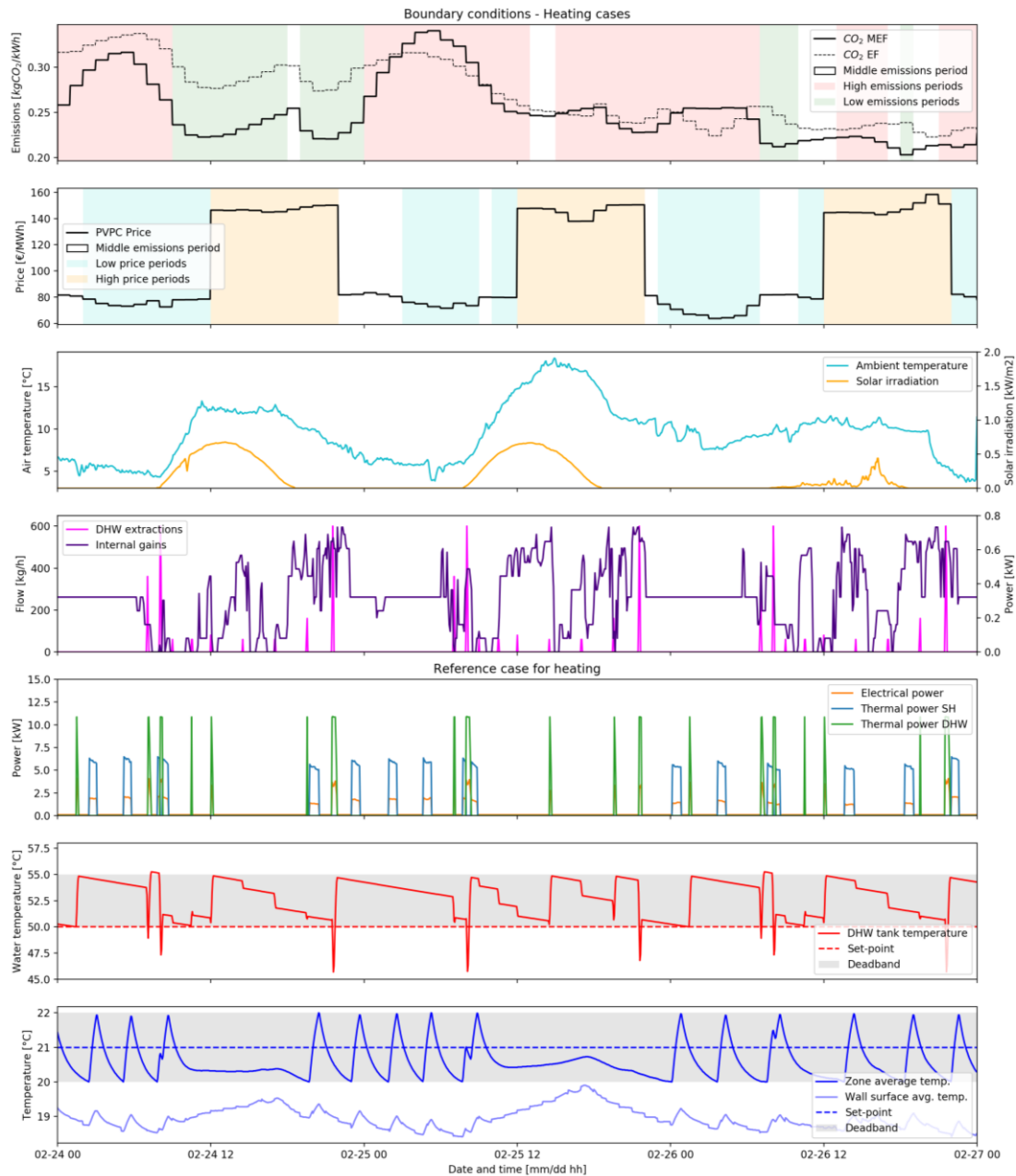


Figure 14. Boundary conditions and reference heating case. The first four graphs display the boundary conditions: CO₂ emissions and price signals, weather parameters and DHW extractions profile. The last three graphs show the reference heating case: the electrical and thermal powers of the heat pump, the resulting temperature in the TES tank and in the dwelling.

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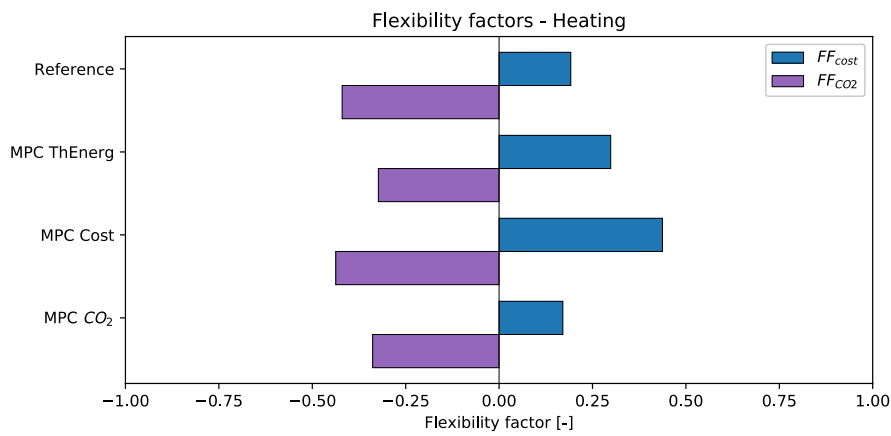
637 3.1.1. Flexibility factors

638 One major goal of implementing energy flexibility control strategies consists in shifting the loads
639 towards periods of lower electricity price or lower CO₂ emissions from the grid. To quantify this
640 shifting, the flexibility factor (FF) as defined in [38] is utilized. This indicator is calculated both with
641 regards to the electricity price (FF_{cost}) and the CO₂ marginal emissions input signal (FF_{CO_2}). The
642 generic formulation is shown in Eq. (17), p referring to the penalty signal being used (price or
643 emissions); with hp and lp respectively the high and low penalty periods. FF varies between -1 (all
644 the electricity use of the heat pump occurs during hours of high price/emissions) and 1 (all the
645 electricity use of the heat pump occurs during hours of low price/emissions).
646

$$FF_p = \frac{\int_{lp} P_{el} dt - \int_{hp} P_{el} dt}{\int_{lp} P_{el} dt + \int_{hp} P_{el} dt} \quad (17)$$

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The flexibility factors are presented in Figure 15. As previously analyzed, the reference case benefits more from the price signal than from the CO₂ signal in heating mode: for that case, $FF_{cost} = 0.19$ and $FF_{CO_2} = -0.42$. The low values of FF_{CO_2} are also caused by the fact that the amount of high CO₂ MEF hours is larger than the amount of high price hours (see Figure 14). As expected, the case MPC Cost increases FF_{cost} the most, since this is its main objective: it reaches the value $FF_{cost} = 0.44$, while its $FF_{CO_2} = -0.44$ is further degraded compared to the reference case. The results of the MPC CO₂ case are less satisfactory in terms of flexibility factors. This case fails to increase significantly the value of FF_{CO_2} and thus to achieve its declared objective: $FF_{CO_2} = -0.34$, at a similar level than MPC ThEnergy. This could be due to the low variations of the penalty signal in this case, which complicates the optimization process. Analyzing solely the flexibility factors, the MPC Cost configuration appears like the most efficient control strategy to achieve load-shifting.



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Figure 15. Flexibility factors of the studied heating cases, both in terms of cost and marginal CO₂ emissions.

661 3.1.2. Electrical and thermal energy

662 To understand how the MPC strategies affect the operation and efficiency of the systems, it is
663 important to analyze the energy balance of the heat pump. In this regard, the delivered thermal
664 energy $Q_{SH} + Q_{TES}$ (whether in space heating or DHW production mode) is calculated, as well as the
665 overall electricity use of the heat pump during the three days of the analyzed cases, including a
666 standby power of 95 W when the compressor is off (as measured with the real heat pump system in
667 a laboratory setup). The ratio between these energy quantities represent the overall coefficient of
668 performance of the system.

669 Furthermore, when analyzing the thermal energy balance over the simulation period, it is
670 important to consider the energy stored or discharged within the building. In fact, if we consider the
671 building and its water tank as storage elements, their state of charge is not equal at the beginning and
672 at the end of the simulation, and this energy gap must be taken into account in the overall energy
673 balance analysis. For this reason, we define the energy difference ΔE between the initial and final
674 moments for the three states, as shown in Eq.(18).

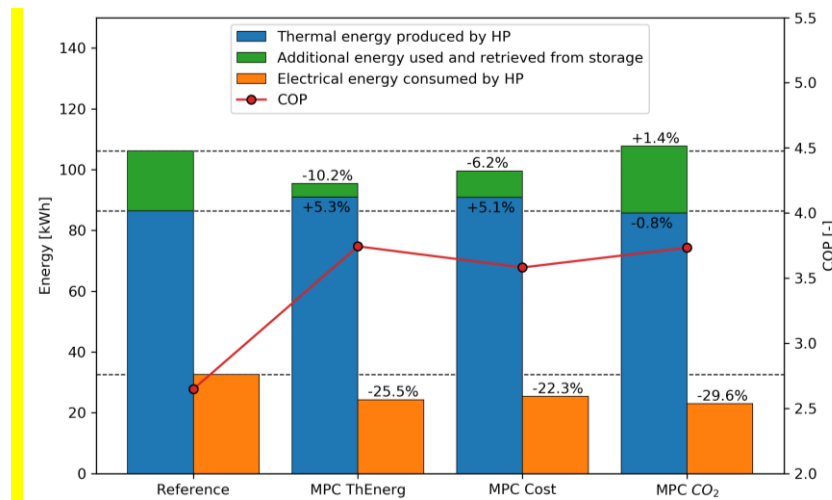
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$$\Delta E = C_{int}(T_{int,init} - T_{int,fin}) + C_w(T_{w,init} - T_{w,fin}) + C_{TES}(T_{TES,init} - T_{TES,fin}) \quad (18)$$

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All the energy balance parameters are represented for each analyzed case in Figure 16. It is observed that for every MPC case, the thermal energy produced by the heat pump is slightly larger than the reference case, although the electrical energy use is lower, which results in a higher efficiency. The MPC controller usually chooses to operate the heat pump at a lower supply temperature, which means a higher COP of the heat pump, as shown previously in Figure 6. This

682 result already proves the benefits of choosing an MPC controller: by operating the system at a higher
 683 COP, the heat pump actually becomes a more sustainable option (the European Union notably
 684 considers electrically-driven heat pumps as a renewable energy option only if their seasonal COP
 685 surpasses a value of 2.5 [40]). This corroborates the findings of [41]. DHW is always produced with a
 686 supply temperature of around 55°C, therefore the COP during the tank charging operation would
 687 take lower values (in a range from 2 to 3 as seen in Figure 6). This naturally affects the overall COP
 688 of the system, as well as the standby losses which are not considered in the static tests or by the
 689 manufacturer data, where the heat pump only operates in steady-state conditions.
 690



691
692 **Figure 16.** Energy analysis of the heating cases.

693 3.1.3. Cost and emissions

694 The actual outputs of the energy flexibility strategies can be measured in terms of monetary
 695 savings or CO₂ emissions avoided. These metrics are presented in Table 5, as savings compared to
 696 the reference case. For this reason, the choice of the reference case is crucial: in the present work, a
 697 simple thermostatic case was chosen as the reference since it is the most common type of controller.
 698 The monetary cost represents the money spent on the electricity use of the heat pump, but it does not
 699 include the other loads of the dwelling, nor the other parts of the electricity bill (e.g. taxes or grid
 700 connection fees).

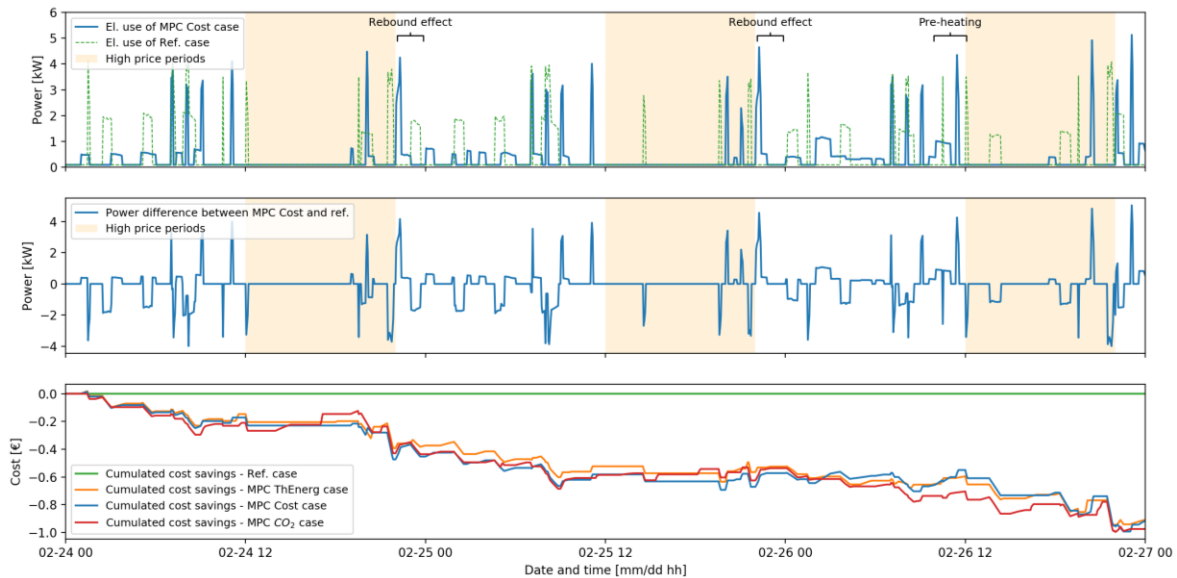
701 If analyzing only the thermal energy produced by the heat pump, it appears that the case MPC
 702 ThEnergy does not achieve its minimization objective: it is in fact increased by 5.3% compared to the
 703 reference case. However, when considering the total energy use (hence also the energy ΔE retrieved
 704 from the storage), MPC ThEnergy presents the lowest value among the MPC cases, a reduction of
 705 10.2% compared to the reference case. It retrieves less energy from the storage than the other cases,
 706 to preserve it and to minimize the overall energy use in the long term.

707 For a more detailed cost analysis, Figure 17 is plotted. On the top graph, the electricity use of the
 708 reference case and the MPC Cost case (the most relevant when analyzing the cost savings) are
 709 represented, highlighting the periods where the electricity price is higher. Even though the reference
 710 case already uses little electricity during these periods, a certain load shifting can be observed, as the
 711 MPC controller tends to avoid them to operate the systems. As a result, a “rebound effect” can
 712 sometimes occur when the high price period terminates: the system then needs to compensate for a
 713 prolonged reduced operation by turning the system on when the price becomes low again. A pre-
 714 heating effect also happens on the last day of the simulation: since on that day the solar radiation and
 715 the outside temperature are particularly low (see in Figure 14), the MPC controller anticipates the
 716 consequent increased heating needs combined with the high price, and decides to pre-heat the
 717 building when the price is still low. In this regard, the MPC controller behaves as expected. The
 718 bottom graph of Figure 17 presents the cumulated costs of all the analyzed cases: the three MPC cases
 719 perform better than the reference case and display a very similar behavior among them.

720
721**Table 5.** Savings of the heating MPC cases in terms of cost and CO₂ marginal emissions.

MPC objective case		MPC ThEnergy	MPC Cost	MPC CO ₂
Cost variation compared to the reference case	[€]	-0.91	-0.92	-0.98
	[%]	-27.9%	-28.1%	-29.9%
Thermal energy use J_{en} compared to the reference case	[kWh]	+4.59	+4.44	-0.67
	[%]	+5.31%	+5.14%	-0.78%
Energy difference between initial and final state ΔE	[kWh]	4.4	8.7	22.0
Total energy ($J_{en} + \Delta E$) variation compared to the reference case	[kWh]	-10.8	-6.6	+1.5
	[%]	-10.2%	-6.2%	+1.4%
Electricity use variation compared to the reference case	[kWh]	-8.33	-7.27	-9.67
	[%]	-25.5%	-22.3%	-29.6%
Average CO ₂ emissions variation compared to the reference case	[kgCO ₂]	-2.41	-2.21	-2.79
	[%]	-26.8%	-24.6%	-31.1%
Marginal CO ₂ emissions variation compared to the reference case	[kgCO ₂]	-2.31	-2.03	-2.64
	[%]	-25.7%	-22.6%	-29.4%

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Figure 17. Electricity use of the heat pump in the reference and the MPC Cost cases (top graph), resulting difference (middle graph) and cumulated cost savings of the four studied cases (bottom graph).

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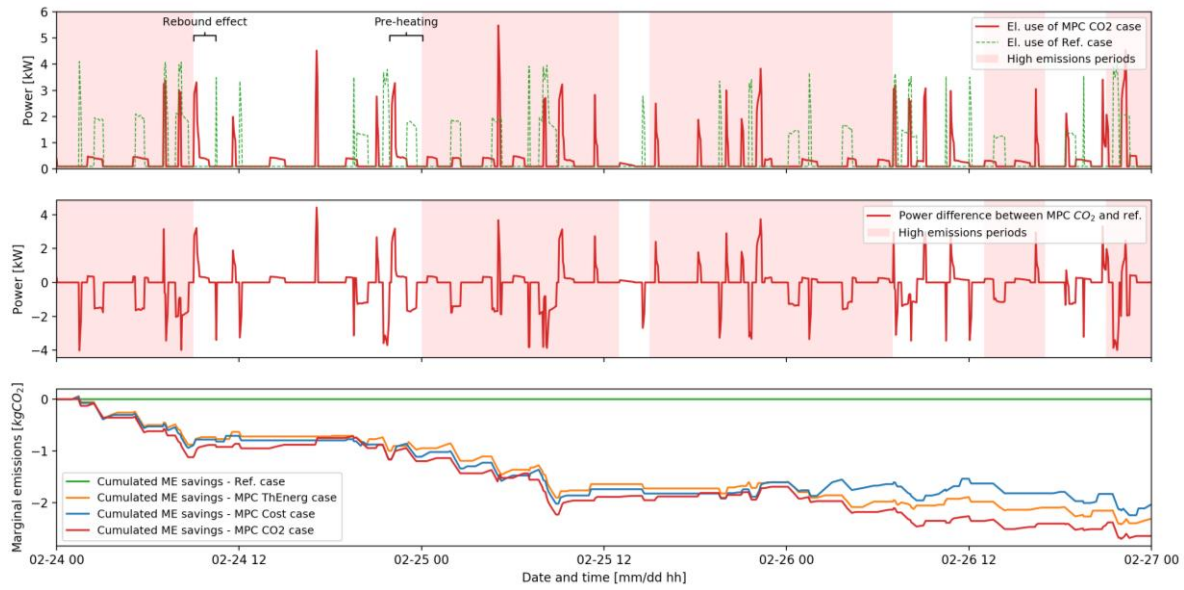
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For a more detailed analysis of the CO₂ emissions savings, Figure 18 is plotted. On the top graph, the electricity use of the reference case and the MPC CO₂ case (the most relevant when analyzing the emissions savings) are represented, highlighting the periods where the marginal emissions are higher. The expected load shifting towards periods where the grid emits less CO₂ is less clearly visible than in the MPC Cost case previously analyzed. In fact, the input signal of the CO₂ marginal emissions becomes almost flat during the second half of the experiment (see Figure 14): this could have complicated the optimization task of the MPC in this configuration. However, emissions savings are still achieved in all MPC cases, but they are mainly due to the operation of the heat pump at a lower supply temperature (i.e. at a higher efficiency), reducing the overall electrical energy used by the systems. Among them, MPC CO₂ logically yields the highest marginal emissions savings: -2.64 kgCO₂ (-29.4%). Table 5 also reveals that the average emissions calculation slightly underestimates the benefits compared to the marginal emissions calculation, although the two methods give close results. The MEF signal is still preferred as an input signal for its variations of larger amplitude.

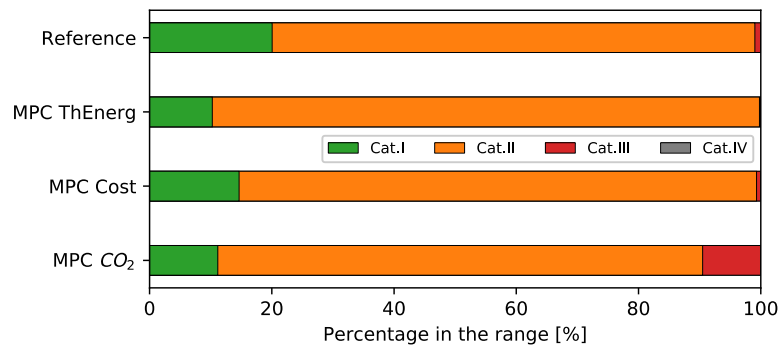


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Figure 18. Electricity use of the heat pump in the MPC CO₂ and reference cases (top graph), resulting difference (middle graph) and cumulated marginal emissions savings of the four cases (bottom graph).

743 3.1.4. Comfort

744 The comfort of the occupants is of utmost importance when interfering with the control of the
745 HVAC systems. To ensure acceptability of the users, the flexibility control strategies must not
746 jeopardize their thermal sensations [4], [42]. For this reason, the resulting indoor temperature T_{int} is
747 analyzed, in terms of time spent in the comfort categories defined by the standard EN 15251 [43]. It
748 should be noted that thermal comfort is a much more complex topic, and that it depends on many
749 other parameters (humidity, air velocity, activity level). However, the indoor temperature remains
750 the most significant parameter and the easiest to analyze, therefore it provides meaningful insights
751 about the thermal comfort. Figure 19 reveals that all the cases present similar comfort conditions than
752 the reference cases, with a majority of the time spent in Cat.II (between 20 and 21°C), which is logical
753 given the lower boundary of 20°C. Case MPC CO₂ presents a slight degradation of comfort, with
754 incursions in the lowest acceptable comfort category (Cat. III: operative temperature between 18 and
755 20°C in the heating season), but Cat. IV (less than 18°C) is however never reached.
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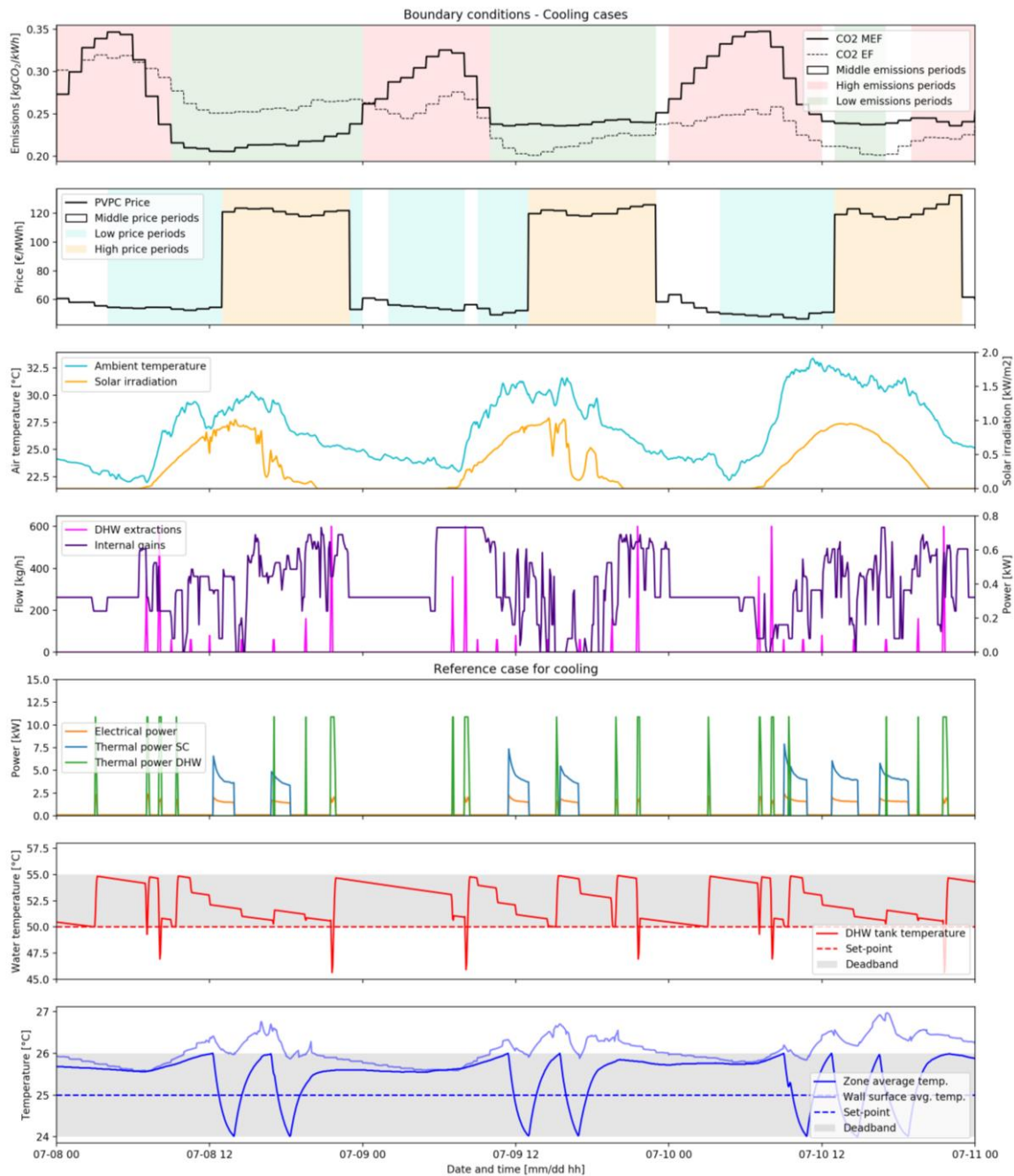
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Figure 19. Comfort analysis of the heating cases.

759 3.2. Cooling cases

760 The boundary conditions and the reference case for cooling are presented in Figure 20. For the
761 reference case, the set-point of the thermostat is fixed to 25°C, with the deadband of ±1°C, so that the
762 upper bound is 26°C, as in the MPC cases. The MPC strategies are then analyzed in the following
763 sections under the angles of the same KPIs than the heating cases. In the cooling season, the
764 symmetric behavior of the two input signals (see the two top graphs of Figure 20) is accentuated:

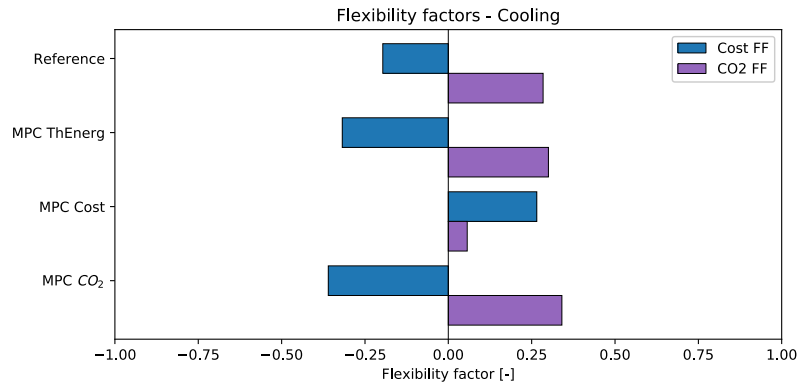
765 during daytime where solar energy takes up a large part of the electricity production, the marginal
 766 emissions are low while the price is high, following the same pattern than in winter. Conversely at
 767 night, the price is low while the marginal emissions are high due to the use of more polluting energy
 768 sources. Furthermore, in summer the cooling loads are concentrated in the afternoon due to high
 769 solar heat gains entering the buildings, therefore the cooling configuration represents a more
 770 favorable situation with regards to the reduction of emissions rather than the costs. Over these three
 771 summer days, the heat pump uses 31.1 kWh of electricity corresponding to a cost of 2.78 € and
 772 average emissions of 7.29 kgCO₂.
 773



774 **Figure 20.** Boundary conditions and reference cooling case. The first four graphs display the boundary
 775 conditions: CO₂ emissions and price signals, weather parameters and DHW extractions profile. The last three
 776 graphs show the reference cooling case: the electrical and thermal powers of the heat pump, the resulting
 777 temperature in the TES tank and in the dwelling.
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780 3.2.1. Flexibility factors

781 As previously mentioned, the reference case in the cooling season presents more favorable
 782 characteristics for the reduction of CO₂ emissions than for the reduction of costs, according to the
 783 respective input penalty signals. As a result, $FF_{CO_2} = 0.28$ while $FF_{Cost} = -0.20$ in that base case.
 784 When implementing the MPC Cost strategy, the FF_{Cost} increases significantly to reach a value of
 785 0.27, which confirms the effectiveness of this configuration. MPC CO₂ only improves FF_{CO_2} by +0.06:
 786 since it is already relatively high in the reference case, the margin for improvements is greatly limited.
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Figure 21. Flexibility factors of the studied cooling cases, both in terms of cost and CO₂ emissions.

790 3.2.2. Electrical and thermal energy

791 In cooling mode, the definitions need to be slightly adapted: since the thermal energy delivered
 792 to the space Q_{SC} is negative, the total energy considered is calculated as $|Q_{SH}| + Q_{TES}$. Dividing this
 793 quantity by the total electricity use of the heat pump over the three days duration gives the overall
 794 COP of the systems. The definition of ΔE must also be slightly updated: in cooling mode, a lower
 795 temperature corresponds to a higher state of charge while it is the opposite in heating mode, therefore
 796 minus signs are included, as shown in Eq.(19).
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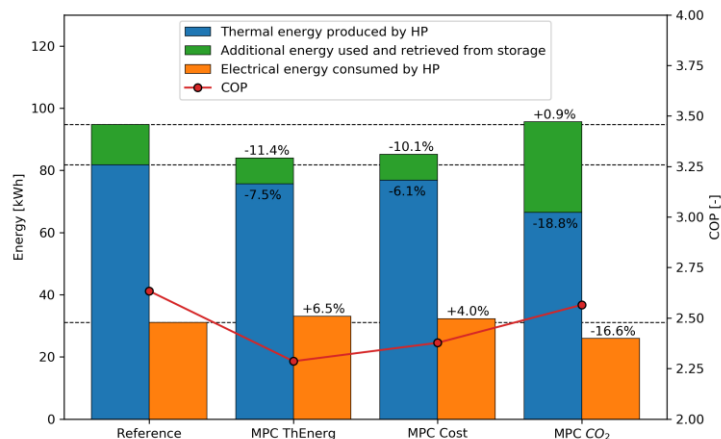
$$\Delta E = -C_{int}(T_{int,init} - T_{int,fin}) - C_w(T_{w,init} - T_{w,fin}) + C_{TES}(T_{TES,init} - T_{TES,fin}) \quad (19)$$

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800 As observed in Figure 22, all configurations reduce the amount of thermal energy produced by
 801 the heat pump, while their electricity use remains at the same level, which causes a small drop in
 802 COP. The MPC CO₂ case presents the highest COP of the MPC cases (at a similar level than the
 803 reference), and reduces both the thermal and electrical energy, similarly to what was observed in
 804 heating mode.

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Figure 22. Energy analysis of the cooling cases.

807 3.2.3. Cost and emissions

808 The costs and emissions savings are summarized in Table 6. MPC ThEnergy provokes poor results
 809 both in economical and environmental terms: it increases both the costs (+12.9%) and the CO₂
 810 emissions (+5.7%). Even though the heat pump thermal energy is not the lowest for that
 811 configuration, the total energy used for conditioning the building (including energy retrieved from
 812 the storage ΔE) still achieves the lowest value, with 11.4% saved compared to the reference. This
 813 result is coherent with the observations made in heating mode.

814 MPC Cost achieves the highest cost reduction, of -13% in that case, and it corresponds to the
 815 expectations since this is the actual objective function of that MPC. Similarly, MPC CO₂ achieves -
 816 19.1% reduction in the emissions and thus also achieves its objective. It should be noted that the
 817 calculated savings are greater when considering the marginal emissions rather than the average
 818 emissions: the latter calculation would result in only -16.8% emissions savings. In the present work,
 819 both MPC Cost and MPC CO₂ have shown considerable potential, and they can be equally used
 820 depending on which objective one aims towards.
 821

822 **Table 6.** Savings of the cooling MPC cases in terms of cost and CO₂ marginal emissions.

MPC objective case		MPC ThEnergy	MPC Cost	MPC CO ₂
Cost variation compared to the reference case	[€]	+0.36	-0.36	-0.31
	[%]	+12.9%	-13.0%	-10.97%
Thermal energy J_{en} produced by the HP compared to the reference case	[kWh]	-6.16	-5.03	-15.35
	[%]	-7.5%	-6.1%	-18.8%
Energy difference between initial and final state ΔE	[kWh]	8.3	8.4	29.1
Total energy ($J_{en} + \Delta E$) variation compared to the reference case	[kWh]	-10.8	-9.5	0.8
	[%]	-11.4%	-10.1%	0.9%
Electricity use variation compared to the reference case	[kWh]	+2.03	+1.24	-5.15
	[%]	+6.5%	+4.0%	-16.6%
Average CO ₂ emissions variation compared to the reference case	[kgCO ₂]	+0.40	+0.39	-1.22
	[%]	+5.5%	+5.4%	-16.8%
Marginal CO ₂ emissions variation compared to the reference case	[kgCO ₂]	+0.42	+0.37	-1.39
	[%]	+5.7%	+5.0%	-19.1%

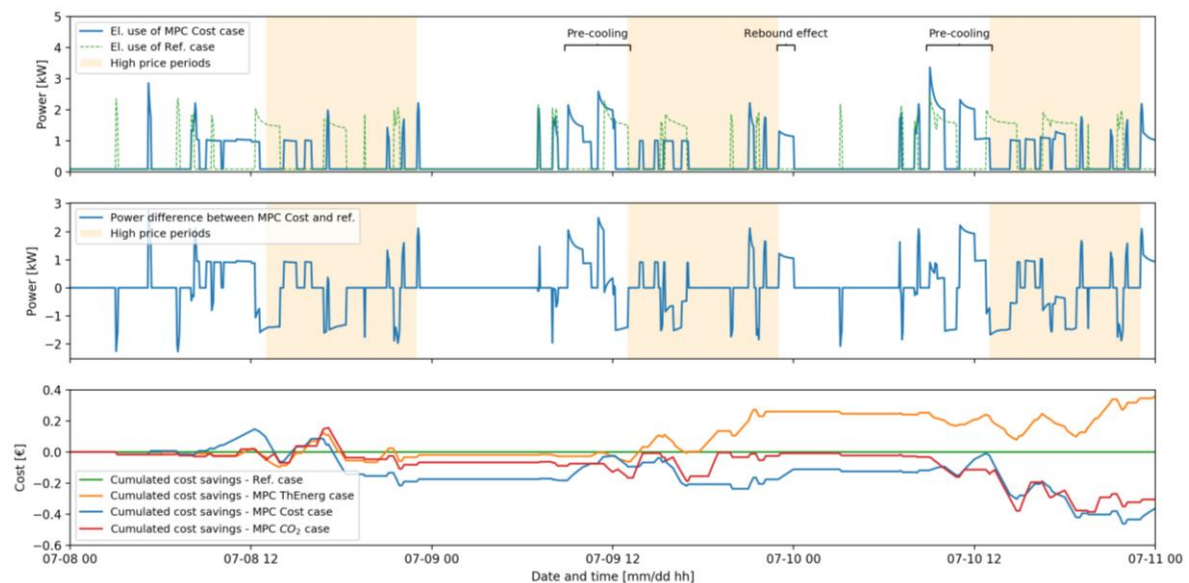
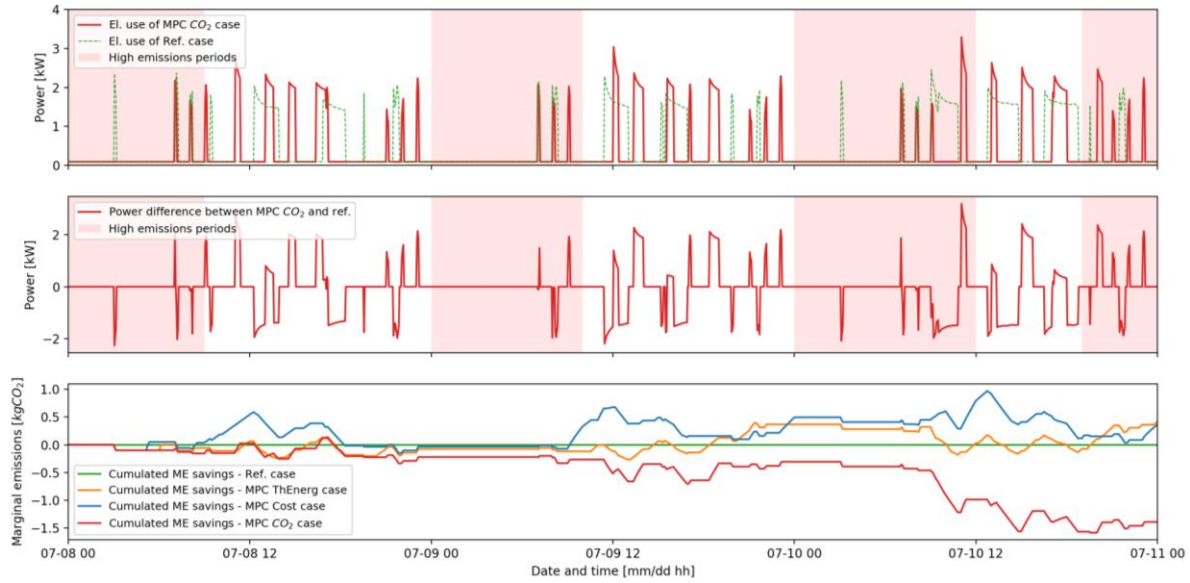
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Figure 23. Electricity use of the heat pump in the reference and the MPC Cost cases (top graph), resulting difference (middle graph) and cumulated cost savings of the four studied cases (bottom graph).



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Figure 24. Electricity use of the heat pump in the MPC CO₂ and reference cases (top graph), resulting difference (middle graph) and cumulated marginal emissions savings of the four cases (bottom graph).

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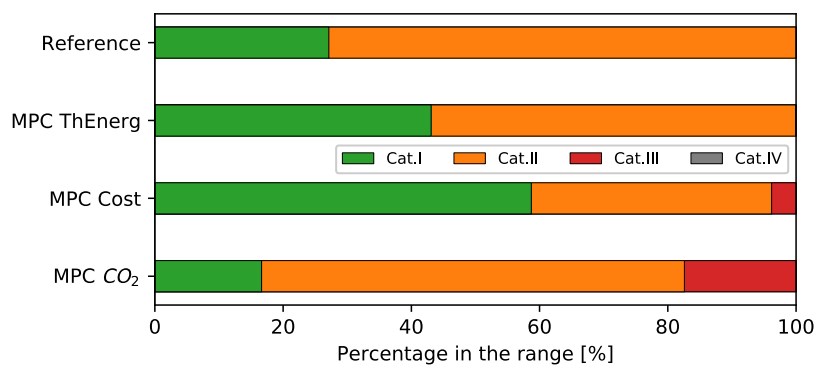
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Analyzing detailed plots of the costs and emissions outputs helps to understand and endorse the findings of Table 6. For the cost analysis, Figure 23 shows the satisfactory performance of MPC Cost in cooling mode: similarly than in heating mode, the effects of pre-cooling and rebound effect are observed, as a result of the predictive behavior of the controller. During the last day, where the outdoor temperature and solar heat gains are the highest, the cooling load is higher and therefore cannot be shifted entirely to the low price period, some cooling still needs to be provided during the high price period. For the emissions analysis in Figure 24, the load shifting is less evident, but still occurs. MPC CO₂ is the only configuration that manages to reduce the CO₂ emissions, logically achieving its declared objective and saving -1.39 kgCO₂ compared to the reference case, hence a reduction of -19.1%.

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3.2.4. Comfort



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Figure 25. Comfort analysis of the cooling cases.

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The comfort analysis for cooling is presented in Figure 25. The comfort categories are adapted for the summer season (Cat.I for instance corresponds to an operative temperature below 25.5°C), still from the European standard EN 15251. It appears that some MPC configurations improve the comfort conditions: in the case of MPC ThEnerg, this improvement obviously has a cost in terms of energy and lack of flexibility. In the case of MPC Cost, comfort is also improved (+31.6% of the time in Cat.I), simultaneously with the previously analyzed indicators: such results highlight the joint benefits that can be attained with predictive controllers. In the case of MPC CO₂, the comfort is slightly degraded due to the low value assigned to α_ϵ , the weighting coefficient associated with the

854 comfort objective. As a result, few excursions happen in Cat.III (+17.4%), suggesting that larger
855 fluctuations occur in the indoor environment. However, in all configurations the temperature always
856 stays within the range of Category III, which is considered as the acceptable threshold (operative
857 temperature below 27°C).

858 4. Discussions on MPC for heat pump control and energy flexibility

859 4.1. Sensitivity of MPC

860 The development steps of the MPC controller have been recounted in the present article.
861 Undergoing this process enabled to highlight the large development efforts still needed to build such
862 controllers. For instance, the weighting coefficients required fine tuning for every MPC
863 configurations, and the MPC outcome was greatly influenced by the choice of these parameters. In
864 particular, the value of the coefficient α_ϵ , associated with the objective J_ϵ determines whether the
865 controller will rather emphasize comfort or the flexibility objective; it should thus be chosen with
866 specific care. For example in the MPC Cost configuration in cooling mode, $\alpha_\epsilon = 0.15$ was still a high
867 value since comfort was significantly increased; decreasing it further could have led to even higher
868 savings and comfort conditions closer to the reference case. Considering hard constraints rather than
869 soft ones (hence eliminating the discomfort term J_ϵ in the objective function) could solve this
870 sensitivity issue, however the J_ϵ objective considerably improves the robustness of the controller [44]
871 and therefore it remains interesting to keep it.

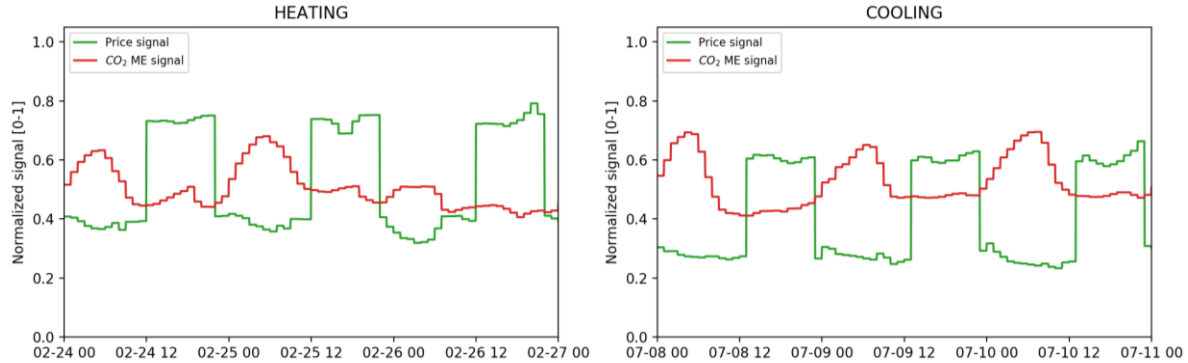
872 Adjustments were also needed between the heating and cooling configurations. For example,
873 the weighting coefficients and the RC model parameters have significantly different values for MPC
874 Cost in the two seasons. This could be due to the fact that the electricity price level changes seasonally
875 (the average price is 22% lower in the cooling case than in the heating case), and thus the Pareto
876 analysis compensates for this difference by decreasing accordingly the α_ϵ coefficient. A more
877 meticulous sensitivity analysis could be conducted on these weighting parameters as a further
878 research topic, for instance trying to obtain coefficients independent from the utilized penalty signal.
879 This could be done by dynamically adapting the coefficients to the level of the input signal, or a prior
880 normalization of the input signal realized in a more dynamic way than the present study (i.e. not
881 considering a fixed maximum cost E_{max}).

882 4.2. MPC as a tool to activate the energy flexibility of buildings

883 Despite the identified barriers previously discussed, the proposed MPC framework has shown
884 a good performance for activating the energy flexibility of residential buildings in the Mediterranean
885 area. Operating a building flexibly is a subtle compromise between different aspects that are all
886 related and sometimes contradictory. The strength of MPC is that such control is capable to quantify
887 and balance different objectives. Furthermore, it can sometimes lead to improving several objectives
888 at a time: for instance, the MPC Cost configuration enables simultaneously to realize some load
889 shifting towards low-price periods, to reduce the electricity bill of the users, while maintaining
890 comfortable conditions indoors. These findings are of utmost importance since the deployment of
891 flexibility at a large scale will require the acceptance of all parties involved: the occupants of the
892 buildings (interested in their comfort and energy bills), the grid stakeholders (interested in load
893 shifting and the moments when electricity is consumed) and the society as a whole (which should be
894 concerned about the reduction of the CO₂ emissions and climate change).

895 The penalty signals play an important role in the activation of building energy flexibility. In the
896 present work, two different signals have been used: the time-varying electricity price and the
897 marginal CO₂ intensity of the grid. From the analyzed cases, it appears that they often display
898 opposite behavior: the high penalty occurs in the afternoons for the price (the grid operators want to
899 incentivize peak shaving in this way), while it corresponds to the low penalty for CO₂ (due to the
900 high share of solar and renewable energy at this moment). The results also show that the patterns of
901 these signals greatly affect the outcome of the MPC controller: the price signal presents large day-
902 night variations, and thus already provides a pre-defined pattern for the electricity use, which

903 facilitates the consequent optimization of the MPC. On the other hand, the CO₂ signal presents
 904 smaller variations, and therefore gives little prior information to the MPC as to which periods are
 905 more interesting for operating the systems. The marginal emissions signal was chosen precisely
 906 because it varies more than the average emissions signal, but it appeared that this was not sufficient
 907 in some cases. Both normalized signals can be seen in Figure 26 for comparison.
 908



909
 910 **Figure 26.** Normalized signals in heating and cooling modes.

911 Conclusions

912 From development to application, the present study has covered many aspects of using Model
 913 Predictive Control for heat pump control and enhancing the energy flexibility of building thermal
 914 loads. Several steps were followed for creating the MPC controller: identification of simplified linear
 915 models of the building envelope and of the heat pump performance, definition of different objective
 916 functions, software implementation and tuning of the algorithm parameters. This process enabled to
 917 highlight the specificities of a controller used for both heating and cooling, and the still consequent
 918 development costs of such controller.

919 A co-simulation framework was then created between TRNSYS and MATLAB to test the created
 920 MPC controller. This framework can be reused to test many different aspects of MPC and energy
 921 flexibility, and to perform sensitivity analysis on the numerous parameters present in the MPC
 922 algorithm and models. In the present case, the MPC controller with three different objective functions
 923 (minimization of the thermal energy, of the electricity costs or the CO₂ marginal emissions) was tested
 924 on a Spanish residential building in heating and cooling seasons. Among these 3 configurations, MPC
 925 Cost performed better in comparison to a traditional thermostatic control: it enabled notably to shift
 926 the loads towards low-price periods (FF_{cost} was increased from 0.19 to 0.44 in heating and from -0.20
 927 to 0.27 in cooling), resulting in monetary savings in the range of 13 to 28%. The electricity used by the
 928 heat pump controlled by the MPC Cost was also reduced, due to an operation at lower supply
 929 temperature, which resulted in a higher efficiency, mostly in heating mode. The MPC controller
 930 achieved these positive results without affecting the thermal comfort of the occupants, and therefore
 931 constitutes a very promising control technique for enhancing the energy flexibility of buildings. The
 932 MPC CO₂ configuration also performed well, although its load-shifting behavior was less evident: it
 933 achieved marginal emissions savings in the range of 19 to 29%. On the other hand, MPC ThEnerg did
 934 not present the lowest amount of thermal energy produced by the heat pump, even though this was
 935 its minimization objective. However, when considering the total thermal energy used to condition
 936 the building (hence including also the energy which had been previously stored in the building mass
 937 and the water tank, and retrieved during the studied cases), MPC ThEnerg did actually present the
 938 highest savings, in the range of 10 to 11%. This reveals that MPC ThEnerg retrieved less energy from
 939 the storage than the other MPC cases, leading to a better thermal energy management on the long
 940 term. The complexity of the MPC controller and its sensitivity to tuned parameters have additionally
 941 been discussed: the good results obtained with the MPC controllers required several adjustments and
 942 extensive expertise, which makes a broader implementation still delicate.

943 Given the potentially important benefits brought by MPC controllers and demonstrated in the
 944 present work, it is hoped that the computation barriers will become less limiting with the ever
 945 increasing calculation capacities. A consequent amount of research has already been dedicated to
 946 MPC for building climate control, therefore the further efforts should focus in applying these
 947 strategies to real heat pump systems. In this way, potential obstacles in the implementation can be
 948 identified, and the performance can be verified against more realistic conditions. In particular, the
 949 dynamic effects of the heat pump were neglected in the present work (i.e. we considered that the heat
 950 pump reaches the desired set-point always). The discrepancy between the sent commands and the
 951 actual operation of the heat pump (delayed response, ramping) will thus be the object of further work
 952 based on laboratory experiments.

953 Nomenclature

Variables		Indices	
C	Thermal capacity	S	Space heating or cooling
e	Vector of external inputs (disturbances)	SH	Space Heating
E	Cost (price or emissions)	SC	Space Cooling
f	Frequency	TES	Thermal Energy Storage (DHW tank)
FF	Flexibility factor	DHW	Domestic Hot Water extractions
gA	Aperture area	el	Electricity
I _H	Solar irradiation	sup	Supply
J	Objective	ret	Return
m	Flow rate	amb	Ambient
M	Coefficient of heat conversion	occ	Occupants
N	Prediction horizon	w	Water
P	Electrical power	eff	Effective
Q	Thermal power (negative for cooling)	eq	Equivalent
R	Thermal resistance	obj	Objective function: "en", "cost" or "CO ₂ "
T	Temperature	en	Objective: minimization of thermal energy
u	Vector of controlled variables	cost	Objective: minimization of the costs
x	Vector of states	CO ₂	Objective: minimization of the CO ₂ emissions
y	Vector of output variables	det	Detailed (heat pump model)
α	Weighting coefficient	simpl	Simplified (heat pump model)
δ	Binary variable (on/off switching)	tot	For both space heating/cooling and DHW
ΔT	$T_{sup} - T_{ret}$ Water temperature difference	int	Relative to the internal zone state
ε	Slack variable (comfort violations)	w	Relative to the wall state
		ε	Relative to the comfort objective
		Δu	Relative to the smoothing objective
		p	Penalty signal (price or emissions)
		lp	Low penalty
		hp	High penalty
		e	Relative to the exogenous inputs
		u	Relative to the controllable inputs

Abbreviations

COP	Coefficient of Performance	MEF	Marginal Emissions Factor
DHW	Domestic Hot Water	MILP	Mixed Integer Linear Programming
EER	Energy Efficiency Ratio	MPC	Model Predictive Control
FCU	Fan-Coil Units	OCP	Optimal Control Problem
(VS)HP	(Variable Speed) Heat Pump	PLR	Part-Load Ratio
HVAC	Heating, Ventilation & Air Conditioning	PRBS	Pseudo Random Binary Signal
KPI	Key Performance Indicator	RES	Renewable Energy Sources
LP	Linear Programming	(N)RMSE	(Normalized) Root Mean Square Error

955 **Conflicts of Interest:** The authors declare no conflict of interest.

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