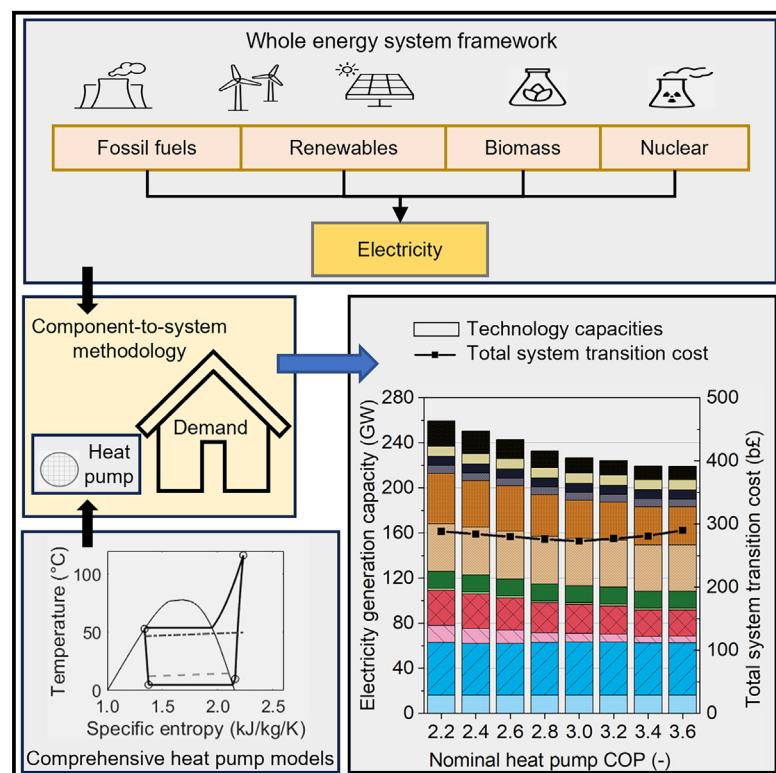


Toward optimal designs of domestic air-to-water heat pumps for a net-zero carbon energy system in the UK

Graphical abstract



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In brief

Olympios et al. investigate the implications of various domestic air-to-water heat pumps on the whole UK energy system. Heat pump cost and performance are shown to be correlated, and adopting higher-performance designs (e.g., with larger heat exchangers and more efficient compressors) reduces the required electricity generation capacity. However, an optimal design exists that minimizes overall system transition costs. Any investment in improving performance further increases the total cost, making it more cost effective to invest in centralized energy generation and storage.

Highlights

- Technoeconomic heat pump models are integrated within a whole-energy system model
- The system model reveals how technology design influences decarbonization pathways
- The approach allows for optimal investments in heat pumps and system infrastructure
- Trade-offs between conflicting system implications guide future technology development



Article

Toward optimal designs of domestic air-to-water heat pumps for a net-zero carbon energy system in the UK

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SCIENCE FOR SOCIETY Reducing the carbon footprint associated with domestic heating remains a challenge in many economies. Whole-energy system models are used to identify national decarbonization pathways, but many of them share a limitation: the cost and performance of competing technologies, especially with respect to heating, are represented by single efficiency and cost values or simplified models. In this work, detailed models that capture the cost and performance characteristics of heat pumps for different designs are integrated within a whole-energy system model. This integration extends the capabilities of the system model: besides optimizing network infrastructures, it also provides information on the optimal technology designs required to meet the system-wide objectives. Our findings reveal that there is an optimal heat pump design that minimizes the system transition cost. Further performance improvements increase overall costs, favoring investment in centralized energy generation and storage.

SUMMARY

Air-to-water heat pumps come with diverse design options whose cost and performance are correlated, giving rise to a crucial question: should manufacturers aim at designing higher-performance yet higher-cost heat pumps, reducing the wider energy infrastructure cost but increasing the upfront cost to end users, or more affordable yet lower-performance alternatives? Comprehensive heat pump performance and cost models are integrated within a whole UK energy system framework to capture how different heat pump designs influence the decarbonization pathway. We find that an uptake of higher-performance heat pumps leads to a reduced national electricity generation capacity. However, there is an optimal design that minimizes the total system transition cost, indicating a point of diminishing returns, beyond which, instead of investing in even higher heat pump performance, it is more cost effective to invest in centralized energy generation and storage. Insights are valuable for locations with low heat pump adoption and high electricity-to-gas price ratios.

INTRODUCTION

In an effort to meet worldwide energy and sustainability goals, major economies including the UK, EU, New Zealand, Canada, Korea, and Japan have set net-zero carbon emission targets for 2050 into law,^{1–3} although tens of other countries have stated equivalent targets in their energy-policy documents. Space heating and hot water provision account for a high proportion of the global energy consumption and emissions. For example,

natural gas is still responsible for more than 70% of the provision of heat to buildings in the Netherlands and the UK, with Italy, Canada, the United States, Germany, and France being close behind. At the same time, Belgium, Ireland, Portugal, Greece, and many others still experience a high penetration of oil products (>20%) for heating.⁴

Decarbonizing heating is a challenging component of energy transition strategies and requires an in-depth understanding of the candidate technology options.^{5–7} Most proposed heat



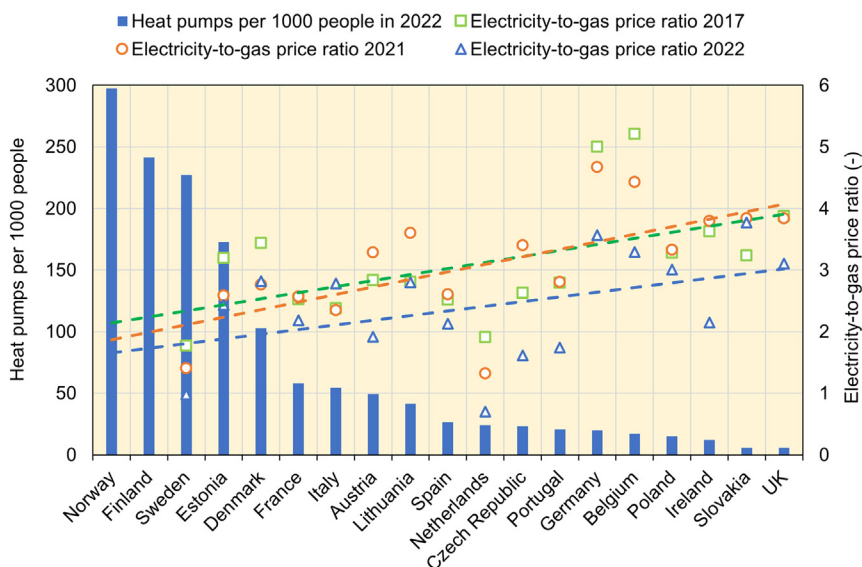


Figure 1. Number of electricity-driven heat pumps per 1,000 households in 2022 and ratio of electricity to natural-gas price for domestic consumers in major European economies between 2017 and 2022

A linear line best fit is plotted through electricity-to-gas price ratio points for 2017, 2021, and 2022. Note: there is little gas-distribution infrastructure in Finland and Norway; therefore, no gas price is recorded.^{28,29}

decarbonization pathways focus on electricity and hydrogen. Electricity is already a significant contributor to heating in several countries like Sweden and Norway,⁸ and recent national plans in the Netherlands, UK, and Germany^{8,9} have set new technology upgrade schemes to support electrification. These policy documents share the view that although hydrogen can be an option in the longer term, short-term policies should focus on achieving a high uptake of electricity-driven technologies.

For a large uptake of new technologies to be adopted, new technology designs should appeal to both manufacturers and consumers. Along with being cost effective, new technologies should comply with new environmental regulations as well as be as reliable in meeting demand as their predecessors. In the context of electrification, electricity-driven air-source heat pumps are a commercially mature technology able to harness “renewable” energy taken from the environment.¹⁰ In many countries, the process of energy transition has started: according to the International Energy Agency (IEA), air-source heat pumps are becoming the most common technology in newly built houses in many countries.¹¹ In Europe, the annual sales of air-source heat pumps have been steadily increasing by more than 10% per year since 2012.¹²

Electrification through heat pumps is a key route for heat decarbonization, but this transition is complex because of two main reasons: (1) the electricity used to drive domestic heat pumps should be produced centrally by net-zero carbon sources and (2) the magnitude of the total national electricity demand of countries advancing to a large uptake of electric heat pumps would be significantly increased.¹³ A fully renewable electricity system is expected to require high proportions of wind and solar technologies,¹⁴ an expansion and reinforcement of the power grid¹⁵ and large-scale energy storage.^{16,17} These system implications largely depend on the cost and performance of heat pumps, which are in turn influenced by the choice of components, heat demand, and operating conditions.¹⁸

Countries pursuing a net-zero carbon energy system have a range of pathways to choose from. In energy systems, various

technologies are interconnected and influenced by decisions made across different levels, ranging from centralized to decentralized energy generation, distribution, storage, and utilization technology options. Choices that are optimal for end users may have unintended consequences for the broader energy system, and vice versa. Whole-energy-system models are used to assess and compare different decarbonization pathways and provide recommendations on the system-wide policies required to achieve the energy transition. In the UK, for example, such models include the UK market allocation (MARKAL) model,¹⁹ the whole electricity system investment model (WeSIM),^{20,21} the modular energy system simulation environment (MUSE),²² and the electricity systems optimization (ESO) model.²³ Each of these models has its own advantages (e.g., high spatial resolution, high temporal resolution, and inclusion of different investor types), but they all share a limitation when it comes to integrating heat pumps: the technical and economic characteristics of these technologies are represented by simple mappings between inputs (e.g., ambient temperature) and outputs (e.g., efficiency). Available heat pumps on the market involve various designs (e.g., different working fluids, heat exchanger sizes, and compressor types), meaning that the use of simplified relationships overlooks interactions and trade-offs when selecting technologies in the broader energy context and results in high uncertainties and no guidance on technology design.²⁴

Heat pumps in Europe

The number of electricity-driven heat pumps per 1,000 people installed by 2022²⁵ and the ratio between the electricity and natural gas prices^{26,27} for domestic consumers for some of the largest economies in Europe between 2017 and 2022 are shown in Figure 1. A linear line of best fit is plotted through the electricity-to-gas price ratio points corresponding to 2017, 2021, and 2022. Norway, Finland, Sweden, and Estonia have by far the highest penetration of heat pumps in the domestic heating market (>150 heat pumps per 1,000 people), whereas the UK comes last (6 heat pumps per 1,000 people). Several countries are taking drastic measures to shift away from fossil fuels. The Norwegian government banned heating installation based on fossil fuels in 2017.²⁸ In Finland, the government announced that the country will be carbon neutral by 2035 and the significant rise in heat pump installations can be attributed to the fact that

heat pumps are clearly a profitable investment.²⁹ Both Norway and Finland lack widespread gas-distribution infrastructure.^{28,29}

As shown in Figure 1, there is an inverse relationship between the uptake of heat pumps and the electricity-to-gas price ratio reported in European countries. This is attributed to the fact that a low ratio increases the competitiveness of electric heat pumps in terms of operational costs compared with gas-fired options. In countries like the UK, Germany, Slovakia, and Belgium, this ratio in the last 5 years has been consistently above 3. This means that in these countries, assuming no incentives are provided, a heat pump would only provide any operational cost savings for the end user compared with a gas boiler if its annual coefficient of performance (COP), which is the ratio of the useful heat output over the electricity input, is more than 3 times higher than a boiler's efficiency. This is often not the case and the heat pump uptake in these countries is low (<20 heat pumps per 1,000 people). It is noteworthy that the significant increase in gas prices observed during 2022 led to a decrease in electricity-to-gas-price ratios in many locations (as evidenced by the blue line of best-fit trend compared with the green and orange lines). This phenomenon highlights the growing competitiveness of electric heat pumps in the European context.

Novelty and relevance

In energy systems, decisions at various levels, from household to energy-system level, affect interconnected technologies. In light of the recent vast development of policies aiming at the wide update of air-to-water heat pumps worldwide,²⁵ this study represents the first known attempt to provide design guidance for low-temperature residential air-to-water heat pumps from both an end user and a whole-energy system perspective. To achieve this, data for more than 100 commercially available products are used to develop and validate comprehensive thermodynamic and component-costing models of variable-speed compressor air-to-water heat pumps.³⁰ Using these, a set of optimal heat pump designs is obtained representing competing components, all of which can meet heating requirements across the entire range of considered temperatures. The designs are first compared in terms of price, payback time, and levelized cost of heat (LCOH). Then, the characteristics of different heat pump designs are integrated into the heat, electricity, and gas infrastructure and technology (HEGIT) model, a whole-energy system capacity-expansion and unit-dispatch model focusing on heat electrification. The latter model, which is described in detail in the work of Hoseinpoori et al.,^{31,32} is an expanded version of the ESO model described in the studies of Heuberger et al.,^{23,33} and it is here used to identify the cost-optimal transition pathways for decarbonizing heat and meeting the UK 2050 net-zero emission targets. Different heat pump designs are compared in terms of their effect on the energy system's electricity generation portfolio and system transition cost toward heat decarbonization.

Given the remarkable role of air-to-water heat pumps in transition pathways¹³ and the importance of appropriately capturing technology developments in energy-system models,³⁴ this work provides useful insights to energy planners, system operators, and heat pump manufacturers about how to best choose and design domestic heat pumps in net-zero carbon energy systems.

In the rest of this work, the UK is used as a case study, as it is one of the countries with the highest electricity-to-gas price ratios and lowest uptake of electric heat pumps in Europe (Figure 1). The UK experiences significant seasonality in its heat demand. During cold winter days, the peak demand for heating of the UK energy system (in kW_{th}) exceeds 6 times the peak demand for electricity (in kW_e).³⁵ The UK government aims to intervene decisively and is now aiming to install 600,000 new heat pumps per year by 2028,⁹ which makes the UK a well-suited and relevant case study to compare domestic heat pump designs. Valuable insights can be derived not only for locations with similar uptake and electricity-to-gas price ratio characteristics (e.g., Germany, Belgium, and Poland) but also for locations that share similar net-zero carbon emission targets and are highly dependent on fossil fuel-driven heating (e.g., the Netherlands, Italy, and France). Nevertheless, the numerical data presented here are susceptible to fluctuations depending upon the characteristics of different geographical areas, as well as other uncertainties, and thus, they should be viewed as general reference points and not definitive empirical benchmarks.

RESULTS AND DISCUSSION

In this section, an analysis of different domestic air-to-water heat pump designs is presented concerning their thermodynamic and economic performance. This includes a comparison of existing and prospective components and working fluid choices and a consideration of environmental considerations as well as the trade-offs between achieving high efficiency and low cost. Heat pump designs are assessed in terms of price, payback time, and LCOH. Then, the implications of different designs on the energy system are examined, and the ways in which these affect design choices are discussed.

Heat pump component and working fluid selection

In most domestic applications, electricity-driven air-to-water heat pumps comprise four main components: a compressor, a condenser, an evaporator, and an expansion valve.²⁴ The thermodynamic and component-costing model presented in detail in the experimental procedures is used to provide and compare a wide range of optimal air-to-water heat pump designs. Following an extensive market analysis, these involve three different compressor types found on the heat pump market (reciprocating-piston, rotary vane, and scroll), fifteen current and prospective working fluids, and a large range of heat exchanger areas (between 0.5 and 4 m²). All designs, which are based on state-of-the-art component models, encompass optimizing heat pump cycle parameters (heat exchanger pressures, superheating, and subcooling degrees) with the objective to maximize the COP under nominal operating conditions. These nominal conditions are set as the industry-standard benchmarks used by European manufacturers to report heat pump performance: an ambient air temperature of 7°C and a hot-water delivery temperature of 55°C (referred to as "A7/W55").³⁶ By using an inverter-driven variable-speed compressor, all heat pump designs are able to produce a maximum thermal output of 10 kW_{th} across all operating conditions. The compressor is intentionally sized to meet this output requirement. This heat

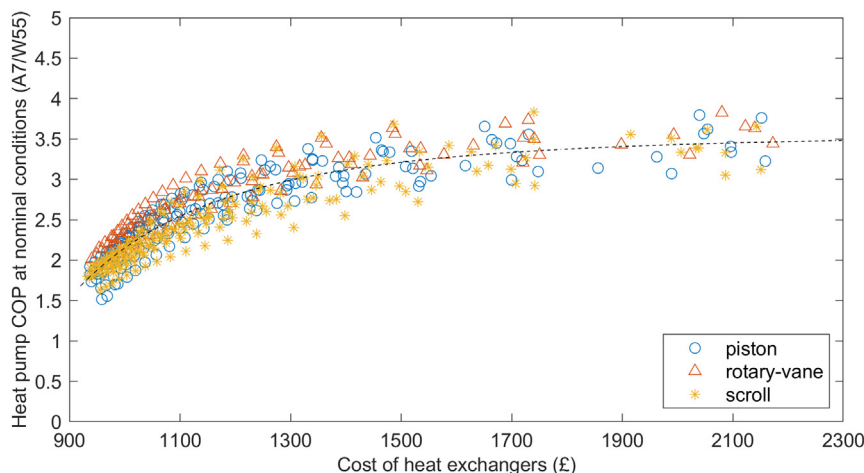


Figure 2. COP of domestic 10 kW_{th} air-to-water heat pumps at nominal operating conditions (A7/W55) as a function of heat exchanger cost

A change in heat exchanger cost (which is the sum of the evaporator and condenser costs) represents a change in heat exchanger size. Large heat exchangers cost more than small heat exchangers, but they also allow for greater heat transfer and enhanced performance (i.e., higher COP). Different symbols show different compressor types.

pump thermal output aligns with typical capacities of commercially available domestic heat pump products found on the market³⁰ and is also equal to the peak heat demand observed in an average UK household, according to the “cold” temperature profile of Sansom.³⁷

Figure 2 shows the heat pump COP at nominal operating conditions as a function of heat exchanger costs as obtained from the thermodynamic and component-costing models for different investigated component combinations. Every scatter point represents an optimal heat pump design for a selected compressor type, heat exchanger area, and working fluid. Different compressor types are represented by different symbols. For simplification purposes, only designs for which the minimum temperature differences between heat exchanger fluids are the same in the condenser and evaporator are shown (although all combinations are investigated).

As shown in Figure 2, the choice of components can have a significant effect on the COP of domestic heat pumps, which varies between about 1.6 and 3.8 depending on the chosen design. Furthermore, Figure 2 reveals that the cost and performance of heat pumps are not independent. Better performance (i.e., a higher COP) can be attained with a greater capital investment in components such as the heat exchangers.

Although Figure 2 is interesting mainly in understanding the degree to which heat exchanger size affects heat pump performance, Figure 3 is useful in comparing the costs of different compressor types. It shows the average compressor cost and associated standard deviation for each type. The average cost of reciprocating piston, rotary vane, and scroll compressors is equal to £2,560, £790, and £2,690, respectively, and as shown by the standard deviations, the cost for most piston, and scroll designs varies between about £1,000 and £4,000, whereas it varies between about £650 and £900 for rotary vane compressors. When rotary vane compressors are an available option, they are significantly cheaper than the other two types, which is the main reason that most domestic-scale heat pumps on the market are based on this compressor type. More details on the cost and performance of different compressor types are provided in the [experimental procedures](#).

Figure 4 is useful to examine the effect of a large range of possible working fluids on the heat pump performance and cost. The ten best-performance fluids are shown. Figure 4A shows the average

heat pump COP at nominal conditions for different fluids. Figure 4B shows the heat pump LCOH, which is a measure of the average cost per unit of heat generated over the system’s lifetime, and the global warming potential (GWP) of each fluid, which is a measure of a fluid’s contribution to global warming. For the calculation of the LCOH, we assume a lifetime of 20 years, installation costs of £2,300,³⁸ a maintenance cost of £100,³⁹ an electricity price for domestic consumers equal to 0.28 £/kWh (average in the UK in 2022⁴⁰), and a real discount rate of 3% (as suggested by IEA for air-to-water heat pumps⁴¹). Although some of the shown fluids have already been phased out from domestic applications (R22 and R134a), their technoeconomic potential is evaluated for comparison purposes.

Hydrochlorofluorocarbons (HCFCs) and hydrofluorocarbons (HFCs), which are synthetic in nature, have until now been the most widely used working fluids in air-conditioning and heat-pumping applications. R22 was one of the main options in the past and, as shown in Figure 4, is one of the highest-performing fluids. It is associated with one of the highest average COPs across the investigated working fluids and an average LCOH lower than 0.19 £/kWh. However, its use in domestic heating has been dramatically reduced due to its high ozone depletion potential (ODP), equal to 0.055, and its high GWP index, equal to 1,960.^{42,43}

R134a has been another widely used fluid that does not damage the ozone layer and has a lower GWP index than R22 (1,530; Figure 4B), but it is also being phased out of low-temperature heating applications. It is associated with an average COP of 2.5, which is competitive with other options, but it requires larger components and the estimated LCOH is higher than its successors. The analysis of commercially available products in the work of Olympios et al.³⁰ shows that, in recent years, R410a has been the working fluid in more than 70% of the commercially available domestic heat pumps in the UK. As shown in Figure 4B, R410a shows to have a lower average LCOH than R134a. However, R410a exhibits a remarkably high GWP (2,256). This has led to further research focusing on the development and comparison of new fluid solutions with lower environmental impacts.^{44,45}

R152a shows competitive performance with a GWP of 164 and an average LCOH of 0.19 £/kWh. Since 2019, there has been an

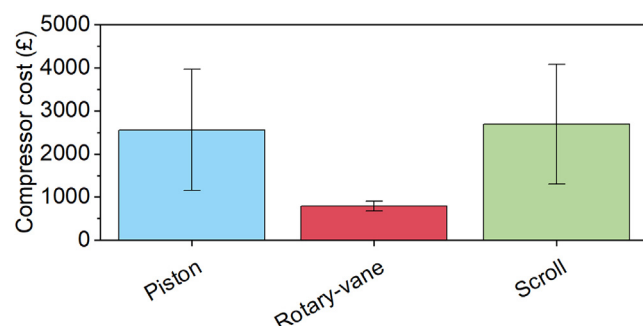


Figure 3. Compressor cost for domestic air-to-water heat pumps for different compressor types (piston, rotary vane, and scroll)

The error bars represent the standard deviation based on all simulated component combinations.

increasing trend toward R32, which has a GWP index of 771. Due to its excellent heat-transfer characteristics,⁴⁶ heat pump components can be compact, and therefore, the estimated average LCOH is the second lowest (0.18 £/kWh) of the investigated options. R32 is now dominant in newly advertised units.⁴⁷ Although the GWP of R32 is lower than its previous contenders, it is still substantial, and stricter regulations may require even lower-GWP fluids.

Natural working fluids are a sustainable alternative to HFC options, benefiting from zero ODP and negligible GWP. These include hydrocarbons (HCs), ammonia, and CO₂. CO₂ is not considered in this work, as it has a low critical temperature (31°C), and transcritical CO₂ systems achieve lower performance than the subcritical systems investigated in this work in low heat delivery temperature applications (i.e., <65°C).^{48,49} Nevertheless, it is important to note that CO₂ systems have a low GWP of 1, zero ODP, non-toxicity, non-flammability, and the ability to generate hot-water delivery temperatures up to 90°C,^{49–51} which makes them suitable for colder locations and buildings with outdated central heating systems, avoiding the need for radiator replacement.

The three best-performing HC fluids shown in Figure 4 (butane, propane, and isobutane) have competitive performance. Butane shows a high average COP close to 2.7, but it is demonstrated in Figure 4B that propane is associated with the lowest average LCOH of the three of them (close to 0.19 £/kWh). One of the main reasons for the latter result is that the properties of propane are such that a lower mass flow rate is required during the heat pump's operation, and therefore, a smaller compressor can be selected compared with other HC fluids. Propane-based compression machines have been proven to be reliable⁵² and are increasingly appearing on the market.⁵³

Ammonia has the potential to play an important role in energy-transition pathways.⁵⁴ As shown in Figure 4, it is the fluid with the best thermodynamic performance (average COP equal to 2.8) and the lowest cost (heat pump LCOH equal to 0.17 £/kWh). However, it is toxic and corrosive,⁵⁵ being considered "extremely hazardous" by the U.S. Environmental Protection Agency (EPA).⁵⁶ These limitations often necessitate the use of complex heat pump designs, which explains why ammonia is currently predominantly employed in large industrial plants and commercial facilities,⁵⁷ as opposed to domestic hot-water sys-

tems (no domestic electricity-driven ammonia-based heat pumps are currently available on the market). In a scenario of high uptake of ammonia-based heat pumps, components must be sufficiently proofed, and strict safety inspections should be regularly performed.

The analysis of current and potential components and working fluid choices for low-temperature air-to-water heat pumps offers valuable insights for heat pump designers. Most importantly, it quantifies how heat pump cost and performance are correlated, which lays the groundwork for the development of a comparative analysis of a diverse range of optimal heat pump designs from the energy system perspective in the upcoming sections of this paper.

Trade-off between heat pump efficiency and cost

Based on the analysis and discussion of the potential of different working fluid options, the rest of the results in this work are focused on four main working fluids: (1) R410a, which is the currently most widely used fluid; (2) R32, which has been replacing R410 in recent years; (3) propane, which has the most promising technoeconomic potential between the HC options; and (4) ammonia, which is shown to be the best-performing fluid but is associated with some safety concerns.

In the subsequent analysis, we categorize heat pumps as high- or low-performance based on their nominal COP. Specifically, high-performance heat pumps have COPs equal to or greater than 3.2, and low-performance heat pumps have COPs equal to or less than 2.8. High-cost heat pumps are those with specific prices greater than or equal to 750 £/kW_{th}, and low-cost heat pumps are those with specific prices less than or equal to 600 £/kW_{th}.

Figure 5 summarizes the main characteristics associated with the above four fluid options. Characteristics include each fluid's health (H) and flammability (F) indexes, which are ratings on a scale from 0 (no hazard) to 4 (severe hazard) provided by the U.S. National Fire Protection Association (NFPA).⁵⁸ The heat pump COP and specific price shown in Figure 5 correspond to the average values from the range of investigated designs. The price reflects the expenditure for the heat pump unit itself and does not include supplementary costs related to the hot-water cylinder, labor, or radiator replacement costs.

From the four fluid options shown in Figure 5, R410a has by far the highest GWP, whereas its COP is similar to R32 and propane. R32 has the lowest specific heat pump cost, and although it has a high flammability index of 4, it is already widely employed in new heat-pumping systems mainly due to advancements in the design of hermetically sealed components.⁵⁵

Ammonia has the best thermodynamic performance (average nominal COP of 2.8), and it does not contribute to global warming. On the other hand, ammonia is the only investigated fluid that has been given a health index as high as 3 by NFPA.⁵⁸ It is also important to state that this analysis does not account for the fact that ammonia is not compatible with several copper components that can lead to design complexities and thus additional costs.

Propane, which, as in the case of ammonia, does not contribute to global warming, is shown to have a slightly higher price than the other options, but it has a competitive COP. The

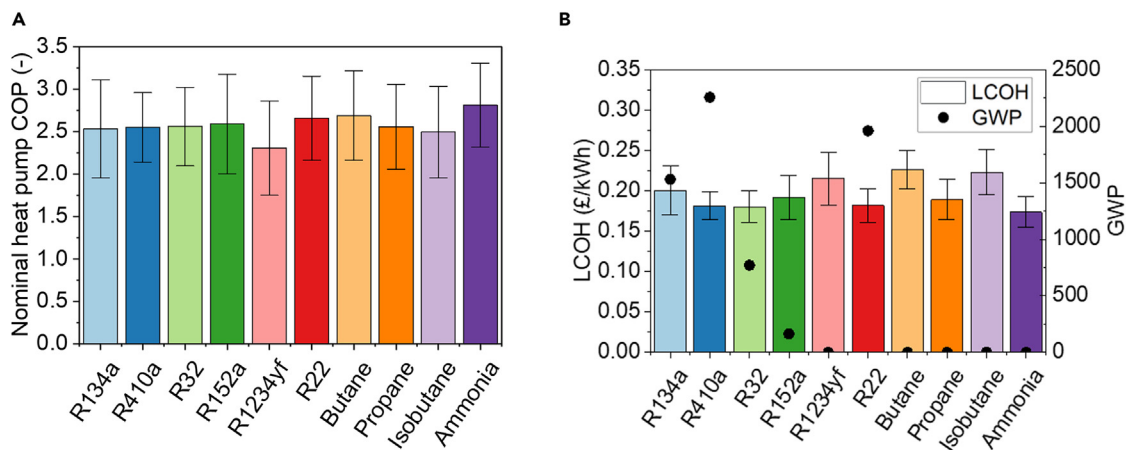


Figure 4. Comparison of air-to-water heat pump technoeconomic performance for a range of different fluids

(A) COP at nominal operating conditions (A7/W55) and (B) LCOH and working fluid GWP (100 years). The error bars represent the standard deviation based on all component combinations.

flammability index of 4 and the A3 classification according to BS EN378⁵⁹ indicate that propane, due to its low quantity required for combustion in air, necessitates careful handling. It is crucial to consistently implement safety protocols to ensure that it is used safely and effectively.

The trade-off between choosing high-efficiency/high-cost or low-efficiency/low-cost heat pumps is demonstrated in Figure 6, which shows the nominal COP and specific price (excluding supplementary costs such as labor, cylinder, and radiators) associated with different designs for the four discussed fluid options. All designs including those with a different minimum temperature difference in each heat exchanger are shown. All three compressor types commonly found in the domestic heat pump

market are examined, along with a wide range of heat exchanger sizes spanning from the minimum feasible size, determined by the critical temperature of each fluid, to the maximum size, which represents a minimum temperature difference of 1°C between heat exchanger fluids.

The drawn lines represent the Pareto fronts associated with each fluid. These represent the sets of optimal heat pump designs that are not dominated by any other solution with respect to both the objectives of COP and price. Essentially, for every solution on the Pareto front, there is no alternative solution that can improve one objective without diminishing the other. Any heat pump design within the feasible region not on the Pareto front is suboptimal, indicating the presence of solutions that could improve either the COP or the price without negatively impacting the other. Notably, even when a heat pump is designed in an optimal way (i.e., positioned on the Pareto front), a remarkable spread in the nominal COP (ranging from 2.2 to 3.8) and specific price (ranging from 510 to 830 £/kW_{th}) are observed. The disparities in these ranges are noteworthy, given that all analyzed heat pump designs share identical nominal capacities and configurations. As all solutions on the Pareto front are optimal, the optimal design choice depends on the set objectives, which can vary when looking at the problem from the perspective of the end user or from that of the whole energy system.

An interesting observation from Figure 6 is that most of the heat pump designs found on the Pareto fronts involve a rotary vane compressor. This is because rotary vane compressors found on the market are in general cheaper than piston or scroll compressors. As the COP increases, piston and scroll compressors become more competitive. In fact, scroll compressors appear on the Pareto fronts for maximum COP designs of R410a, R32, and ammonia-based heat pumps. As demonstrated by the Pareto fronts in Figure 6, ammonia achieves the best combinations of COP and specific price, whereas R32 can be competitive with ammonia for low-performance, low-cost designs. Propane can be used to design similar-efficiency heat pumps to R32, but this happens at a higher price.

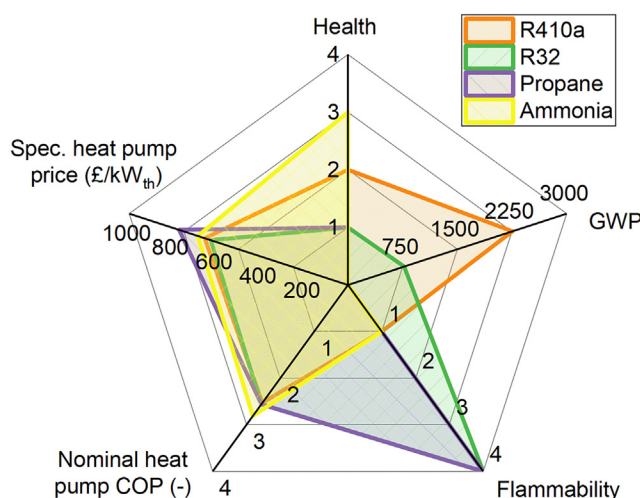


Figure 5. Specific air-to-water heat pump price, COP at nominal operating conditions (A7/W55), and fluid characteristics (health, flammability, and GWP indices) for four optimal heat pump designs with different working fluids

Health and flammability indexes are ratings on a scale from 0 (no hazard) to 4 (severe hazard) according to NFPA classification.⁵⁸

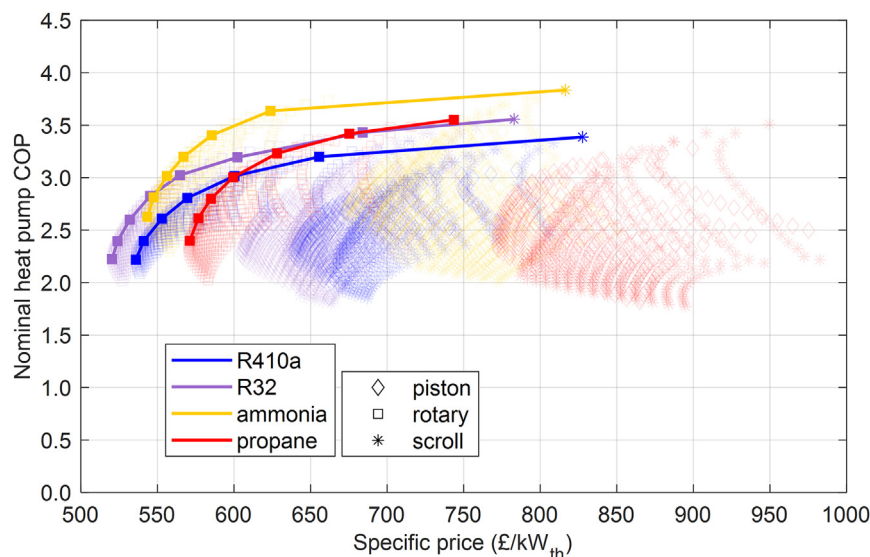


Figure 6. Air-to-water heat pump COP at nominal operating conditions (A7/W55) versus specific retail price for different designs based on alternative compressor types, working fluids, and heat exchanger (condenser and evaporator) areas
The different lines show the Pareto fronts for the investigated fluids.

Overall, the analysis in this section shows that most high-performance (nominal COP ≥ 3.2) and high-cost (price ≥ 750 £/kW_{th}) heat pumps involve large heat exchangers (with a total cost $\geq$ £1,300) and rotary vane or scroll compressors, whereas most low-performance (nominal COP ≤ 2.8) and low-cost (price ≤ 600 £/kW_{th}) designs involve small heat exchangers (with a total cost $\leq$ £1,300) and rotary vane compressors. Reciprocating-piston compressors are shown to achieve lower heat pump COPs than rotary vane and scroll compressors for the investigated conditions, and therefore, they do not appear on the Pareto fronts of Figure 6. However, reciprocating piston compressors are associated with high-pressure capabilities and are competitive at higher pressure ratios and colder climates.⁶⁰

High-cost or low-performance heat pumps do not inherently signify poor design, especially if they are positioned near or on the Pareto front. Instead, this positioning indicates deliberate design decisions aimed at maximizing performance or cost-effectiveness, respectively. The quantification of this performance-cost trade-off was never explored in the context of domestic air-to-water heat pumps and the large variety of possible designs shows the significance of this section.

Heat pump selection from the end-user perspective

When considering heat pump selection from the end user's perspective, the payback time and LCOH are useful performance indicators to account for both investment and operation costs. Figure 7 shows the calculated heat pump unit price, LCOH, and payback time associated with specific points along the Pareto front of each fluid from Figure 6. Although several end users often base their technology choices on investment costs (Figure 7A), it is wiser to use performance indicators that account for both investment and operation costs. The payback time (Figure 7B) is the period required to break even following the initial heat pump investment, and the LCOH (Figure 7C) is a measure of the average cost of heat generation. For the payback time estimation, cost savings associated with the installation of a

heat pump are calculated assuming switching from an electric boiler, as recent legislations on gas boilers for domestic applications show that these will soon not be an available option.⁹ For the calculation of payback time and LCOH, labor and radiator replacement costs are included and assumed to be the same for all heat pump designs.

LCOH considers the entire lifetime of a technology. Consequently, the operational

performance and thus operational costs are more significant factors in this metric compared with payback time. Conversely, payback time places greater emphasis on the initial investment cost. As demonstrated in Figure 7, for all four investigated fluids, the minimum payback time and LCOH are obtained for nominal COPs in the range of 3.2–3.6. At this range, rotary vane compressors are the optimal compressor option, but scroll compressors are also competitive, achieving a LCOH lower than 0.17 £/kWh. Furthermore, optimal designs at this COP range involve large condensers and evaporators, often with a total cost higher than £1,300 (Figure 2).

Although the analysis from the end user's perspective provides useful insights, it is of interest to compare this with how heat pump designs compare with those from a whole-energy system's perspective. This is performed by integrating the designs corresponding to the points along the fluid Pareto fronts within the HEGIT model, a novel whole-energy system model that is used to explore how the energy system would look for different domestic heat pump component choices. The results of this analysis are presented and discussed in the next section.

Energy system implications

Different domestic heat pump designs can convert heat demand into different power demand profiles, which can in turn have an effect on the energy system technology mix, the requirements for electricity generation, the heat decarbonization transition cost, and the way heating technologies should be operated within a multi-vector energy system. HEGIT is an integrated multi-scale heat, electricity, and gas-system capacity-planning and unit-commitment model used to simultaneously optimize the installation and operation strategies of electricity-driven, gas-driven, and heat-driven technologies of the whole energy system. The objective of the model is to minimize the total system cost required to reach a net-zero energy system while complying with all environmental objectives and maintaining the security of supply. By using the technoeconomic heat pump models to inform HEGIT, the role of different heat pump designs is investigated over the planning

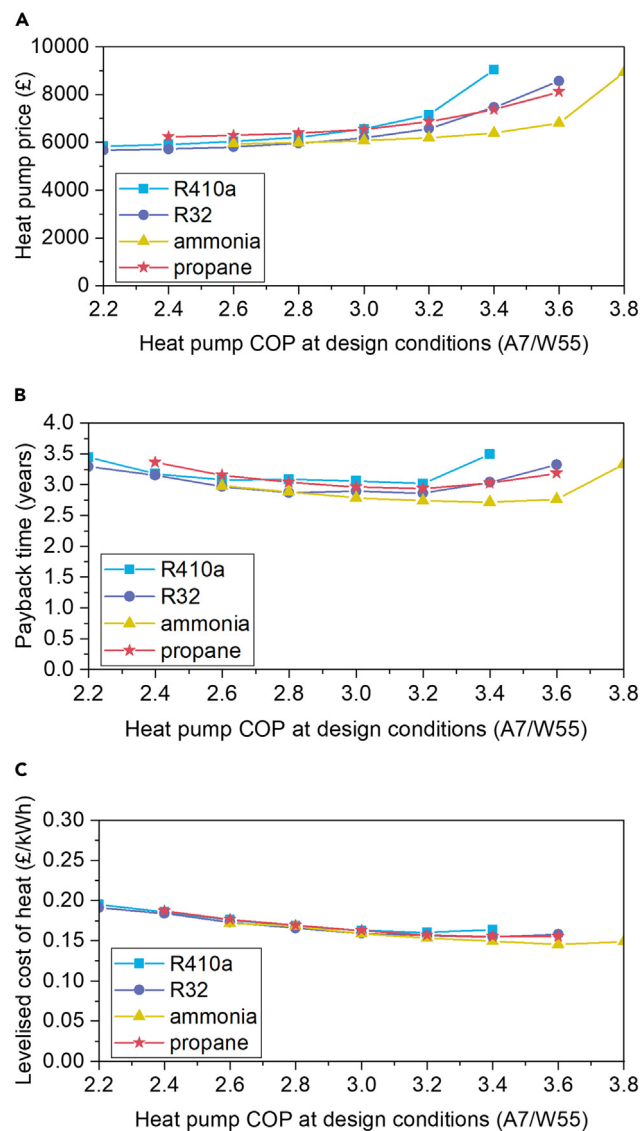


Figure 7. Comparison of air-to-water heat pump designs of varying COP and price in terms

(A) Investment cost; (B) payback time when switching from an electric boiler; and (C) LCOH. Different designs correspond to those shown on the Pareto fronts of Figure 6.

horizon extending from now to 2050, which is the year by which most countries are targeting to achieve net-zero carbon emissions.

In all whole-energy system results of this section, the decarbonization of both hot water and space heating is assumed to take place only through electrification and the uptake of domestic air-to-water heat pumps. The heat pumps are assumed to have the same size as in the previous section (corresponding to a heat output of 10 kW_{th} at nominal conditions). Whenever a new heat pump is installed in a household, it is accompanied by a hot-water cylinder, which stores water at the required temperature. The cylinder is sized so that the heat pump can charge it in 1 h⁶¹ and is costed based on the analysis of commercially available products on the market.³⁰ HEGIT can identify the

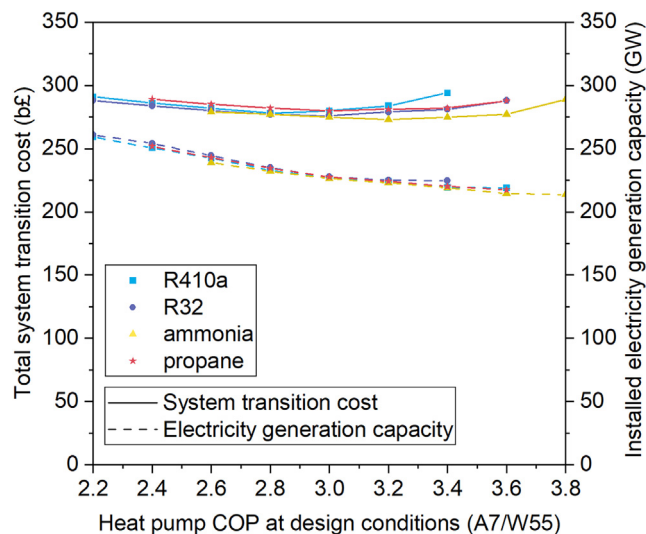


Figure 8. Total system transition cost (in present value) to decarbonize the domestic heating sector over the planning horizon (2020–2050) and installed electricity generation capacity in 2050 for different air-to-water heat pump designs of varying COP and price

optimal operation of all considered technologies, thus capturing load-shifting capabilities associated with the hot water cylinder.

Electricity system generation capacity and heat decarbonization transition cost

In Figure 8, the total system transition cost of decarbonizing domestic heating by 2050 is shown along with the installed electricity generation capacity in 2050 assuming that the domestic heating sector is decarbonized through different-performance heat pumps. The system transition cost of decarbonizing heating is the sum of all upstream investment and operation costs associated with energy generation and storage, as well as all heat pump investment, maintenance, and operation costs over the planning horizon. This cost is quantified as the difference between the total cost in a scenario where all households are decarbonized using air-to-water heat pumps by 2050 and a counterfactual scenario with no net-zero carbon domestic heating. The investigated designs correspond to the Pareto fronts for the four investigated fluids in Figure 6. Non-optimal designs (appearing below the Pareto fronts of Figure 6) are not investigated from the system perspective as they would not lead to any additional system benefits.

Depending on the chosen heat pump design, the total system transition cost and the installed electricity generation capacity are shown to vary in the ranges 273–297 b£ and 213–263 GW, respectively.

The use of high-performance/high-cost heat pumps (nominal COP ≥ 3.2), which are often designed with rotary vane or scroll compressors and large heat exchangers, can lead to a substantial reduction in the required electricity generation capacity of up to 50 GW (~20%) compared with low-performance/low-cost units (nominal COP ≤ 2.8), which are often designed with rotary vane compressors and small heat exchangers. This is important, as it means that a large uptake of high-performance heat pumps can

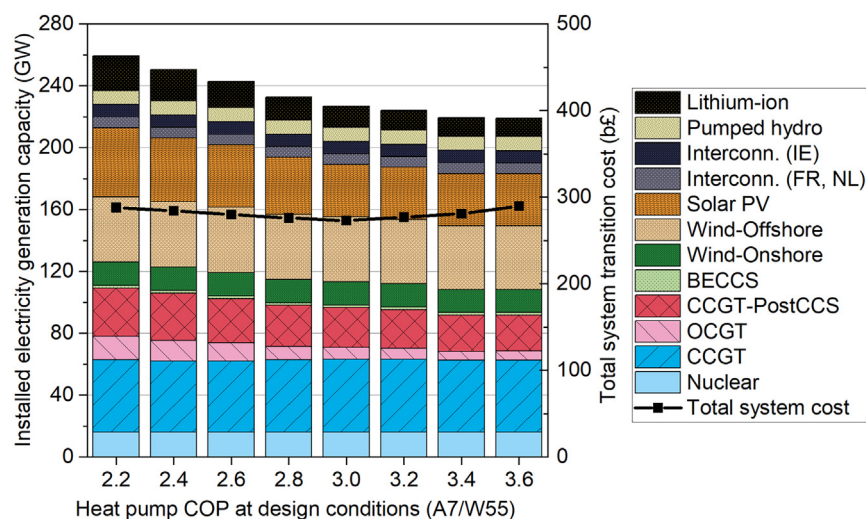


Figure 9. Installed electricity generation capacity by technology in the UK energy system in 2050 and system cost of heat decarbonization for different domestic air-to-water heat pump designs of varying COP and price

The different designs correspond to those shown on the Pareto front of Figure 6 with R32 as the working fluid.

As shown in Figure 9, the majority of electricity generation capacity is attributed to nuclear power, open-cycle gas turbines (OCGTs), closed-cycle gas turbines (CCGTs) with or without carbon capture and storage (CCS), and onshore and offshore wind and solar photovoltaic (PV) systems. For the emissions attributed to unabated gas-based generation

(OCGTs and CCGTs) to be offset, a small capacity of negative-emission technologies, and in particular, bioenergy with CCS (BECCS), is also present. In addition, the model also accounts for power imports through interconnectors with Ireland (IE), France (FR), and the Netherlands (NL). The energy system also includes grid-scale energy storage in the form of pumped hydro and lithium-ion batteries.

A significant capacity of OCGTs and CCGTs without CCS is shown to exist in the energy system. In detail, the two technologies together account for about 20% (52–60 GW) of the total electricity generation capacity (Figure 9). However, the actual amount of electricity produced by these sources during a year is much lower than that, accounting for less than 1% of the total annual electricity output (Figure 10). The reason for this is that during peak heat-demand periods, rapid heat-demand variations introduce notable ramping service requirements for the system. Ramping services are primarily supplied by backup gas turbine plants. This means that although a significant capacity of backup generators is required to ensure the security of supply, these are not in operation most of the time. Nuclear plants, on the other hand, which only account for 5% of the total electricity generation capacity (Figure 9), provide constant and reliable power and are therefore responsible for more than 20% of the annual electricity output (Figure 10).

Overall, the performance of domestic air-to-water heat pumps has three main implications for the set of technologies comprising the country's electricity generation and storage infrastructure, as indicated in Figures 9 and 10. First, the higher the heat pump COP, the less the system's dependence on grid-scale energy storage. The main reason for this is that the domestic heat demand is highly fluctuating and seasonal. A high uptake of high-performance heat pumps would lead to reduced electricity demand compared with low-performance alternatives, consequently reducing the necessity for centralized electricity grid flexibility, which demonstrates the interlinked nature of electricity and heat vectors. Grid-scale energy storage is acknowledged to have a vital role to play in maintaining the variability and uncertainty of the demand,^{16,62} and as our analysis demonstrates, its role is largely

significantly lower the power-grid expansion and technology uptake rates that are required to achieve the country's environmental objectives. In terms of financing and materials, this in turn means that a more practical and realistic system transition may lie ahead.

Although high-performance heat pumps are shown to significantly reduce the need for electricity generation, they are also more expensive. As shown in Figure 8, the minimum system transition cost is obtained for heat pumps with a nominal COP in the range of 2.8–3.2 for the four investigated fluids (273 b£ for ammonia-based heat pumps and 276 b£ for R32-based heat pumps). This is up to 23 b£ lower than the system transition cost obtained for the highest-performance heat pumps, corresponding to 9% of the total cost. Heat pumps with a nominal COP in the range 2.8–3.2 also have the advantage that they result in a reduction in the electricity generation capacity by 15–40 GW compared with low-performance/low-cost units.

In the case that R32 and ammonia are not widely adopted in the near future due to GWP or safety concerns, propane is one of the most likely alternatives, but it is associated with a higher total transition cost (281 b£ at best). This means that compared with current refrigerant solutions (R410a and R32), the cost of using natural refrigerants in new heat pump designs can be expected to be close to 5–8 b£.

In order to understand how the energy system would look for different designs, we here choose as an example to focus on the optimal heat pump designs that correspond to the Pareto front which involves R32 as the working fluid (similar trends were also obtained for the other fluids). The optimized breakdown of the installed electricity generation capacity in the UK energy system in 2050 is presented in Figure 9 together with the specific heat pump price associated with each design. The annual electricity output per technology and the energy-system power load factor in 2050 are shown in Figure 10. The total electricity output is equal to the total electricity demand for the entire year, including that required for heating during the heating season. The power load factor is defined as the ratio of the average annual electricity demand over the peak electricity demand.

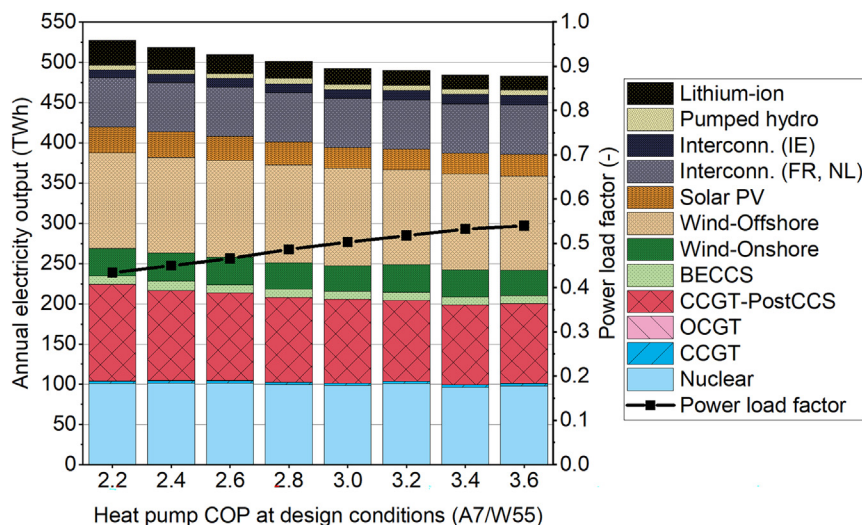


Figure 10. Annual electricity output by technology in the UK energy system in 2050 and associated power load factor (average annual electricity demand over peak electricity demand) for different domestic air-to-water heat pump designs of varying COP and price

The different designs correspond to those shown on the Pareto front of Figure 6 with R32 as the working fluid.

affects the grid's flexibility requirements and thus the role of grid-scale energy storage and CCS.

It is important to also consider how end users are economically affected by heat pump design choices. In Figure 11, the total system transition cost to decarbonize heating by 2050 is broken down into two

affected by the chosen heating technologies. Specifically, the capacity of lithium-ion batteries in 2050 is shown to vary greatly between 17 and 30 GW for different R32-based heat pump designs.

The second important effect of heat pump design on the energy system is the change in the requirements for electricity generation from natural gas. In fact, the required capacities of OCGT plants without CCS and CCGT plants with CCS reduce significantly when installing higher COP heat pumps. The higher the overall performance of heat pumps, the lower the peak heat demand, and the smoother the fluctuations in demand, which means lower ramping requirements. Although, according to current assumptions, this combination of technologies seems to offer a cost-effective method to avoid exclusive dependence on lithium-ion batteries, it is crucial to note that CCS technologies have not yet been widely deployed and are thus subject to limitations regarding the rate at which new energy infrastructure can be currently constructed. As shown, the capacity of OCGT reduces by more than 50% when using the highest-performance R32 heat pumps compared with the lowest-performance ones, going down from 13 to 6 GW, whereas the capacity of CCGT with CCS also reduces significantly from 30 to 24 GW (Figure 9). The annual electricity production based on CCGT technology with CCS varies between 100 and 130 TWh for different heat pump designs (Figure 10), which demonstrates that the higher the heat pump performance, the lower the dependence of the energy system on CCS technologies.

The third effect of different heat pump designs is associated with the renewable electricity generation capacity and, especially, that of solar PV. Low-performance heat pumps are associated with up to 9 GW more renewable electricity generation capacity (out of which 7 GW is solar PV) installed in the energy system than high-performance heat pumps.

A high load factor means that the difference between the average and peak electricity generation is small, resulting in a more efficient use of resources. As shown, the load factor varies between 43% and 55% for the heat pump designs shown in Figure 10. The fact that low-performance heat pumps result in a lower load factor shows the degree to which heat pump design

parts: (1) the cost associated with upstream electricity generation and storage technologies and (2) the cost that homeowners would pay for heating systems. The latter cost involves the investment, installation, and maintenance costs associated with domestic heat pumps and thermal storage.

The total system transition cost for end users is shown in Figure 11 to vary between 106 and 122 b£ for different heat pump designs. This is an interesting observation as it means that wide use of more affordable heat pumps would shift a significant portion of the total system transition cost that is required for heat decarbonization from the end users to the government compared with high-performance units. Consequently, this would result in reduced upfront expenses for all homeowners, regardless of their income level, potentially enhancing accessibility and affordability for a wider range of households. It becomes imperative for the government to play a pivotal role in devising mechanisms to ensure a fair distribution of the upstream energy system costs among taxpayers and ratepayers. It is interesting to compare the transition cost for end users to the total system transition cost required for heat decarbonization. As shown in Figure 11, from an energy system perspective, it is not cost-optimal to promote a wide uptake of the higher-performance/higher-cost (nominal COP ≥ 3.2) heat pumps, as this would increase both the cost that needs to be paid by end users and the total system cost compared with medium-performance/medium-cost units with a nominal COP in the range of 2.8–3.2.

Investing in heat pump performance or whole system flexibility?

Our findings reveal that uptake of high-performance heat pumps results in a lower LCOH from an end-user perspective and a reduced required national electricity generation capacity compared with low-performance heat pumps. However, from an energy-system perspective, there is a point of diminishing returns, beyond which, instead of investing in even higher heat pump COP, it becomes more cost effective to invest in increased centralized energy system generation and storage technologies.

In detail, it is shown that rather than investing in high-cost heat pumps with a nominal COP higher than 3.2, it is overall

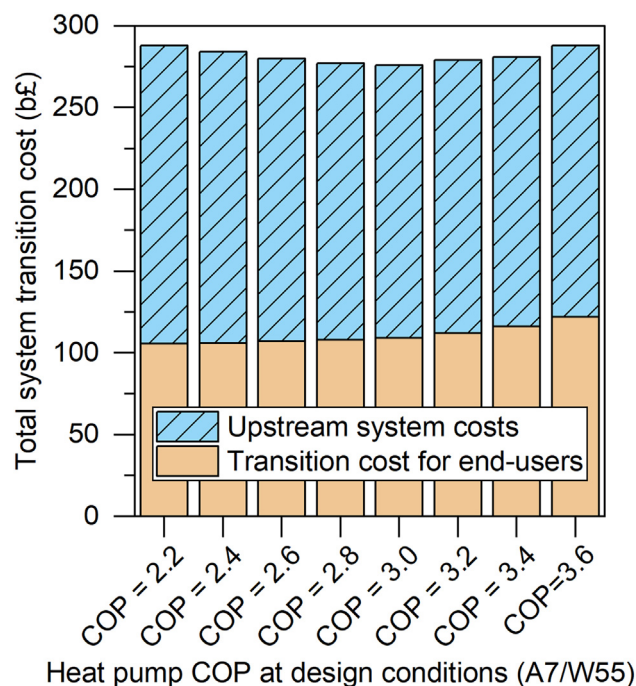


Figure 11. Total system transition cost (in present value) to decarbonize the domestic heating sector over the planning horizon (2020–2050) for different air-to-water heat pump designs of varying COP and price, broken down into the total cost associated with upstream electricity generation and storage technologies and the cost that household owners would pay for heating systems (investment, installation, and maintenance costs associated with domestic heat pumps and thermal storage)

The different designs correspond to those shown on the Pareto front of Figure 6 with R32 as the working fluid.

cost-optimal to keep heat pump costs relatively low (e.g., ≤ 750 £/kW_{th}), even if that means investing in a fair amount of battery storage, CCGT with CCS, and solar PV. Such an approach also means that transferring a large part of the transition cost to the end users is avoided. The difference in the transition cost for homeowners when comparing heat pumps with a nominal COP below 3 (Figure 11) is not significant, varying between only 1% and 3%. On the other hand, the transition cost for homeowners increases by more than 13% when increasing the COP from 3 to 3.6. Due to this, and since medium-performance/medium-cost heat pumps with a nominal COP in the range of 2.8–3.2 were shown to achieve the minimum total system cost for most fluids (Figure 8) and are also associated with lower total electricity generation requirements than lower-performance heat pumps (Figure 9), it makes sense that investing in medium-performance ($2.8 \leq \text{nominal COP} \leq 3.2$) heat pumps provides a good compromise between achieving a practical energy system transition and minimizing the required government and end user investments.

It is interesting to compare the above conclusions to those drawn when only considering the payback time or LCOH associated with each fluid option (Figure 7). As shown in Figure 12, from an end user's (homeowner's) perspective, and depending on whether the minimization of the payback time or LCOH is consid-

ered the main objective, heat pump designs with a COP of 3.2, 3.2–3.4, 3.4–3.6, and 3.2–3.4 are optimal when the working fluids are R410a, R32, ammonia, or propane, respectively.

From an energy system's perspective, the designs that minimize the total system cost have COPs of 2.8, 3, 3.2, and 3 when using R410a, R32, ammonia, or propane as the working fluid, respectively. Instead of investing in further heat pump COP enhancements beyond these designs, the findings indicate that it is economically favorable to invest in increased centralized energy storage, CCS, and renewable energy generation.

The additional system transition cost when designing heat pumps for objectives other than the total system transition cost is also shown in Figure 12. Using payback time as the objective function leads to higher COPs than when using the whole-energy system transition cost as the objective function. Meanwhile, using LCOH, which places more emphasis on operational performance, often results in even higher nominal COPs and consequently, higher overall energy system transition cost compared with when using the latter as the objective function. Depending on the chosen fluid and objective, additional system costs of up to 5 b£ can be observed when an end user perspective is adopted, demonstrating the notable impact of heat pump design on the total cost of energy transition pathways.

When considering heat pump component choices, it can be concluded that although from an end user's perspective, high-performance compressors (scroll or rotary vane) and large heat exchangers (often costing $\geq$ £1,650 in total for a 10 kW_{th} heat pump as shown in Figure 2) are competitive options, from an energy-system perspective, it is beneficial to focus on medium-performance compressors (rotary vane) and smaller heat exchangers (costing less than £1,300 for the obtained optimal designs of Figure 12).

Results from this section have energy system implications and can be translated into certain energy policy measures. For example, the government could set measures that encourage consumers to buy heat pumps with certain characteristics. These could involve grants to household owners that are only applicable for heat pumps that meet certain design and cost specifications. Furthermore, the government could help manufacturers make design choices that are optimal from an energy system perspective by subsidizing specific components or by providing grants to those who design heating technologies that meet the required cost and performance criteria.

Limitations and further discussion

All heat pumps examined in this paper were designed to be able to meet heating requirements across the whole considered temperature range. Even the least efficient heat pumps are sized so that they could provide the required heat at the coldest average temperature in the UK. The only difference between low- and high-performance heat pumps is that the former are associated with a higher electricity consumption than the latter.

The need for supplementary electric resistance heaters or natural gas boilers is found to be minimal in the UK, primarily since outdoor temperatures rarely drop below -10°C . However, in locations with considerably colder climates, the role of backup technologies can differ significantly and could potentially change some of the results.

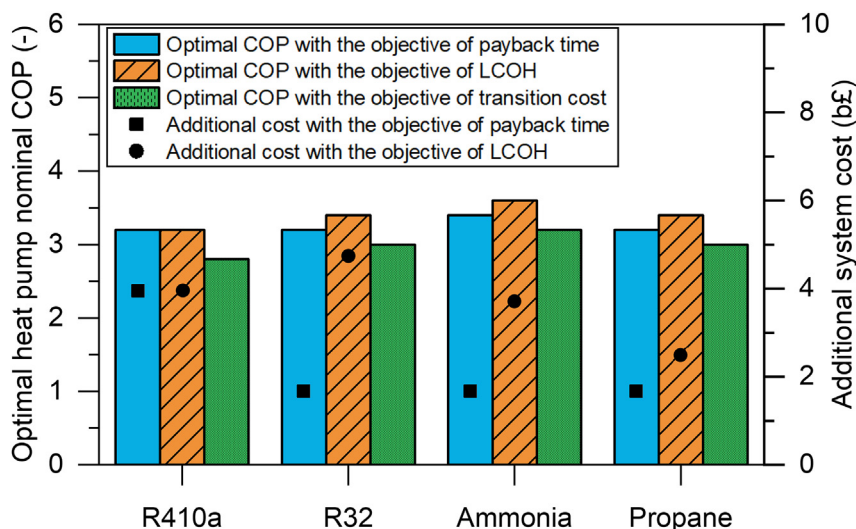


Figure 12. Optimal heat pump nominal COP at design conditions (A7/W55) for different working fluids when looking at the design problem from an end-user's perspective (with the objective to minimize being the payback time or LCOH) and a whole-energy system perspective (with the objective to minimize being the total system transition cost)

The additional system transition costs to decarbonize heat when using the payback time or LCOH as the objectives compared with when using the total system transition cost are also shown.

Technology prices are notably influenced by economic, demographic, and technological changes, posing challenges. Technological learning from the extended deployment of various technologies is likely to drive down prices in the future,

Furthermore, we acknowledge that although electricity-driven heat pumps are likely to dominate the heating market of many countries worldwide, they are unlikely to be the sole heating technology in use. For example, solar thermal could be an option in some locations, but it is anticipated to be limited in the UK, and the UK Sixth Carbon Budget⁶³ indicates that solar thermal combined with electric resistance heating are likely to contribute less than 5% of the heating technology mix. In terms of hydrogen, in the Heat and Buildings Strategy report,⁶⁴ it is stated that further “testing, trialing, research, and development to help assess the feasibility, costs, and benefits of widespread use of hydrogen in heat and buildings” is required. At the same time, in a recent work of the authors,⁶⁵ we demonstrated that given current hydrogen production costs, electricity-driven heat pumps are significantly more cost effective for decarbonizing residential heat demand. The Heat and Buildings Strategy report⁶⁴ also recognizes the viability of district heat networks as an alternative pathway in “areas of high-density heat demand and where there are large low-carbon heat sources,” and the UK government’s recent evaluation report⁶⁶ suggests that heat networks could potentially address up to 20% of the heat demand. It is stated, however, that this serves as an upper limit and should not be considered an indicative target, due to local limitations and the potential economic infeasibility of projects reliant on waste-heat sources.

Another interesting technology in specific types of buildings involves high-temperature heat pumps, which could potentially deliver higher temperatures than 55°C (e.g., up to 90°C). Although such heat pumps are typically more expensive and less efficient than low-temperature heat pumps that would be expected to be found in typical UK households, they could be a method to avoid replacing central heating systems and radiators in properties characterized by uninsulated solid floors, very exposed places, unusual construction, no room for a hot water cylinder, or minimal-tenant-disruption targets.

It is also important to acknowledge that although our energy system model is informed by detailed thermodynamic and component-costing models, all data related to heat pumps and other technologies and systems still possess uncertainties.

with each technology affected differently.

HEGIT simplifies the UK energy system by representing it as a single node, without considering the geographical distribution of resources and demand. Although this is a common simplification in whole-energy system models, we acknowledge that the UK often experiences air temperature variations, which introduce a degree of uncertainty into the model.

In addition, an analysis of methods related to modifying heat demand through shifts in consumer behavior is not included in the scope of this work, but it is acknowledged that if a considerable number of end users were to shift some of their heating demand to lower demand hours, the peak electricity demand of the system could reduce, influencing the energy system technology mix. Several other mechanisms also play a role in the performance and competitiveness of heat pumps, including the characteristics of the physical limitations and thermal properties of different houses (radiators, insulation, thermal inertia, etc.) and control approaches. Although smart heat pump and thermal storage integration and control (a topic explored in various other papers) are useful, our aim here is to demonstrate that heat pump design choices themselves, even at the component level, have a substantial influence on energy transition pathways, and therefore, an exploration of various hot-water cylinder sizes was not conducted in this study.

Considering the aforementioned limitations, it is important to acknowledge that the specific numerical data presented in this paper concerning energy system costs and installed capacities should only be considered general reference points. This applies to all forms of whole-energy system model analyses, given the inherent uncertainties associated with input parameters. However, these limitations do not diminish the substantial impact of the heat pump physical characteristics on both efficiency and cost (even for identical configurations and capacities) and thus on the whole energy system.

Finally, it is crucial to emphasize that although our analysis indicates a clear correlation between heat pump cost and performance, this is not an absolute rule. Innovation has the potential to enable manufacturers to enhance component heat pump

performance without increasing costs. Thus, research and development in novel heat pump components and systems should remain a top priority in all electrification pathways.

Conclusions and outlook

Electricity-driven air-to-water heat pumps have the potential to play a dominant role in decarbonizing domestic heating and meeting global energy and environmental objectives. In this study, we developed a component-to-system framework that considers a wide range of domestic heat pump designs. Starting with an examination of their technoeconomic potential from the end user's perspective, detailed thermodynamic and component-costing heat pump models were used to quantify the significance of design decisions on heat pump performance and cost and compare different designs in terms of investment cost, payback time, and LCOH. Then, by integrating outputs from these models within the whole-energy system model HEGIT, the effects of different designs on the national electricity generation technology portfolio and heat decarbonization transition cost were identified, demonstrating the trade-offs inherent in different design choices.

The findings of this work revealed that the selection of heat exchanger size, compressor type, and working fluid has a significant effect on the cost and COP of a heat pump. Specifically, the heat pump COP at nominal conditions (ambient air temperature of 7°C and hot-water delivery temperature of 55°C) was shown to vary between 1.6 and 3.8 depending on the chosen heat pump design, whereas the specific cost was shown to vary between 510 and 990 £/kW_{th}. Furthermore, there is a Pareto front of multiple optimal heat pump designs that trade off performance and cost, rather than a single best design. When comparing different heat pump designs from an end user's perspective, the minimum payback time and LCOH were obtained for heat pumps with nominal COPs in the range of 3.2–3.6. The question that arises is, among all the available heat pump designs, which one is associated with the minimal whole energy system heat decarbonization cost?

When different optimal heat pump designs were compared in terms of their implications for the UK energy system, it was shown that progressively higher-performance/higher-cost heat pumps monotonically reduce the required national electricity generation capacity. Higher-performance/higher-cost heat pumps (nominal COP > 3.2), which are often designed with rotary vane or scroll compressors and large heat exchangers (often costing >£1,300 in total), can lead to a substantial reduction in the required electricity generation capacity of up to 50 GW (~20%) compared with lower-performance/lower-cost heat pumps (nominal COP < 2.8), thus reducing power-grid expansion and technology-uptake rate requirements. However, as the heat pump COP increases, the (end-use) heat pump investment required also rises, leading to an optimal design that minimizes the total system transition cost. Beyond that optimal point, further COP improvements become financially ineffective, and those resources could be more effectively allocated elsewhere in the energy system. Specifically, we show that from an energy system perspective, it is overall cost-optimal to design heat pumps with nominal COP in the range of 2.8–3.2, which typically has a specific cost lower than 650 £/kW_{th}, and simultaneously to invest in increased capacities of renewable energy

generation technologies and batteries, in the first instance, followed by OCGT and CCGT with CCS. We estimate that such an approach would lead to a total system transition cost reduction that, depending on the working fluid, can be more than 20 b£ (corresponding to almost 10% of the total cost) and also means that transferring a large part of the transition cost to the end users can be avoided, potentially accelerating the uptake of low-carbon heating technologies.

Given that optimal heat pump designs can enable a 20% reduction in the required electricity generation capacity and a 10% decrease in total system transition costs relative to the use of lower- or higher-performance alternatives, respectively, it can be concluded that heat pump design selection holds as much or, arguably, even greater significance for the decarbonization of the UK energy system because the inclusion of technologies that are considered crucial to the future evolution of the system, such as CCGT with CCS, batteries and BECCS, are projected to represent about 10%, 7% and 1% of the UK's total installed electricity generation capacity in 2050.

EXPERIMENTAL PROCEDURES

Resource availability

Lead contact

Further information and requests for resources should be directed to and will be fulfilled by the lead contact Christos N. Markides (c.markides@imperial.ac.uk).

Materials availability

This study did not generate new unique materials.

Data and code availability

The published article and its supplemental information include all data analyzed during this study. Any additional information required to reanalyze the data reported in this paper is available from the [lead contact](#) upon request.

Heat pump models and data

A spatially lumped thermodynamic and component-costing model of a domestic air-to-water heat pump was developed in previous work published by the authors.^{24,65} The heat pump model, which predicts the performance and cost of each heat pump component, is validated based on an analysis of more than 100 commercially available heat pumps (<20 kW_{th}) found on the UK market in 2019–2021.³⁰ The data used for this analysis is provided in [Note S1](#). The detailed description of the heat pump cycle, the governing equations, and defrosting assumptions are provided in [Note S2](#). Component cost correlations and model validation are provided in [Notes S3](#) and [S4](#), respectively.

The basic components of a domestic air-to-water heat pump along with a temperature (*T*)–specific entropy (*s*) diagram of the heat pump cycle are shown in [Figure 13](#). Process 1–2 represents the working fluid compression, 2–3 the heat transfer from the working fluid to hot water, 3–4 the isenthalpic expansion, and 4–1 the heat transfer from the heat source to the working fluid.

The (first-law) thermodynamic performance of heat pumps is characterized using the COP, which is the ratio of the useful heat output $\dot{Q}_{out}$ to the required electricity input $\dot{W}_{in}$:

$$COP = \frac{\dot{Q}_{out}}{\dot{W}_{in}} \quad (\text{Equation 1})$$

In this work, we have extended the previously developed heat pump model to capture the effect of four independent design parameters on the heat pump's performance and cost: (1) compressor type; (2) condenser size; (3) evaporator size; and (4) working fluid choice.

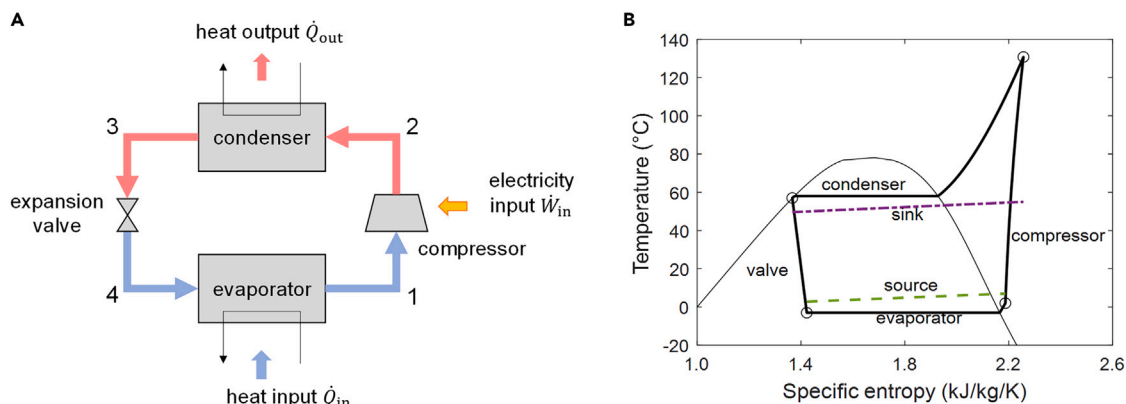


Figure 13. Vapor compressor heat-pump cycle
(A) Basic components and (B) temperature (T)—specific entropy (s) diagram.

Compressor types

The performance of a heat pump depends crucially upon the design of the compressor. The analysis of the heat pump market shows that heat pumps in domestic applications involve three main compressor types: rotary-vane, scroll and reciprocating-piston. An understanding of the performance of these types at various operating conditions is necessary to properly model design and off-design heat pump performance. We use a similar methodology to that of As-tolfi,⁶⁷ who reported data of various commercially available screw compressors to examine the relationship of maximum isentropic efficiency as a function of the volume ratio between compressor inlet and outlet and the volumetric flowrate. Screw compressors are usually found in larger heat-pumping systems than those required for domestic applications, therefore they are excluded from our analysis. Furthermore, since our analysis focuses on typical domestic applications, only compressors that can attain the necessary compression ratio through a single compression step are considered. All these compressors are equipped with inverters, allowing for variable-speed operation.

Rather than collecting information only related to the maximum efficiency of each commercially available unit, in this work we instead focus on gathering information for both the design and off-design performance of available units. This is useful to predict compressor isentropic efficiency at any operating condition. Using manufacturer data for 40 currently commercially available units for each of the three compressor types,⁶⁰ we use 2nd order polynomial fits to form compressor efficiency maps that can predict their behavior for various working conditions. Rotary-vane compressors available on the market are associated with volumetric flowrates below $5 \cdot 10^{-3} \text{ m}^3/\text{s}$ and, therefore, they are not included in designs requiring higher flowrates. The developed maps and associated equations are found in [Note S5](#).

Condenser and evaporator sizes

In traditional technoeconomic optimization of power or heat pump cycles, the size of heat exchangers is often optimized based on a specified performance indicator (e.g., specific investment cost or LCOH). As this approach does not account for implications of the different designs on the energy system, the obtained designs may be suboptimal from the whole-energy system's perspective. To obtain the wide spread of possible heat pump designs, we parametrically and independently vary the minimum temperature difference between heat exchanger fluids, often referred to as the pinch-point temperature difference (PPTD), in the condenser and evaporator. The minimum considered heat exchanger size is based on the critical temperature of each fluid; designs with heat exchangers that would require the working fluid to operate at supercritical temperatures to deliver the required heat are not investigated due to the performance deterioration and additional complications associated with such conditions.^{48,49} At the same time, a maximum heat exchanger size is set based on the space available for heating systems in typical UK homes. In detail, the length and width of the heat exchangers are constrained to be lower than 0.5 m, so that heat pump systems could replace traditional boilers in typical homes (which most often

have widths and depths lower than 0.5 m^{68,69}) without requiring significantly more space.

In order to investigate various heat exchanger sizes between these two stated limits, the PPTD is varied in steps of 1°C, between a minimum value as low as 1°C (based on the maximum heat exchanger size constraint) and a maximum possible value often close to 15°C–20°C depending on the critical temperature and pressure of the chosen working fluid). As the PPTD gets smaller, the heat pump COP increases, but the required heat exchanger area increases and leads to higher component costs. Conversely, as the PPTD gets larger, both the COP and heat exchanger costs reduce. Designs with even larger heat exchangers (lengths or widths larger than 0.5 m) were also tested for comparison purposes, however, in addition to being unrealistically large for domestic applications, these were shown to lead to insignificant COP improvements (<3% for all investigated fluids); therefore, further analysis for such designs is not presented.

The heat pump model incorporates comprehensive heat exchanger models comprising of different zones based on the flow characteristics. In the case of the condenser, a plate heat exchanger is used. Plate heat exchangers are characterized by compactness and high performance, which are both vital in small-scale applications.^{24,70} In the case of the evaporator, a plate fin-and-tube heat exchanger is used to enhance the heat transfer area between air and the working fluid, in line with the vast majority of domestic heat pumps.²⁴ Details about heat exchanger models are found in [Note S6](#).

Working fluids

The extent to which a heat pump can be designed for maximum achievable performance largely depends on the choice of working fluid. Working fluids, also referred as refrigerants, undergo repeated phase transitions in a heat pump cycle and should be effective at heat exchange. The fluid choice depends on the fluid thermophysical characteristics, the environmental impact, and the associated legislative regulations.⁷¹ The leakage of working fluids to the earth's atmosphere during the operational lifetime of heat pumps can have two negative effects: (1) contribute to the destruction of the ozone layer which protects the earth from ultraviolet radiation; and (2) warm the earth by absorbing infrared radiation.⁷² Regulations recently become stricter^{73,74} and the phase-down of a large range of options is expected in the next years.⁷⁵ The full list of working fluids under investigation in this work and their main characteristics are provided in [Table 1](#). It should be mentioned that the fluids with the worst thermoeconomic potential have been excluded from [Figure 4](#) in the [results and discussion](#) section.

LCOH and payback time

The LCOH and payback time are calculated as shown in [Equations 2 and 3](#) according to IEA⁷⁷ and the discounted payback time methodology,⁷⁸ respectively:

$$C_{\text{LCOH}} = \frac{C_{\text{inv}} + \sum_{k=1}^n C_{\text{op,ann}} (1+r)^{-k}}{\sum_{k=1}^n Q_{\text{ann}} (1+r)^{-k}} \quad (\text{Equation 2})$$

Table 1. List of working fluids under investigation and their main properties

Working fluid	Type	T_{crit} (°C)	P_{crit} (bar)	M (kg/kmol)	ODP	GWP (100 years)	H	F
R22	HFC	96	50	87	0.055	1,960	1	0
R134a	HFC	101	41	102	0	1,530	1	0
R410a	HFC	71	49	73	0	2,256	2	1
R32	HFC	78	58	52	0	771	1	4
R152a	HFC	113	45	66	0	164	1	4
R245fa	HFC	154	36	134	0	962	2	0
R1234yf	HFO	95	34	114	0	0.5	1	4
R404a	HFC	72	37	98	0	4,728	2	1
R125	HFC	66	36	120	0	3,740	2	0
Butane	HC	152	38	58	0	0.006	1	4
Propane	HC	97	42	44	0	0.02	1	4
Pentane	HC	197	34	72	0	0	1	4
Iso-butane	HC	135	36	58	0	0	0	4
Iso-pentane	HC	187	34	72	0	0	1	4
Ammonia	–	132	113	17	0	0	3	1

T_{crit} and P_{crit} represent the fluid critical temperature and pressure, respectively; M is the molar mass; and H and F are the health and flammability indexes according to NFPA classification⁵⁸ (0 is no hazard, and 4 is maximum hazard). The GWP is given for a 100-year time horizon and is based on the 6th Assessment Report of the Intergovernmental Panel on Climate Change (IPCC).⁷⁶ HFO stands for hydrofluoroolefin.

$$t_{PBT} = \frac{\ln \left[\frac{C_{sav,ann}}{C_{sav,ann} - rC_{inv}} \right]}{\ln[1+r]} \quad (\text{Equation 3})$$

where C_{inv} is the sum of the heat pump investment (equipment) and installation (non-equipment) costs, $C_{op,ann}$ is the sum of the annual operational and maintenance costs, k is the year, n is the heat pump lifetime, r is the real discount rate, Q_{ann} is the annual thermal energy produced, and $C_{sav,ann}$ is the annual cost savings.

All collected heat pump cost data are corrected for inflation and other economic conditions using the chemical engineering plant cost index (CEPCI) method.⁷⁹ For cost savings, it is assumed that the heat pump is used to replace an electric heater. For installation costs, we have based our assumptions on the recent report used by the UK Department for Business, Energy & Industrial Strategy,³⁸ which includes installation costs for various heating technologies and installation types. The installation cost is the sum of labor fees and the cost for replacement of “a few” radiators (without completely replacing the heating system or installing underfloor heating) as provided to correspond to a simple heat pump installation in a typical house in the UK. The annual maintenance cost is a constant value and consistent across all designs, as they all share similar components.

Heat pump design and off-design optimization

Two different heat pump models are used for the analysis shown in this paper: (1) a design optimization problem which involves optimal sizing of components under specific design condition with the objective to maximize the COP; and (2) an off-design optimization model used to optimize heat pump operation to maximize the COP for fixed component sizes but under varying temperature conditions by adjusting the compressor speed and the opening of the electric expansion valve.

The off-design model is necessary for the evaluation of the LCOH, payback time, and whole-energy system implications. This model identifies the optimal COP for different temperatures throughout the year by using the hourly temper-

ature and heat demand profiles corresponding to the cold temperature scenario from the work of Sansom.³⁷ The time-varying COP obtained is utilized to convert the hourly heat demand profile into an electricity demand profile, which is used to obtain annual operational costs and to determine energy system requirements. It is presumed that the heat demand is completely fulfilled in this analysis.

Heat pump design and off-design optimization problems are solved using MATLAB's interior-point algorithm *fmincon*⁸⁰ and the optimization variables are provided in Note S7.

Whole-energy system model

The methodology involves the heat pump price and time-varying COP values obtained using the developed design and off-design thermodynamic and component-costing models being used as inputs in HEGIT to quantify the influence of heat pump characteristics to the energy system. The different heat pump designs not only impact the cost of heat generation (via the heat pump price) but also the electricity generation and operational costs, as the COP affects the electricity demand, which subsequently impacts the required electricity generation technologies and the associated start-up costs, maintenance costs, and imports.

HEGIT is an integrated model of heat, electricity, and gas networks based on mixed-integer linear programming. A schematic of the model is available in Note S8. The model captures interactions between energy generation, network, storage, and utilization technologies, simultaneously optimizing investment and operation strategies for all considered technology options in the whole energy system. Thus, it can provide the cost-optimal heating and electricity generation portfolio as well as optimal dispatch profiles for the whole transition period from now to the end of the planning horizon (set as 2050). The main components of the objective function, which is to minimize the total system cost C_{tot} over the planning horizon, are shown in Equation 4:

$$\min C_{tot} = \sum_{i,k} \frac{(C_{inv,i} d_{i,k} + C_{op,i,k} n_{i,k} + C_{re,k} + C_{dec,k})}{(1+r)^k}, \quad (\text{Equation 4})$$

where $C_{inv,i}$ is the investment and installation cost of technology i (which includes electricity, gas and heat generation, conversion, and storage technologies), $C_{op,i,k}$ is the fixed and variable operation, maintenance, and start-up cost of technology i in year k including imported electricity costs, $d_{i,k}$ is the number of installed units of technology i in year k , $n_{i,k}$ is the number of units of technology i in operation in year k , $C_{re,k}$ is the grid-reinforcement cost in year y , $C_{dec,k}$ is the cost of decommissioning the gas grid in year k , and r is the real discount rate. The grid-reinforcement factor is a function of newly installed capacity of electricity generation technologies.

The model is subject to technology-operation and system-wide constraints (energy and mass balances, technology build-up rates, storage state of charge and charging/discharging rates, reserve and frequency control requirements, and carbon emissions). The k-means clustering method with an “energy-preserving” approach as proposed in the work of Heuberger et al.³³ is used to identify representative days for the annual electricity and heat demand, wind power, solar availability, price of imported electricity, and outside air temperature, while at the same time retaining the original profiles’ intermittency and variability. The model considers long-term changes in fuel prices, technologies, and carbon taxes and the time horizon is divided into 5-year investment periods. We use the model to identify the impact but also the optimal timing of heat decarbonization (i.e., how many households should change their heating technologies and when) based on the prices and objectives of each investment period.

The whole-energy system analysis includes supplementary costs related to thermal energy storage, labor, and radiator replacement costs, and these are assumed to be the same for all heat pump designs. The model also includes a backup electrical resistance heater but, given that we have sized the heat pumps based on the peak heat demand of typical UK households and configured them to provide hot water at the desired output temperature under all investigated environmental conditions, the use of the electric resistance heater in this context is found to be unnecessary. This aligns well with the findings of the recent work of Gibb et al.,⁸¹ who demonstrated that standard heat pumps can achieve suitable COPs for providing efficient heating in most locations in Europe where temperatures rarely fall below -10°C without the need for back-up heating capacity.

Addressing energy security and the ability to meet demand during extended cold periods is of paramount importance. Based on this, the annual heat pump performance is determined based on the hourly UK outside air temperature and typical heat demand profile as proposed for the cold temperature scenario from the work of Sansom,³⁷ which represents the coldest year from data collected between 1998 and 2010. By aggregating heat demand data collected during a comprehensive field trial conducted by Carbon Trust in 2007 and using a heating degree day analysis, Sansom categorized the years with minimal and maximal heating degree days as “mild” and cold temperature scenarios, respectively. The choice of the cold temperature scenario, which coincides with the year 2010, is used to capture potential peak heat demands (and the same rationale is found in earlier studies which focus on the same temperature scenario from Sansom^{82–86}). Additionally, to ensure grid security during extreme events, in HEGIT we assume the absence of renewable energy sources during the peak heat demand day.

The heat demand profile is adjusted to consider the changes in the UK’ population over the planning horizon. An average household size is used to size the heat pumps and detailed house segmentation is not performed. The heat-supply profiles generated by heat pumps involve differences compared to the heat-demand profiles, primarily due to the presence of decentralized thermal energy storage. The model distinguishes between buildings connected or not connected to the gas grid. For detailed information on the formulation and equations of the model, the reader is directed to the work of Hoseinpouri et al.^{31,32}

SUPPLEMENTAL INFORMATION

Supplemental information can be found online at <https://doi.org/10.1016/j.crsus.2024.100021>.

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AUTHOR CONTRIBUTIONS

A.V.O. wrote the paper with contributions from P.H. and C.N.M. A.V.O. and P.H. wrote the main code, ran the simulations, and provided formal analysis. C.N.M. led the research, conceptualized the ideas, defined the aims, provided resources, and managed research activities.

DECLARATION OF INTERESTS

The authors declare no competing interests.

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