Optimal design of low-temperature heat-pumping technologies and implications to the whole-energy system

Andreas V. Olympios\textsuperscript{a,b}, Pooya Hoseinpoori\textsuperscript{c,b}, Matthias Mersch\textsuperscript{a,b}, Antonio M. Pantaleo\textsuperscript{a,b,d}, Michael Simpson\textsuperscript{a,b}, Paul Sapin\textsuperscript{a,b}, Niall Mac Dowell\textsuperscript{c}, and Christos N. Markides\textsuperscript{a,b}

\textsuperscript{a} Clean Energy Processes (CEP) Laboratory, Department of Chemical Engineering, Imperial College London, London SW7 2AZ, UK. \textsuperscript{b} Centre for Process Systems Engineering (CPSE), Imperial College London, London SW7 2AZ, UK. \textsuperscript{c} Centre for Environmental Policy, Imperial College London, London SW7 2AZ, UK. \textsuperscript{d} Department of Agro-Environmental Sciences, University of Bari, Via Amendola 165/A, 70125 Bari, Italy

Abstract:
This paper presents a methodology for identifying optimal designs for air-source heat pumps suitable for domestic heating applications from the whole-energy system perspective, accounting explicitly for a trade-off between cost and efficiency, as well as for the influence of the outside air temperature during off-design operation. The work combines dedicated brazed-plate and plate-fin heat-exchanger models with compressor efficiency maps, as well as equipment costing techniques, in order to develop a comprehensive techno-economic model of a low-temperature air-source heat pump with a single-stage-compressor, based on the vapour-compression cycle. The cost and performance predictions are validated against manufacturer data and a non-linear thermodynamic optimisation model is developed to obtain optimal component sizes for a set of competing working fluids and design conditions. The cost and off-design performance of different configurations are integrated into a whole-energy system capacity-expansion and unit-dispatch model of the UK power and heat system. The aim is to assess the system value of proposed designs, as well as the implications of their deployment on the power generation mix and total transition cost of electrifying domestic heat in the UK as a pathway towards meeting a national net-zero emission target by 2050. Refrigerant R152a appears to have the best design and off-design performance, especially compared to the commonly used R410a. The size of the heat exchangers has a major effect on heat pump performance and cost. From a whole-system perspective, high-performance heat pumps enable a \textasciitilde 20 GW (\textasciitilde 10\%) reduction in the required installed power generation capacity compared to smaller-heat-exchanger, low-performance heat pumps, which in turn requires lower and more realistic power-grid expansion rates. However, it is shown that the improved performance as a result of larger heat exchangers does not compensate overall for the increased technology cost, with low-performance heat pumps being associated with the lowest system transition cost (£470 billion).

Keywords:
Distributed energy, Energy system, Heat pumps, Optimisation, Part-load performance.

1. Introduction
The carbon intensity of electricity generation is reducing rapidly, while space heating and hot water provision still mostly rely on natural gas boilers and account for a significant proportion of the world’s total fossil-fuel consumption and CO\textsubscript{2}-equivalent emissions [1]. The UK became the first major economy to pass laws aiming for net-zero emissions target by 2050 [2]. Currently, more than 75\% of the UK heating emissions originate from space heating and hot water demand in the residential and commercial sectors, while natural gas is responsible for about 70\% of the UK heat demand [3].

The decarbonisation of heating is a challenging component of the transition strategy and requires an in-depth understanding of the candidate technologies and the strategies that can be used to integrate these into whole-energy systems. Low-temperature heat pumps are amongst the most promising options for decarbonising the heat sector, while facilitating heat-electricity integration [4,5]. They have great potential to replace energetically wasteful boilers and their role is therefore gaining increasing importance [6]. However, the optimal integration of such technologies in energy systems implies operational flexibility and, consequently, high-performance capabilities at off-design
conditions. In addition, unlike competing technologies like gas-fired CHP systems [7], the off-design performance of heat pumps is strongly influenced by the temperature difference between heat source and sink, meaning that optimal designs are not only affected by peak-energy demand needs, but also by the selected operating strategies and ambient temperature conditions.

Electrifying domestic heat demand through heat pumps will have significant implications on the electricity generation portfolio of the country’s energy system and will require an expansion and reinforcement of the power grid. These implications depend on the heat pumps’ cost and performance, which in turn are functions of the chosen heat pump components. In traditional system modelling, heat-pump cost and performance have been mostly represented by single values, or, in the best case, with the use of simple mappings between inputs and outputs. For example, in the work of Anandarajah et al. [8], although it is clearly stated that heat pumps should take a key role in decarbonisation, their performance characteristics and their variation in different periods of the year are not addressed.

In the report of Strbac et al. [9], distributed heat pumps emerge as one of the core decarbonisation strategies, since a hydrogen-only pathway without electrification seems to have higher system costs for a net-zero carbon target. However, the latter work utilises a simplified representation of the heat-pump performance, while the sensitivity analysis presented demonstrates that different assumptions on the performance and cost of end-use heating technologies can completely change the recommended pathway that the model selects. To overcome this, some studies have defined the performance of heat pumps as a function of temperature. In the work of Zhang et al. [10], data collected from one single heat pump is used to define a linear relationship between performance and temperature, while the work of Qadrdan et al. [11] also proposes a linear relationship for a typical heat pump. These relationships provide rough estimates of the performance variations during different periods of the year and are therefore more accurate. However, an in-depth consideration of concepts including the performance and cost of heat-pumping technologies being dependant on the component choice, size and operating conditions in whole-energy system models does not appear in literature, giving rise to two main drawbacks: (i) given the significant uncertainty in the assumptions, no clear lowest-cost pathway is identified; and (ii) whole-energy system models cannot guide technology-level decisions, as they cannot provide manufacturers with system-level insights into how to optimally design a heat pump.

This paper proposes a multiscale modelling framework for the design of low-temperature heat pumps for residential heating from the whole-energy system perspective. First, a comprehensive techno-economic model of single-stage-compressor air-source heat pumps based on the vapour-compression cycle is developed, utilising dedicated brazed-plate and plate-fin heat-exchanger models, as well as screw-compressor efficiency maps. An equipment costing technique is used to cost components. The heat pump model is validated through relevant market research and used to define a set of optimal designs for competing working fluids. Then, the off-design operation characteristics of the different configurations are determined and integrated into a power-and-heat system capacity-expansion and unit-dispatch model focusing on the electrification of heat in the UK. The system model, which is an expanded version of the Electricity Systems Optimisation (ESO) Framework model described in the works of Heuberger et al. [12,13], aims to identify the cost-optimal transition pathway for decarbonising heat in order to meet the UK 2050 net-zero emission targets. To achieve this, Section 2 describes the heat-pump model and how the cost and performance of different designs are integrated into the whole-energy system model. Section 3 presents the characteristics and system implications of the developed designs and Section 4 draws conclusions and defines future objectives.

### 2. Model design

An electrically-driven low-temperature heat pump is composed of four basic components: a compressor, a condenser, an expansion valve and an evaporator. The heat pump performance is denoted by its coefficient of performance (COP), which is the ratio of useful heat output to the required electric power input. Unlike boilers, which exhibit efficiencies between 75-94%, heat pump COPs are in the range of 2 to 5 depending on the chosen design and operating conditions [6].
The most common type is the air-source heat pump (ASHP), where the heat source is air. Ground-source heat pumps (GSHPs), which use the ground as the heat source, benefit from the fact that the annual variation in the ground temperature is much smaller than that of the air. This means that they experience more steady COPs than ASHPs, something particularly important in winter [14]. However, GSHPs involve high installation costs, require space, and heat requires time to replenish [15]. In this paper, focus is placed on electrically-driven ASHPs, which are widely-adopted in both high-population and low-population density areas and are easy to install.

2.1. Heat pump model

A spatially-lumped model of a heat pump with a single-stage-compressor is constructed, operating according to the typical vapour-compression cycle. The model assumes steady-state operation of the heat pump components, isenthalpic expansion through the expansion valve and no pressure losses in the heat exchangers and piping. The heat pump cycle is presented in Fig. 1. Process 1-2 corresponds to the compression of the working fluid; 2-3 is the heat rejection from the working fluid to the hot water, 3-4 is the isenthalpic expansion; and 4-1 is the heat addition from the air to the working fluid.

![Heat pump cycle](image)

*Fig. 1. Vapour compression heat pump cycle on a temperature (T) – specific entropy (s) diagram.*

Most heat pump studies assume a fixed isentropic efficiency for the compressor. However, the compressor efficiency depends on the working fluid, the flow rate through and pressure ratio across the component. Using a fixed value can lead to performance estimations that are challenging to achieve. In this work, the heat pump model includes compressor efficiency maps, capturing both the design and off-design performance of the device at different operating conditions. The maps are adopted from the work of Astolfi [16] and refer to screw compressors, providing relationships for the isentropic efficiency as a function of volume ratio and volumetric flowrate. The surrogate models were defined based on data for more than 100 Bitzer screw compressors [17].

The heat pump model also incorporates dedicated heat exchanger (HEX) component models, which capture the performance and cost of different HEX designs. The condenser, where heat is transferred to the circulating hot water, is a brazed-plate heat exchanger comprising three distinct zones: (i) the desuperheating zone (Process 2-2a); (ii) the condensing zone (Process 2a-2b); and (iii) the subcooling zone (Process 2b-3). The evaporator, where heat is transferred from the ambient air into the cycle, is a plate-fin heat exchanger and comprises two zones: (i) the evaporating zone (Process 4-4a); and (ii) the superheating zone (Process 4a-1). Dividing the HEX into the above zones is necessary as the heat transfer coefficients heavily depend on the flow (single-phase liquid, vapour, or two-phase flow).

The main governing equations for the heat pump cycle are presented in the following section.

2.1.1. Vapour compression cycle

The working fluid vapour enters the compressor (Process 1-2) at temperature $T_1$ and specific enthalpy $h_1$, where it is compressed to temperature $T_2$ and specific enthalpy $h_2$. For a given isentropic
efficiency $\eta_{\text{is,comp}}$, the discharge enthalpy $h_2$ of a well-insulated compressor is calculated using:

$$ h_2 = h_1 + \frac{h_{2,\text{is}} - h_1}{\eta_{\text{is,comp}}} , $$

where $h_{2,\text{is}}$ represents the specific enthalpy for a perfectly isentropic compression. The isentropic efficiency $\eta_{\text{is,comp}}$ is estimated from an empirical correlation provided by Astolfi [16]:

$$ \eta_{\text{is,comp}} = c \left[ 0.940 + 0.0293 \ln(V_i) - 0.0266V_i \right] , $$

where $V_i$ is the isentropic volumetric flow rate at the inlet of the compressor, $V_i$ the volume ratio across the compressor and $c$ is given by:

$$ c = 1 - 0.264 \ln \left( \frac{V_i}{V_i} \right) \text{ for } V_i > 7 . $$

Given a working-fluid mass flow rate $\dot{m}_{\text{w}}$, the electrical power required by the compressor is:

$$ \dot{W}_\text{in} = \dot{m}_{\text{w}}(h_2 - h_1) = \frac{\dot{m}_{\text{w}}(h_{2,\text{is}} - h_3)}{\eta_{\text{comp}}} . $$

The vapour leaving the compressor enters the condenser, which is at a higher temperature than the heat sink. Therefore, heat is rejected from the refrigeration cycle (Process 2-3). The vapour is condensed and can be also subcooled to a degree of subcooling that is defined by:

$$ d_{\text{SC}} = T_{2b} - T_3 . $$

The heating rate can be determined by calculating the enthalpy reduction of the working fluid:

$$ Q_\text{out} = \dot{m}_{\text{w}}(h_2 - h_3) , $$

which is equal to the rate at which heat is rejected to the heat sink (indoor space that is heated):

$$ \dot{Q}_\text{out} = \dot{m}_{\text{sink}}c_{\text{p,sink}}(T_{\text{sink,out}} - T_{\text{sink,in}}) , $$

where $\dot{m}_{\text{sink}}$ corresponds to the mass flow rate of the heat sink (indoor water stream), $c_{\text{p,sink}}$ its specific heat capacity and $T_{\text{sink,out}} - T_{\text{sink,in}}$ the temperature increase of the heat-sink stream. The condensed working fluid then passes through an expansion valve (Process 3-4). The process is assumed to be isenthalpic, so that:

$$ h_4 = h_3 . $$

The working fluid entering the evaporator (Process 4-1) is at a temperature below that of the heat source (ambient air), meaning that the working fluid absorbs heat from the surroundings. Vapour is condensed and slightly superheated. Superheating is necessary in order to ensure that the compressor operates at its intended capacity, as well as to protect it from possible mechanical damage due to liquid ingestion [18]. The degree of superheating is given by:

$$ d_{\text{SH}} = T_1 - T_4 . $$

The rate of heat addition can be calculated using the enthalpy increase of the working fluid:

$$ \dot{Q}_\text{in} = \dot{m}_{\text{w}}(h_1 - h_4) , $$

and is equal to the rate of heat rejected by the heat source:

$$ \dot{Q}_\text{in} = m_{\text{source}}c_{\text{p,source}}(T_{\text{source,in}} - T_{\text{source,out}}) . $$

The energy balance between the rate of heat input, heat output and work input is given by:

$$ \dot{Q}_\text{out} = \dot{Q}_\text{in} + \dot{W}_\text{in} . $$

Finally, the heat pump’s COP is calculated by dividing the heat provided by the condenser to the heat sink by the work required to drive the compressor:
\[ \text{COP} = \frac{Q_{\text{out}}}{W_{\text{in}}} \]  

(13)

### 2.1.2. Heat exchangers

The purpose of the development of detailed HEX models is two-fold: (i) to estimate their cost for different heat pump designs; and (ii) to examine the system’s behaviour at off-design operating conditions. The geometrical parameters of brazed-plate and plate-fin HEXs are obtained based on experimental tests conducted by Unamba et al. [19] and Karthik et al. [20], and examples from the work of Shah et al. [21]. The main parameters appear in Table A.1 in the Appendix.

The HEXs are discretised into a series of segments based on either equal temperature increments (single-phase regions) or equal enthalpy increments (two-phase regions). For each increment, the required heat flowrate and temperatures of heat source or sink, as well as the heat transfer coefficients are determined. The overall heat transfer coefficient \( U_i \) of each increment \( i \) can be determined from:

\[
\frac{1}{U_i} = \frac{1}{h_{\text{inner},i}} + \frac{\Delta x}{k} + \frac{1}{h_{\text{outer},i}},
\]

where \( k \) represents the thermal conductivity of the wall and \( h_{\text{inner},i} \) and \( h_{\text{outer},i} \) refer to the heat transfer coefficients at the sides of the working fluid and source/sink stream respectively.

In the heat pump design optimisation model, the logarithmic temperature differences can be used in conjunction with the calculated heat transfer coefficients and heat flows to define the required area for each zone (desuperheating, condensing, subcooling, evaporating and superheating), according to:

\[
Q_i = U_i A_i \Delta T_{\text{lm},i},
\]

where, for each increment \( i \), \( A_i \) is the heat transfer area and \( \Delta T_{\text{lm},i} \) the log-mean temperature difference.

In the operation optimisation model, the total HEX area is fixed and the models are altered so as to provide the cycle and source/sink outlet states. In both model variants, an initial guess is made and the problem is solved in an iterative manner until it converges to a solution within a set tolerance level.

For the single-phase heat transfer in the desuperheating and subcooling sections of the condenser and the superheating section of the evaporator, the Nusselt number is expressed as a function of the Reynolds \( Re \) and Prandtl number \( Pr \):

\[
Nu = a Re^b Pr^c,
\]

with coefficients \( a, b \) and \( c \). To calculate the coefficients, the model switches between correlations of Bogaert et al. [22] for Reynolds numbers lower than 1000 and Chisholm et al. [23] for higher Reynolds numbers. The same correlation is also used for the heat-sink stream.

For the single-phase heat transfer on the air side of the evaporator, the heat exchanger coefficient is instead obtained from the Colburn factor \( j \), which is expressed as a function of the Reynolds number:

\[
j = \alpha Re^b,
\]

with the coefficients \( a \) and \( b \) obtained from Chang et al. [24] for airflow over louvre fins.

In the condenser two-phase flow region, the single-phase Bogaert [22] and Chisholm [23] correlations are again used, but using an equivalent Reynolds number as recommended by Thonon [25].

Lastly, in the evaporator two-phase flow region, the heat transfer coefficient is obtained from:

\[
h = (h_{\text{cb}}^2 + h_{\text{nb}}^2)^{1/2},
\]

where \( h_{\text{cb}} \) corresponds to the heat transfer coefficient attributed to convective boiling and is obtained by switching between the Bogaert and Chisholm correlations, while \( h_{\text{nb}} \) corresponds to the heat transfer coefficient attributed to nucleate boiling and is obtained from Cooper’s correlation [26]. It is worth highlighting that all chosen heat-transfer correlations have been selected following an analysis of relative errors arising from comparing different possible options to experimental data.
2.1.3. Cost estimation

The thermodynamic model developed in Sections 2.1.1 and 2.1.2 would not have a significant value from a whole-energy system perspective, unless it is extended to involve costing estimations of heat pumps and their components. In the work of Olympios et al. [14], a detailed market research was conducted to obtain the costs of available domestic GSHPs in the UK in 2019, which has been extended to involve costs of monobloc, residential and commercial ASHPs. The market research shows that for small ASHPs in the range 5-10 kWth, the average investment cost per unit of power is about £500/kWth. This number is obtained by averaging the cost of more than 30 heat pumps within this size range. While there is a significant spread in the values, the cheapest option appears to be about £200/kWth, while the most expensive one is close to £1000/kWth.

Although heat pumps are readily available, the breakdown of costs into components is not easy to conduct and, in most cases, component manufacturers treat this data as confidential. Most studies utilise well-known costing methods from literature, like Turton et al. [27] or Seider et al. [28]. These correlations are not valid for small-scale components and tend to dramatically overestimate domestic heat pump component costs. For this reason, this work instead utilises component cost correlations as acquired by Quoilin et al. [29] and Lecompte et al. [30], based on the Belgian market in 2010. Based on the results of the analysis of the Department of Energy & Climate Change on ASHP costs [31], Table 1 includes some factors to account for costs for fitting, piping, valves, working fluid, control and heat meters. Adopted correlations have been adjusted based on the conversion from EUR (€) to GBP (£) using a rate of 0.83£/€ and also based on inflation, according to the Chemical Engineering Plant Cost Index (CEPCI) [32]. All adjusted correlations are presented in Table 1.

<table>
<thead>
<tr>
<th>Component</th>
<th>H</th>
<th>Cost (£)</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brazed-plate HEX</td>
<td>Heat exchanger area (m²)</td>
<td>173 + 282A</td>
<td>[29]</td>
</tr>
<tr>
<td>Plate-fin HEX</td>
<td>Heat exchanger area (m²)</td>
<td>270A</td>
<td>[30]</td>
</tr>
<tr>
<td>Compressor</td>
<td>Volume flow rate (m³/s)</td>
<td>204 + 154V</td>
<td>[29]</td>
</tr>
<tr>
<td>Water pump</td>
<td>Electrical power (W)</td>
<td>454(W/300)⁰²⁵</td>
<td>[29]</td>
</tr>
<tr>
<td>Air fan</td>
<td>Frontal area (m²)</td>
<td>578A</td>
<td>[29]</td>
</tr>
<tr>
<td>Piping, refrigerant, valve</td>
<td>-</td>
<td>30%</td>
<td>[31]</td>
</tr>
<tr>
<td>Miscellaneous hardware</td>
<td>-</td>
<td>280</td>
<td>[29]</td>
</tr>
<tr>
<td>Assembly (e.g., welding)</td>
<td>-</td>
<td>20%</td>
<td>[31]</td>
</tr>
<tr>
<td>Control system</td>
<td>-</td>
<td>470</td>
<td>[29]</td>
</tr>
<tr>
<td>Profit margin</td>
<td>-</td>
<td>30%</td>
<td>[31]</td>
</tr>
<tr>
<td>Tax</td>
<td>-</td>
<td>20%</td>
<td>-</td>
</tr>
</tbody>
</table>

2.1.4 Fluid selection

The choice of working fluid can have a significant impact on the performance and cost of heat pumps. The use of R22 in domestic and heating and cooling applications has been dramatically and widely reduced due to its ozone depletion potential (ODP) [33], while R134a has a relatively high global warming potential (GWP) index of 1430, which has driven research into new fluids with preferred environmental characteristics [34]. In 2019, in more than 80% of domestic heat pumps in the UK, the working fluid used was R410a [14]. The latter fluid works at relatively high pressures and is suitable for low-temperature applications, while it exhibits a GWP (equal to 2088), even higher than that of R134a. In recent years, there is an increasing trend towards the use of R32, which has a GWP index of 675 [35]. In this study, the design and off-design performance of domestic heat pumps based on R410a and R32 is investigated and also compared to two other hydrofluorocarbons: R152a and R245fa, both of which have suitable thermodynamic properties and great potential in heat pump systems [36,37]. The main properties of the analysed working fluids appear in Table 2.
Table 2. Main properties of working fluid options: $T_{\text{crit}}$ and $p_{\text{crit}}$ represent the critical temperature and pressure of the fluid, respectively; ODP the ozone depletion potential index; GWP the global warming potential index; and $H$ and $F$ the heat and flammability indexes according to NFPA classification [38] where 4 is maximum hazard and 0 is no hazard.

<table>
<thead>
<tr>
<th>Working fluid</th>
<th>$T_{\text{crit}}$ (°C)</th>
<th>$p_{\text{crit}}$ (bar)</th>
<th>ODP</th>
<th>GWP</th>
<th>H</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td>R410a</td>
<td>71</td>
<td>49</td>
<td>0</td>
<td>2088</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>R32</td>
<td>78</td>
<td>58</td>
<td>0</td>
<td>675</td>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>R152a</td>
<td>113</td>
<td>45</td>
<td>0</td>
<td>124</td>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>R245fa</td>
<td>154</td>
<td>36</td>
<td>0</td>
<td>1030</td>
<td>2</td>
<td>0</td>
</tr>
</tbody>
</table>

2.2. Thermodynamic optimisation

This work involves two separate optimisation tasks. First, the design of a heat pump (size of heat exchangers and compressor) is optimised for each of the four working fluids considered (R410a, R32, R152, R245fa) at a fixed heat demand and heat-source temperature. Then, the off-design performance of the developed designs is optimised under time-varying heat-source conditions. In both the design and off-design optimisation procedures, the heat pump is set to always satisfy the heat demand and provide hot water at a fixed temperature of 55 °C, which is the minimum temperature required to prevent the development of harmful bacteria [39]. All optimisation problems in this work are solved using MATLAB’s interior point algorithm fmincon [40].

2.2.1. Design optimisation

In the heat pump design optimisation problem, given a set of nominal heat-source conditions and constraints, the objective function to be maximised is the COP. A minimum temperature difference between heat exchanger fluids, commonly known as pinch-point temperature difference (PPTD), can be defined during the design stage for both the evaporator ($PP_{\text{evap}}$) and condenser ($PP_{\text{cond}}$). The smaller the temperature difference, the higher the COP. Therefore, small PPTDs result in better-performing cycles. However, they also mean larger heat exchangers and hence increased costs.

The decision variables for the design optimisation are the evaporation pressure $P_{\text{evap}}$, the condenser pressure $P_{\text{cond}}$, the degree of superheating $d_{\text{SH}}$ and the degree of subcooling $d_{\text{SC}}$. The source and sink flow rates are kept fixed. The optimisation problem for a set PPTD is expressed as:

$$\max \{\text{COP}\}$$

subject to all PPTD, energy balance and minimum superheating constraints.

2.2.3. Off-design operation optimisation

The off-design performance of a heat pump depends on the time-varying heat-source temperature. The objective function to be maximised is again the COP, but the size of the components is now fixed. During off-design operation, there are only two degrees of freedom and therefore two decision variables: (i) the compressor speed can be tuned to control the mass flow rate of the working fluid $m_{\text{wf}}$; and (ii) the expansion valve can be electronically controlled to optimise the degree of superheating $d_{\text{SH}}$. The optimisation problem is therefore formulated as:

$$\max \{\text{COP}\}.$$  (20)

Since the heat pump design is fixed, no PPTD constraints are required. The condensing and evaporating pressures adjust themselves according to the decision variable choice.

2.3. Whole-energy system model

The Electricity Systems Optimisation (ESO) Framework [12,13] is used to assess the system implications of a set of different heat pump designs. The model is a mixed-integer linear problem model which minimises the total system cost of decarbonising the electricity and heat system of a
given energy system - the UK in this study. The objective function is decomposed into investment and operational costs and includes a large library of generation, conversion and storage technologies. The readers are referred to the works of Heuberger et al. [12,13] for more details on the model’s main formulation and system-wide constraints. The model has been extended to include domestic heating technologies (heat pumps, electric heaters and hot-water cylinders). The heat-pump COP is specified as a function of temperature. The hot-water cylinder is sized so that the heat pump can fully charge it in one hour and the model optimises its charging and discharging operation.

3. Thermoeconomic analysis and system implications

In traditional thermoeconomic optimisation, the PPTD can be chosen appropriately to optimise a set performance indicator, often the specific investment cost. Here, however, the aim is to test the implication of different possible designs on the whole-energy system and therefore the adopted procedure is as follows: for each of the four considered working fluids, thermodynamic optimisation is used to maximise the COP for three fixed PPTDs: 1 °C, 5 °C and 10 °C, which leads to twelve different designs. The components are sized and the associated costs are calculated. Then, the relationships between off-design COP and heat-source temperature are acquired for all designs and are integrated within the whole-energy systems optimisation framework to assess the system value of each design.

3.1. Analysis of heat pump designs

The design point is chosen at: (i) a heat source temperature of 7 °C, which is the industrial standard for quoting the efficiency of an ASHP [41]; (ii) a heat-sink temperature of 55 °C, which is the minimum required to supply both space heating and hot water [39]; and (iii) a heat demand of 9 kW<sub>th</sub>, which is the average heat demand of a UK household [3]. Fig. 2 displays the results for the cost and COP (at design conditions) for the twelve different heat pump designs (3 PPTDs for each of the 4 working fluids), while Fig. 3 demonstrates how the COP varies for different heat-source temperatures in off-design conditions. It should be noted that the obtained cost ranges are close to heat pump costs obtained from market research (average price for a 9 kW<sub>th</sub> heat pump is £4500), validating the cost estimation model. Similarly, the COP ranges match manufacturer datasheets [14,15]. The requirement for defrost cycles during cold-ambient-condition periods is not considered here. In a pathway dominated by rapid employment of ASHPs, it would be important to consider solutions to deal with the latter issue. Furthermore, the effect of neglecting the pressure drop in the heat exchangers is within the range of uncertainties of this study (the developed model estimates a COP reduction of 3-6% for an evaporator pressure drop of 10%, in line with Ref. [42]).

Fig. 2. COP (at design point) and cost of different heat pump designs, where “high”, “med” and “low” represent high, medium and low performance heat pumps (PPTDs of 1 °C, 5 °C and 10 °C), respectively.

Fig. 2 demonstrates that, for a fixed heat pump output, the size of its components has a very substantial effect on both the cost and performance of the system. Even for a fixed working fluid, the choice
between small or large heat exchangers (which correspond to PPTDs of 10 °C and 1 °C, respectively), can have an effect of about 40-60% on the COP and £2000-3000 on the system price.

Fig. 3. COP of different heat pump designs as a function of heat-source temperature in off-design conditions (heat-sink temperature = 55 °C), where “high”, “med” and “low” represent high, medium and low-performance heat pumps (PPTDs of 1 °C, 5 °C and 10 °C), respectively.

The off-design operation analysis demonstrates that R410a shows inferior performance compared to alternatives like R152a and R245fa, which in most conditions also outperform R32. Fig. 3 reveals that R152a maintains favourable off-design performance for small and medium-size heat exchangers, while R245fa competes well at large sizes. It is observed that at high heat-source temperatures, the COP for high-performance units is substantially higher than low-performance ones, while this difference is smaller in cold weather. Determining which is the optimal design from a system perspective requires the integration of these relationships into the whole-energy system model.

3.2. Implications to the whole-energy system

Different heat pump designs convert domestic heat demand into different power demand profiles and therefore significantly affect the energy system technology mix, operation strategy, electricity generation requirements and total system heat decarbonisation transition cost. In all whole-energy system simulations, it is assumed that the decarbonisation of both hot water and space heating takes place only through ASHPs. All new dwellings are decarbonised through electrification and no GSHPs are included in the analysis. The cylinder size is fixed at 9 kWh, and all twelve heat pump designs are capable of providing the same heat output (9 kWth) at a fixed temperature (55 °C). The off-design performance is determined based on hourly UK outside air temperature and a typical UK residential heat demand profile. Fig. 4a presents the total installed capacity of power generation required at the end of the planning horizon (2050) for the UK to decarbonise the domestic heat sector and achieve net-zero emission targets for the twelve different designs. Fig. 4b presents the total transition cost of heat decarbonisation and the cost of avoided CO₂, which is the cost per tonne avoided compared to a business-as-usual case, in which decarbonisation does not occur.

Fig. 4a reveals an interesting observation: utilising high-performance heat pumps with large heat exchangers (PPTD of 1 °C) means a substantial reduction in required electricity generation capacity of about 20 GW (~10%) compared to low-performance units. This is extremely substantial and means lower required power grid expansion rates and a steadier system operation over peak-demand periods. In terms of financing and materials, this in turn means a more practical and realistic system transition. However, as shown in Fig. 4b, among all designs, low-performance heat pumps made of small heat exchangers (PPTD of 10 °C) achieve the minimum energy system transition cost, with R152a heat pumps achieving a total transition cost of £470 billion and a cost of avoided CO₂ equal to 120 £/tCO₂.
Medium-performance heat pumps, on the other hand, result to significantly lower generation capacity (~5-7 GW) than low-performance units, for a relatively small increase in transition cost (£3-5 billion).

Fig. 4. System implications of decarbonising the UK domestic heat sector by 2050 using different heat pump designs: (a) total installed electricity generation capacity in 2050; and (b) total system transition cost and cost of avoided CO₂ compared to business-as-usual case; where “high”, “med” and “low” represent high, medium and low-performance heat pumps (PPTDs of 1 °C, 5 °C and 10 °C), respectively.

4. Conclusions and outlook

This paper presents a multi-scale modelling methodology for identifying optimal designs for air-source heat pumps suitable for domestic applications. The framework enables comparisons of the effects of different designs on the whole energy system, accounting for possible working fluid and component sizing options. This is achieved through the development of comprehensive design and off-design heat-pump models, composed of dedicated heat exchanger models, screw compressor efficiency maps and costing correlations that capture explicitly the performance and cost of different configurations. The cost and off-design performance of twelve heat pump configurations with the same heat output are determined and integrated into a whole-energy system model representing the UK electricity and heat system, allowing the best heat pump design to be identified from a whole-energy system perspective.

Results show that R152a exhibits the best performance especially at off-design conditions, while R410a experiences inferior performance compared to upcoming alternatives. From a system perspective, it is revealed that high-performance heat pumps require significantly less installed electricity generation capacity (20 GW) to decarbonise domestic heat by 2050, and therefore lower and more realistic power grid expansion rates. However, the increase in performance does not compensate for the increase in cost, with lower-performance heat pumps resulting in a system transition cost which is about £35 billion
lower than that achieved by higher-performance units. Future work will consider more working fluids and component sizes, which will require the use of sophisticated surrogate models suitable for integrating the heat pump optimisation problem within the whole-energy system optimisation model.

Acknowledgments

This work was supported by the UK Engineering and Physical Sciences Research Council (EPSRC) [grant number EP/R045518/1] and UK Natural Environment Research Council (NERC) [grant number NE/L002515/1]. The authors would also like to acknowledge the Science and Solutions for a Changing Planet (SSCP) Doctoral Training Partnership (DTP). Data supporting this publication can be obtained on request from cep-lab@imperial.ac.uk.

Appendix

The main geometrical parameters used in the brazed-plate and plate-fin HEX models of the ASHP are summarised in Table A.1.

Table A.1. Main geometrical parameters used in HEX models.

<table>
<thead>
<tr>
<th>Brazed-plate HEX</th>
<th>Plate-fin HEX</th>
</tr>
</thead>
<tbody>
<tr>
<td>Channel width</td>
<td>2.1 mm</td>
</tr>
<tr>
<td>Fin pitch</td>
<td>1.5 mm</td>
</tr>
<tr>
<td>Chevron angle</td>
<td>22 °</td>
</tr>
<tr>
<td>Fin height</td>
<td>9 mm</td>
</tr>
<tr>
<td>Area enlargement factor</td>
<td>1.2</td>
</tr>
<tr>
<td>Plate thickness</td>
<td>5 mm</td>
</tr>
<tr>
<td>Ratio of fin area to total area</td>
<td>0.75</td>
</tr>
</tbody>
</table>

References