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The case of 100% electrification of domestic heat in Great Britain

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Unlike power sector decarbonisation, there has been little progress made on heat, which is currently the biggest energy consumer in the UK, accounting for 45% of total energy consumption in 2019, and almost 40% of UK GHG emissions. Given the UK's legally binding commitment to "Net-Zero" by 2050, decarbonising heat is becoming urgent and currently one of the main pathways involves its electrification. Here, we present a spatially-explicit optimisation model that investigates the implications of electrifying heat on the operation of the power sector. Using hourly historical gas demand data we conclude that the domestic peak heat demand is almost 50% lower than widely-cited values. A 100% electrification pathway can be achieved with only a 1.3-fold increase in generation capacity compared to a power-only decarbonisation scenario, but only, by leveraging the role of thermal energy storage technologies without which a further 40% increase would be needed.

Introduction

Energy use and emissions from residential heating and cooling are increasingly important in many leading countries in their race to net-zero[1,2]. Recent studies on 1.5°C- compliant scenarios indicate considerably less flexibility in options available to decarbonise the residential sector highlighting the necessity to act now[3–6]. Decarbonising heat in particular is often conceived as a daunting task as natural gas serves between 60-80% of the domestic heat sector in countries like the UK, the Netherlands and United States with high consumer satisfaction[7,8]. By 2019, the UK managed to reduce its greenhouse gas (GHG) emissions by 36% compared to 2008 levels, driven by power sector emissions, which fell by 67%.[9]. While there has been steady progress in decarbonising the power sector, mostly through deploying renewable energy and replacing coal with gas generation, decarbonising the heat sector remains an unsolved riddle on the energy agenda. In 2019, heat was the single biggest energy consumer in the UK, accounting for 45% of total energy consumption and 40% of UK's territorial emissions[10].

The carbon intensity of the heat sector is driven by the incumbent gas-dominated system which serves almost 80% of demand across residential, commercial and industrial sectors[10]. Given the high operational efficiency and low cost of the gas system, decarbonising the heat sector will require judicious decision making and high levels of policy intervention.

Full electrification of the heat sector and replacing natural gas with hydrogen and hybrid systems including district heat networks and cogeneration technologies are the main heat decarbonisation pathways being advanced[11–14]. Each pathway is characterised by distinct trade-offs and a high degree of uncertainty related to the end cost for heating as well as the efficiency and security of the resulting low-carbon system. To date, most research has examined the problem of heat decarbonisation by considering aggregate representations of the spatial and temporal scales of the problem on a national level[15] and the impact of operational and security constraints on the resulting energy infrastructure has been neglected. In its 2018 overview publication, the UK Department of Business, Energy & Industrial Strategy (BEIS), outlined developments and policy initiatives on the topic of heat decarbonisation arguing that no single technology can prevail as dominant so far[16]. Electrification, biomass and hydrogen were advanced as the three main pathways whereas in its 2013 publication electrification was proposed as the dominant pathway[17]. Concerns over electrification often centre on expected pressures on the power grid and the perceived need for a very significant increase in generation capacity by as much as three-fold[18].

We use modelling and optimisation to elucidate the implications of decarbonising the domestic heat sector in Great Britain (GB) through electrification and present for the first time a high-resolution regional analysis. A key contribution of our study is the derivation and modelling of region-specific domestic heat demand profiles across the 13 local distribution zones (LDZs) of the GB gas network. The goal of our study is two-fold: (i) provide a systems-based examination on the implications of electrifying domestic heat in GB and (ii) identify the factors that act as barriers and enablers in the cost-optimal pathways for domestic heat decarbonisation.

Analysing the domestic heat sector in GB

Almost 80% of British households are connected to the gas grid while the remaining 20%, amounting to approximately 3.5 million households, are off-grid. Of the off-gas grid prop-

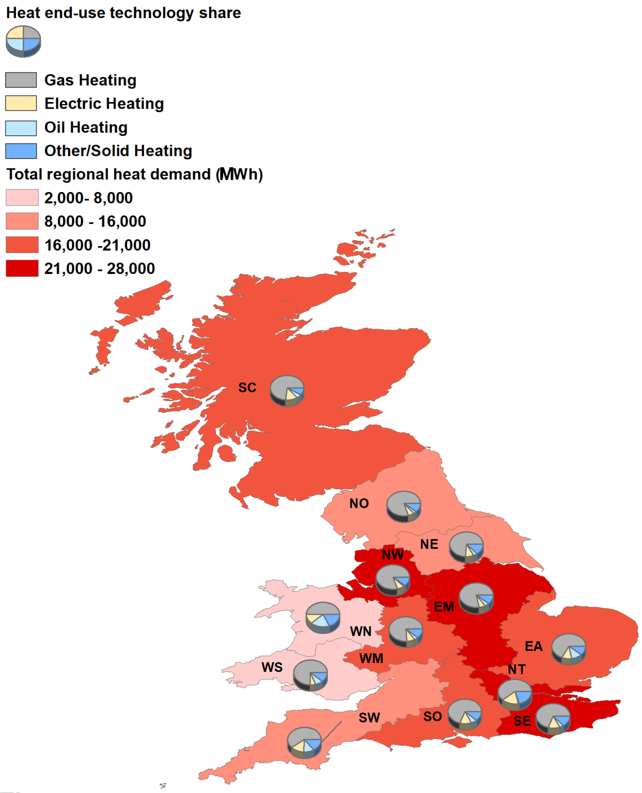


Figure 1. Regional analysis of the share of installed heating systems across the different regions in GB along with the total regional heat demand (MWh, given in red shading. Abbreviations: East Anglia (EA), East Midlands (EM), North East (NE), North (NO), North Thames (NT), North West (NW), Scotland (SC), South East (SE), South (SO), South West (SW), West Midlands (WM), Wales North (WN), Wales South (WS).

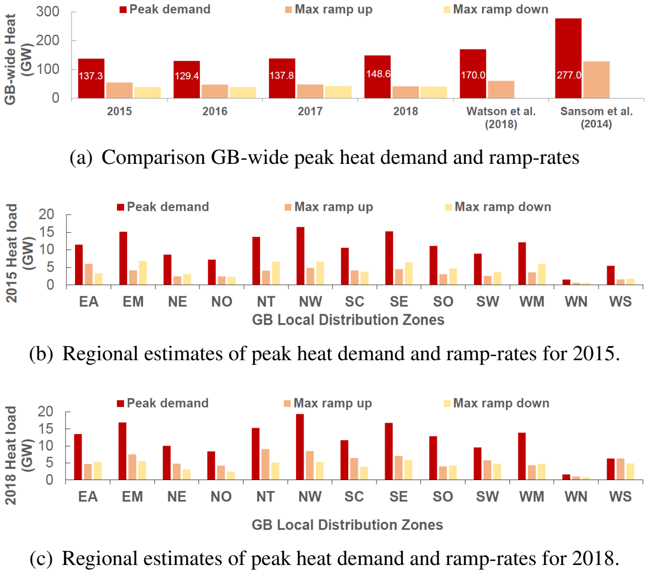
erties, 36.6% use some form of electric heating (mostly in the form of storage heaters), 40.8% utilise solid fuels (e.g. biomass, coal) and 22.4 % use oil burners[19]. Other forms of heating technologies such as district heat networks, ground-source heat pumps (GSHPs), air-source heat pumps (ASHPs) and micro combined heat and power systems (micro-CHP), all of which constitute viable options but to date have experienced limited adoption and taken together represent less than 2.6% of domestic heating systems in the UK[16]. In terms of incumbency, as indicated by Fig. 1 , the regions in the North of England (NO, NE, NW) have the lowest share of electric heating technologies while the South of England (SW, SE, NT) have the largest share. Interestingly in Wales, there is a significant divergence between the two regions, WS and WN, which can be attributed to 50% of WN properties not being connected to the gas grid and hence there are large shares of both electric and oil heating. In Scotland, more than 26% of domestic properties are not connected to the gas grid (13.5% electric heating and 13% oil/solid fuel).

Regional domestic heat demand in GB

Deciphering the impact of heat electrification in GB is explicitly dependent on the underlying heat demand characteristics of the different regions. Compared to non-heat- related electricity loads, heat demand is both highly volatile (in terms of ramp-rate changes) and seasonal. To date, one key challenge has been the lack of heat demand data at high temporal and spatial resolution. In GB, gas consumption data over the 13 different local distribution zones is only publicly available by National Grid with daily resolution[20] which impedes any analysis on the operational implications for the power system. Only a handful of studies make use of (half) hourly heat demand data[15,21,22] to examine heat decarbonisation in GB. However the aforementioned time series suffer from three shortcomings: (i) they are based on a limited number of smart-meter trials[23,24], thus generalising to the actual building stock can be problematic, (ii) the same demand profiles are applied uniformly across regions, thus neglecting differing socioeconomic and climactic factors that affect consumer behaviour and (iii) scaling-up individual profiles on a regional scale is subject to several assumptions about after diversity maximum demand (ADMD) which directly affects the sizing and performance of the resulting energy system infrastructure. ADMD accounts for non-coincident factors that explain the phenomenon under which the actual observed demand from a collection of households is less than the direct summation of their respective loads[25].

To this end, we obtained hourly gas consumption data over a number of years from all British gas network operators (GNOs) and analysed time series so as to develop hourly and region-specific domestic heat demand data. Further details on the data and methodology are given in the Methods section. Noting that previously estimated values cover the year 2010 which based on BEIS' official heating degree days analysis was 20% colder than 2018 and 22% than 2015[26], our analysis indicates that the domestic peak heat demand in GB can be up to 149 GW which is up to 53% less than previously estimated values[27,28] while the maximum hourly increase in heat demand was found to be 54 GW[21]. The importance of taking into account actual regional heat demand characteristics is underscored by Figs. 2(a)-2(c), which highlight the variations in peak load and maximum ramp rate.

Given the striking divergence from previously estimated heat loads, a sliding-window correlation analysis across the spatial and temporal scales was performed to visualise and quantify the importance of region-specific and actual heat demand profiles. As shown by Fig. 3, overall heat demand is as expected strongly dependent on ambient temperature and hence we identify high coincidence in neighbouring regions. Nonetheless, in comparing regions that are not spatially proximal, e.g. NW and SE, we see that their temporal heat map is not uniform (across the x-axis of each square) and hence even though both regions exhibit high heat demand peaks (Fig. 3), the overall peak diverges due to non-coincidence. Of course, non-weather phenomena, such as social factors or differences



(a) Comparison GB-wide peak heat demand and ramp-rates

(b) Regional estimates of peak heat demand and ramp-rates for 2015.

(c) Regional estimates of peak heat demand and ramp-rates for 2018.

Figure 2. Comparison of estimated GB heat demand characteristics for different years and with previous estimates.

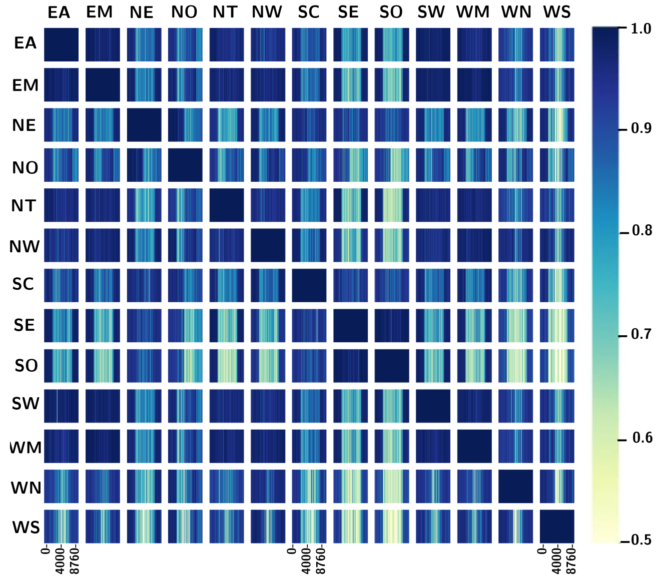


Figure 3. Temporal and spatial heat map of sliding window correlation analysis. Each square block represents the temporal synchronicity of heat demand pattern between two regions. Darker areas indicate synchronous demand pattern while light areas indicate greater divergence.

in building stock, can affect hourly heat demand, which can be seen when comparing the heat demand synchronicity in adjacent regions such as SE and NT, WN and WS or NO and NE. These neighbouring-region pairs experience similar hourly weather patterns so it would be natural to expect high levels of correlation across temporal scales. Instead, we observe significant variation on an hourly basis, which in turn can explain the reduction in heat peak and ramping estimates. The differences are revealed more clearly, once we perform a regression analysis on a daily and hourly basis. After aggregating our historical data on a day-by-day basis, a segmented linear regression explains well the dependence of heat demand on temperature. However, replicating the analysis using a finer (hourly) temporal scale, reveals that the relationship between heat demand and temperature is highly nonlinear, indicating the importance of other factors aside from weather (see Supplementary note 2).

In terms of regional diversity, the largest regions such as North West (NW), East Midlands (EM), NT and SE exhibit peak demand of up to 19 GWh for 2018, which represents the extreme year in our analysis, whereas the smallest regions such as the two Welsh LDZs have peak demand of less than 5 GWh. Focusing on the time series for 2018, while the GB-wide peak domestic heat demand occurs on 1 March between 18:00-19:00, this is not the case in every region. Specifically, while indeed the peak is synchronised with the regions EM, NE, NO, NW, SW and WM; in Wales (WN, WS) peak demand was on the same day but between 17:00-18:00 and 07:00-08:00 respectively, the southern regions (SE, SO) and EA exhibited a morning peak between 07:00-08:00 while the NT and SC regions' peak was the day before (28 February) between 18:00-19:00. Such instances, highlight the necessity of using regional data to evaluate decarbonisation strategies, since their peak occurs at distinctly different days and/or times (see Supplementary note 2).

Scenarios and system description

To accomplish our twin goals of providing a systems-based study of GB heat electrification and drivers of cost-optimal pathways, we propose a new spatially-explicit multi-period mixed integer model (OPHELIA) that simultaneously optimises capacity expansion (on a five-year basis) and operational decisions (on an hourly basis). Final electricity demand is endogenously computed and is divided into heat-driven and non-heat related demand. Assuming that the effects of population growth and improved welfare will be counterbalanced by energy efficiency improvements, which result in reduced demand per capita, future heat demand were derived based on 2015 and 2018 respectively[28]. For non-heat electricity demand, we follow the projections of the GB system operator[29] and consider annual energy requirements of 307TWh (excluding losses) and GB-wide peak demand of 57GW (excluding losses). A detailed overview of the mathematical formulation of OPHELIA along with the list of assumptions is provided in Supplementary note 3. Additional information on the derivation of regional electricity demand as well as the techno economic data is provided in Supplementary note 4.

To analyse the impact of different system assumptions on cost-optimal electrification we consider four main scenarios. In our base scenario “Elec", we assume heat is electrified by deploying ASHPs that are fully flexible and can be used in conjunction with termal energy storage (TES). Scenario "ASHPFlex" differs from "Elec" in that ASHPs are considered to have constrained flexibility and can only ramp-up/ramp-down up to 70% of their nameplate capacity[30]. To quantify the role

Table 1. Impact of heat electrification on capacity and generation by 2050 for different scenarios

	NoHeat	Elec2015	Elec2018	Elec NoTES (2015 heat data)	Elec NoICPeak (2015 heat data)
Nuclear (GW)	6	14.4	16.8	23.4	15.6
CCGT (GW)	18	18.5	18.5	20.5	18.5
CCGTCCS (GW)	19	21.5	21.5	23.5	21.5
Biomass (GW)	7.7	11.2	12.9	13.3	13
BECCS (GW)	1.5	1.5	3	7	4
WindOn (GW)	35	39.6	50	55	46.7
WindOff (GW)	12	38.7	41.9	44.5	42.5
Solar (GW)	26.2	19.3	38.4	45	28
GridStorage (GW)	16	17	19	32.9	20
Total Capacity(GW)	141.4	181.7	222	265.1	210
Total Generation (TWh)	353	530	593	570	563

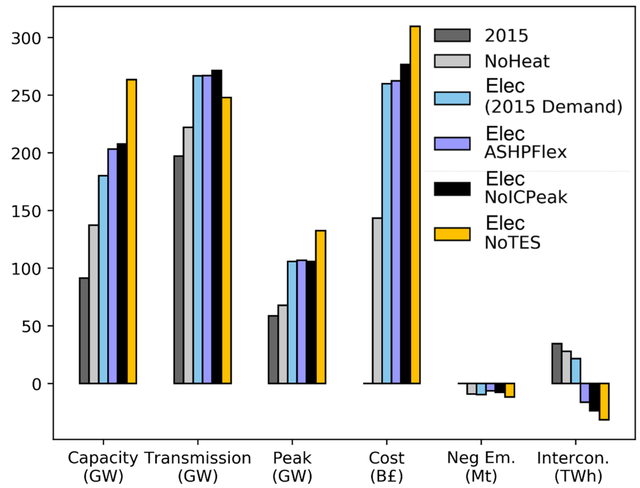


Figure 4. Overview of system-wide impact of domestic heat electrification under different scenarios. NoHeat: Scenario of only power sector decarbonisation. Elec: Base scenario of power and heat decarbonisation through heat electrification. In this scenario, ASHPs are assumed to have full flexibility and TES can be deployed. ASHPflex: Same as the Elec scenario, but ASHPs can ramp up/down only up to 70% of nameplate capacity each hour. NoICPeak: Same as Elec scenario but no interconnection is allowed on the peak heat demand day. NoTes: Same as Elec scenario, but no deployment of TES is considered.

of TES in electrifying heat, we study the scenario "NoTES" in which case electrification is only achieved through ASHPs. The "NoICPeak" scenario is similar to our base "Elec" scenario but no power imports or exports are allowed through interconnection on the peak heat day. Finally, to assess the incremental effect of heat electrification, we consider a "NoHeat" scenario where the power sector is fully decarbonised by mid-century but not heat.

As end-use heating technologies we consider: (i) ASHPs, (ii) TES and (iii) gas boilers. Although GSHPs and resistive heaters (RH) are also suitable electrification technologies, the latter were not considered due to their inferior performance compared to ASHPs and the former would require information on the regional building stock and space availability, two factors that are out of the scope of the present study. As TES, we consider generic insulated hot water tanks. Finally, for the off-gas grid properties we consider full electrification of all related heat requirements (i.e., ASHP adoption).

System-wide implications of 100% heat electrification

Overall, comparing the "NoHeat" and "Elec" scenarios, for 2015 heat demand, electrification could be achieved through a 33% increase in generation capacity and 18% increase in transmission capacity between regions to meet a system-wide peak demand that increases by 56% (106GW vs 68GW). An additional £100bn in capital investments would be needed to deliver sufficient power generation capacity to ensure system security and adequacy under the increasingly seasonal load that a future power sector would have to face under a 100% electrification scenario. A summary of the system-wide changes for the different scenarios is found in Fig. 4.

These differences intensify when system planning is performed under more extreme years, such as 2018, when heat demand data captures the weather variability of a European cold wave (the so-called 'Beast from the East' plus Storm Emma). Specifically during 1 March 2018, gas demand in the distribution networks reached nearly 360 mcm which was higher than the 1-in-20 peak demand forecast that was published as part of GB's gas transmission operator's Ten Year Statement[31]. In "Elec2018", the total system peak reaches 113 GW (a 67% increase compared to the "NoHeat" scenario) while a further 10% increase in TSC is observed compared to the "Elec2015" scenario, with 28% generation capacity (mostly in the form of Nuclear, BECCS and offshore wind) and 4% additional investments in transmission capacity.

Considering only power sector decarbonisation, as shown by Table 1, the optimised generation capacity is dominated by renewable generation technologies (52%), with onshore wind accounting for 25% of the capacity mix. The deployment of combined cycle gas turbines with post combustion carbon capture and storage (CCGT-CCS) begins in 2033 and steadily grows to reach 21.5GW capacity by mid-century, while 1.5GW of of bioenergy with carbon capture and storage (BECCS) is deployed to provide negative emissions. Relative to our central scenario ("Elec") using 2015 (2018) heat demand, the most notable changes are the increase in Nuclear capacity by a factor of 2.4 (2.8) and in offshore wind capacity by a factor of 3.3 (3.6). For the "Elec2018" scenario, aside from those changes, the value of CCS is further highlighted as a source of flexibility in extreme years - BECCS capacity doubles to 3GW and CCGT-CCS capacity increases by 1GW. Electrification of heat also impacts the timing and spatial deployment of CCS technologies, with investments in

CCGT-CCS technologies taking place a half-decade earlier for the "Elec" scenario compared to the "NoHeat" scenario. As an illustration of differences on a regional level, 1GW of CCGT-CCS is deployed in the NT region in the "NoHeat" scenario, but when heat electrification is taken into account, final capacity in the region is increased by a factor of 4.5. As seen in Fig. 2(b), this can be attributed to the high heat demand peak in NT.

Overall, as Table 1 indicates, a potential 100% electrification of heat would require an almost 2-fold increase of firm generation capacity (Nuclear, Biomass) in the best case ("Elec2015") while in the worst case ("NoTES") a direct electrification with limited flexibility would require a 3-fold increase. From a renewable generation perspective, heat electrification appears to favour investments in wind rather than solar generation due to issues related to synchronicity on the availability of solar vs heat demand patterns. Finally, another interesting aspect is the potential competition between grid-level storage technologies and TES as either can be used for absorbing RES intermittent generation (cf. "Elec", "NoTES" scenarios).

Regional drivers and adoption rates

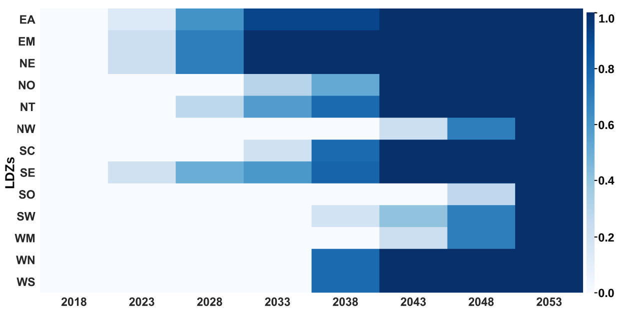
In this section, we delve into the spatio-temporal evolution of the GB energy system towards 100% heat electrification. As indicated by Fig. 5(a), in our base scenarios where no adoption rates constraints are imposed, there is great disparity in regional electrification rates. Eastern regions (EA, EM, NE and SE) appear to be early and steady adopters throughout the planning horizon whereas other regions such as NW, WM, SO and Wales only become electrified towards the end of the time horizon based on very high adoption rates. When adoption rate considerations are not taken into account, the eastern regions can exhibit electrification rates ranging from 35% to 56% over a 5-year period, which far exceeds any previous electrification rollout, and so might be viewed unrealistic[32]. To this end, and to shed light on key barriers/enablers for early electrification, we explore different scenarios whilst imposing a requirement that regional adoption rates lie within either: (i) 10%-20% or (ii) 15%-30% over a 5-year period. The results of these runs are presented in Figs. 5(b)-5(c). It is interesting to note that the 10-15% adoption rate case reflects the UK's government's ambition to install 600,000 heat pumps annually from 2028 following its recent "Ten point plan for a green industrial revolution"[33].

To guide our analysis, let us focus on SE and SO, which, though neighbouring regions, follow completely different paths to electrification, as seen in Figs. 5(a)-5(c). These two regions are also interesting because, apart from similar weather conditions (which affect ASHP performance), they also exhibit very similar heat demand patterns as shown in Fig. 3. In the base scenarios, the SO region is a net importing region while SE is a net exporter, mostly to the NT region. When adoption rates are constrained, however, power flows are reversed in both regions. For example, when adoption rates are constrained, SE exports on a net basis to SO but is a net importer from NT, which, in turn, reduces the electrification rate in NT. The general trend indicates an increase in firm generation, mostly through more nuclear and some biomass power plants, with subsequent reduction in the regional share of intermittent renewable energy sources. This trend is particularly apparent during the early periods (2023-2038) before the uptake of CCS technologies (BECCS or CCGT-CCS). For instance, comparing generation capacities in SO during 2028 we identify an increase of 0.7GW in biomass capacity and 1.5GW in grid-level storage capacity in both constrained scenarios versus the unconstrained case. The same trend is identified in the SW region where solar capacity declines by 1GW in the case of 10-20% and by 2GW when 15-30% rates are imposed. In both scenarios 2.4GW of nuclear capacity is deployed in SW in 2028 whereas in the unconstrained case no nuclear capacity is installed. By contrast, 3GW of additional nuclear is expected in EA by 2033 in the unconstrained case but when adoption rates are constrained, additional installed capacity reduces to 1.8GW and 1.2GW for the 10-20% and 15-30% adoption rate scenarios respectively. Nonetheless, overall RES capacity does not decline in order to meet the decarbonisation targets but instead is complemented in regions with investment in peaker plants (CCGTs, OCGTs) and grid storage. That is the case for NT, where full heat decarbonisation is delayed by a decade in the constrained adoption rate scenario, but both solar power plant capacity (+3GW) and CCGT (+3GW) increase in 2033. Similar insights are derived by examining the NO and NW regions, where firm generation and grid-level storage both increase when adoption rates are constrained (see supplementary note 5).

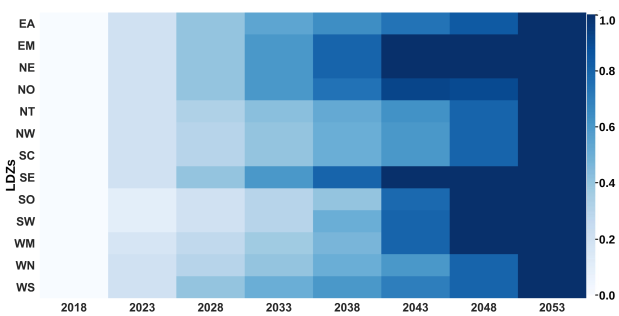
The cost of reduced flexibility in heat electrification

Sources of flexibility become crucial in alleviating the challenges of direct electrification of heat. In particular, we identify and study three different factors: (i) the use of thermal energy storage (NoTES), (ii) the operational flexibility of ASHPs (ASHPflex) and (iii) the ability to import/export power during peak heat demand days (NoICPeak). A decarbonised system without TES deployment requires a total capacity of almost twice that needed for decarbonising the power sector alone due to the doubling in the overall peak the system has to meet (132 GW vs 68 GW). The reduced flexibility due to the absence of TES results in a 35% increase in total system cost (TSC) and leads to asset under-utilisation, with the average utilisation factor for CCGT-CCS dropping to 36% in the "NoTES" from 69% ("Elec" scenario) for the case of 2018 heat demand.

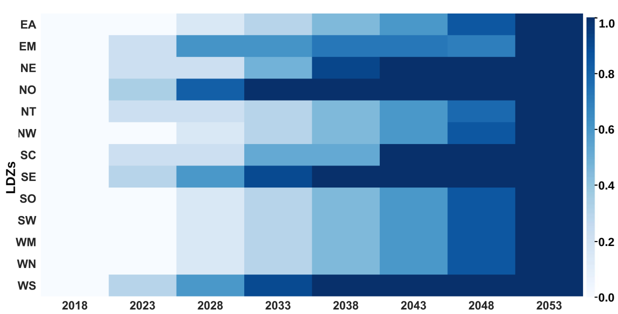
In the "ASHPflex" and "NoICPeak" scenarios, generation capacity increases by 50% compared to the "NoHeat" case, while the absence of interconnection during the peak heat day results in a 22% increase in cross-region transmission capacity utilised to counterbalance the lack of interconnection in coastal regions. In both cases, an additional £10bn and £18bn



(a) Spatio-temporal progress of domestic heat electrification with no constraints on the deployment of ASHPs.



(b) Spatio-temporal progress of domestic heat electrification with adoption rates ranging between 10-20%.



(c) Spatio-temporal progress of domestic heat electrification with adoption rates ranging between 15-30%.

Figure 5. Domestic heat electrification rates under the "Elec" scenario of on-gas grid properties across different regions in GB, following different scenarios for ASHP adoption rate. Progressively darker shades indicate a higher percentage of electrified properties in each region at each time step.

increase is inflected in the TSC while GB ends up being a net power exporter by mid-century mostly to Norway and Denmark due to the increased generation by onshore and offshore wind power plants. Nonetheless, the interconnection flows rely upon future price projections based on European Network of Transmission System Operators for Electricity's Ten-Year Network Development Plan according to their "Global Climate Ambition" (GCA) (or deep-decarbonisation) scenario[34].

Conclusions

Full electrification of heat will be challenging for many reasons apart from the demands placed on the electricity system. Reaching high sustained adoption rates will require significant government incentives and will involve engaging not just early adopters but will require a shift away from gas in large commercial establishments and amongst late adopters and laggard domestic consumers, who will be sceptical of the technology and/or daunted by the capital expense. The economics of maintaining the existing gas infrastructure in the transition to full electrification with ever-smaller volumes of gas is also challenging. Moreover, there are numerous important questions that remain such as how to maintain gas in the system for hybrid heat pumps and what the basis should be for sizing a fully-electrified system. From a carbon reduction perspective in the short run such complications may not be insurmountable, but in the long run they can lead to deadlocks due to the mixed market signals being sent, e.g. on the future of natural gas, as well as undermining a smooth policy-driven transition to low-carbon heat. Future research should build on spatially explicit and multi-period modelling to explore integrated capacity expansion planning and operational optimisation of the integrated heat and power system, particularly in the context of the role negative emissions might play in decarbonising the heat sector. While there is no silver bullet to decarbonise heat, we have shown in the present study that electrification of heat in conjunction with smart operation of thermal energy storage constitute a viable candidate without needing unreasonably rapid growth in overall system capacity. Although we have demonstrated that electrification is not as daunting as some have claimed, this is only one part of the heat puzzle and the potential role for hydrogen and biomass need to be investigated in similar detail so as to decipher the underlying synergies and this constitutes ongoing research within our group.

Methods

OPtimising Heat ELectrificatiOn regIonaL strAtegies (OPHELIA) model description

OPHELIA simultaneously minimises the power and heat system costs to satisfy the related loads on an hourly basis subject to technical constraints for evaluating the impact of domestic heat electrification on the power and gas systems in Great Britain (GB). It is a spatially explicit multi-period model where GB is discretised into the 13 local distribution zones (LDZs) of the gas network. Given existing and projected power generation capacities in GB, the model optimizes: (i) new power generation and storage capacity locations; (ii) hourly dispatch decisions; (iii) power transmission flows within the considered GB regions; (iv) interconnection flows with third countries;(v) hourly upward and downward reserve requirements and commitment; (vi) heat generation and storage capacity investments and location; (vii) hourly heat generation and storage operational decisions. Other key outputs of OPHELIA include: (a) regional share of heat-end use technologies (gas boilers, air-source heat pumps and heat storage); (b) separate monitoring of electricity and heat generation emissions; (c) regional hourly gas flows; and (d) regional hourly marginal cost of electricity. To account for system's flexibility requirements the the ramp-rate constrained unit commitment conditions are employed: (i) minimum up time and down time requirements for thermal generation plants; (ii) thermal generation ramping constraints during the different modes of operations (start-up, committed, shut-down). For the representation of renewable energy sources, we collect hourly availability data as provided by the renewables.ninja platform[35]. The hourly availability reflects the percentage of the installed nameplate capacity that would be generated at a given hour. To capture the variability in RES availability within each region, for solar and onshore wind we sample different spatial intraregional availability and the average of those is used as the final regional availability factor, whilst for the case of offshore wind generation points were considered up to 50km from the shore. While more detailed representations of RES have been presented in recent studies[36], we opt for this approach as our main focus here is the impact of heat electrification and not the integration of renewables in the grid, although our model can readily consider such detailed cases as input data. In terms of reserve requirements, we model upward short-term operating reserve as a function of the forecasting errors in wind generation, electricity demand and the capacity of the largest generator to simulate N-1 security criteria considerations[36]. Downward reserve requirements are modelled as a percentage of the upward requirements[37]. Distribution losses are modelled as a percentage of the resulting regional demand, while transmission and interconnection losses are endogenously calculated as proportional to the transmitted power and distance between the different regions[38]. Transmission corridors between different regions is modelled following the transshipment models conventions which does not account for Kirchhoff's voltage law[39]. One strong point of OPHELIA is the high-fidelity regional demand considerations across the different LDZs. To date, in past studies of heat decarbonization, models have employed the same hourly heat demand patterns and a limited number of representative days when regional decarbonisation strategies are examined[40]. Moreover, we differentiate between emissions reduction requirements for the heat and the power sectors to enable the examination of sector- specific budgets and their impact on heat decarbonisation policies. The overall model is formulated as a mixed integer linear program and is implemented in GAMS and AIMMS. A more detailed description of the model's data, equations and key assumptions can be found in Supplementary notes 3-4.

Deriving regional domestic heat demand data

Understanding and preserving the spatial and temporal variations on heat demand is vital for deriving realistic decarbonisation insights and strategies. In principle, heat demand profiles are determined by a range of aspects such as behavioural, building stock and weather conditions. A primary concern regarding the decarbonisation of heat through electrification is the resulting load variability that the grid operator would face. To this end, a limited amount of works have been presented in the literature that employ half-hourly/hourly heat demand profiles[15,21]. The shortcoming of these previous studies is that the derived heat demand profiles come from either a 2007 Carbon Trust Micro-CHP Accelerator project with 71 domestic buildings[21] or from the Energy Demand Research Project (EDRP) that was carried out between 2007-2010 with around 6000 participants[41]. While these data sets and the resulting heat demand profiles constitute a significant step in the desired direction, using them to evaluate the impact of decarbonisation in a spatial manner for the UK runs into difficulties because of the limited representation of the regional characteristics of heat as well as the end regional heat load is subject to after diversity peak demand considerations which are key in designing the future grid. To this end, in the present work we employ regional hourly gas demand data as a proxy for heat demand that were collected from the GB Gas Distribution Network Operators (DNOs) spanning from 2015-2018. In these time series, gas demand comprises daily metered (DM) demand (associated with large industrial premises) and non-daily metered (NDM) demand (associated with domestic, commercial and medium sized industrial premises). The reader interested in the specific definitions of this components in referred to National Grid's methodology[42] for a comprehensive review. To then derive the related domestic demand from the time series the following methodology was devised by using gas standard load procedures by German Federation of the Gas and Water Industry (BGW)[43] as well as the German Association of Local Utilities (VKU)[44]. Using their methodology, characteristic hourly and temperature-dependent gas demand profiles are presented for a range of different domestic, industrial and commercial units. In conjunction with these profiles, regional hourly temperature data[35], sub-national gas consumption data from BEIS (that also non-gas properties using solid using fuels for heat) in the different regions across GB[45] were employed. Domestic demand is derived then as follows. First, using the gas standard load profiles the daily metered demand as reported in[43,44] is scaled down on an hourly basis for all the LDZs. The resulting hourly DM demand was subtracted from the DNO time series leaving gas demand related to NDM customers. Then, using sub-national gas consumption data statistics about regional domestic and non-domestic percentages together with the master temperature-dependent profiles for non-domestic customers we scale down on an hourly basis the NDM consumption data available from[46]. By subtracting the hourly non-domestic NDM component together with the related DM component from the original time series the domestic hourly gas consumption demand in the different LDZs is retrieved. Finally, for the cases where negative values where encountered in the final time series we interpolated between the neighbouring data points to preserve continuity. It should be noted that for the Welsh regions (WN, WS) we employed existing regional domestic half-hourly data for heat demand[47] because of complications in accounting for different gas flows in those regions. Finally, to derive non-electric heat demand for the proportion of off-gas grid properties within each region, we use the data about household heating technologies as presented by[19] and assume an average of 80% efficiency for both biomass and oil burners. Further assumptions that are employed for the derivation of regional heat demand profiles include: (i) the gas-heated domestic demand is taken as representative for the whole building stock within each region and (ii) the gas boiler demand reflects directly the underlying heat demand. Further to these assumptions, with the regards to the applicability and validity of the German gas suppliers methodology we can expect to have some deviations from the ground-truth heat demand but as indicated by Ruhnau et al.[48] using these standard profiles for the UK results in high consistency between modelled and historic behaviour of the heat sector.

As indicated by Fig.2(a), compared to existing works on estimating the GB heat demand, we are on a national scale, we are in good agreement with the results of Watson et al.[41] with 4% higher estimated peak demand (177GWh) with a larger deviation is observed at 20% for the maximum ramp up in heat demand (72GWh vs 60GWh). Compared to Sansom et al.[24] we derive a significantly lower peak demand (36%) and almost 45% lower maximum ramp up. With regards to the regional aspects of gas-related heat demand, as shown in Figs.2(b)-2(c) the regions EM and NT have the largest contributions to the national peak demand (around 25GW each) while for the case of Wales the profiles derived from Knight et. al[47] indicate a rather interesting behaviour with the scale of peak demand and ramp up, ramp down requirements being quite close especially for WN as indicated by Figs. 2(b)- 2(c). Apart from WN, the smallest heat peak demand is found to be in the NO region (11.3GW) and SW region (12.4GW) and such region-specific insights are useful when deciding regional rollout of electrifying heat as it may be preferable to electrify first those regions where their peak heat demand component is not prohibitively large.

Representative days selection

we use data clustering techniques. In particular, we employ K-Medoids clustering to agglomerate days of the year that exhibit similar patterns with respect to regional demand of electricity and gas, RES availability, interconnection prices and average temperature across the 13 LDZs. To preserve peak electricity and gas demand days, the original time series are pre-processed and these two days are excluded from the clustering and are added at the final stage. Once clustering is completed, an average day is computed and then the representative day is chosen such that it has the minimum geometric distance from that day. While clustering techniques have been widely applied to energy systems models[49,50] the resulting representative days are generally not placed in chronological order. However, for the case of heat decarbonisation preserving the chronological order is important due to the inherent seasonality of demand. To this end, once representative days are selected for each cluster, they are organised in chronological order.

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Author contributions statement

Conceptualization: DMR, KC and VC; Data curation: DMR and VC; Formal Analysis: VC and MF; Funding acquisition: DMR; Investigation VC and MF; Methodology VC, DMR, KC and MF; Project administration: DMR; Visualization: VC and MF; Writing - original draft: VC; Writing - review & editing: VC, DMR, KC and MF.

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Supplementary material: The case of 100% electrification of domestic heat in Great Britain

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Supplementary Note 1: Overview of heat decarbonisation pathways & literature review

Heat decarbonisation would require a major transition of the energy landscape in the UK and in order to secure sustainable, low-carbon and economic heat a number of pathways have been identified. A conceptual visualisation of the individual components that comprise the different pathways is given in Fig. 1.

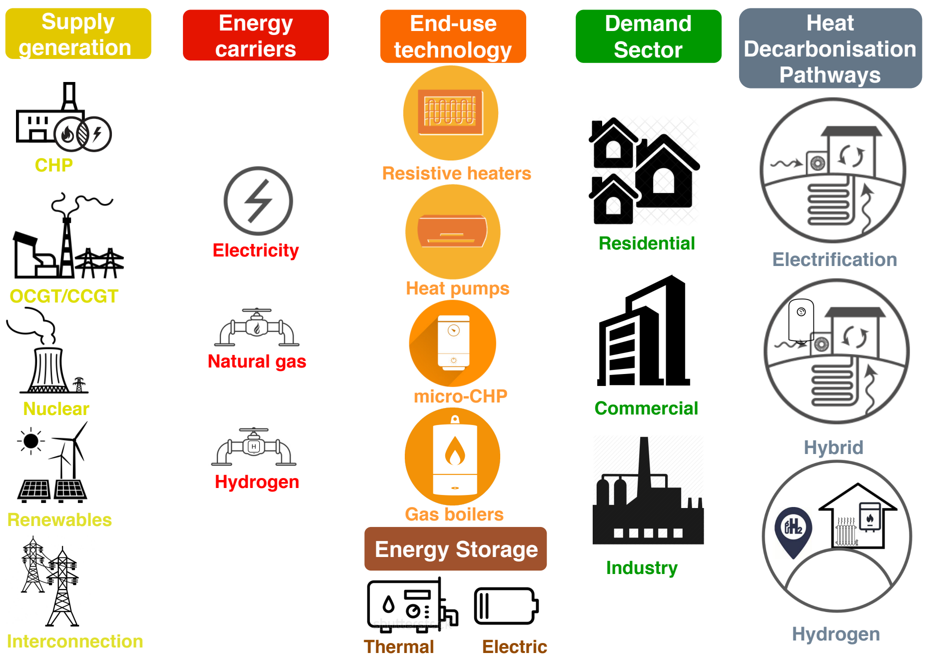


Figure 1: Whole system visualisation of decarbonisation pathways for the GB heat sector

Electrification of heat

Options for heat electrification can be categorised into two broad groups as indicated by Fig.2. In the centralised setting, heat is generated by electricity and is subsequently distributed, through district heat networks (DHN) to the end-users. Research works indicate that DHN have inherent energy storage through their pipelines [1], while additional thermal energy storage can be considered as part of their design. In the decentralised setting, electricity is converted to heat on-site and the main options involve: heat pumps (HPs), either air-sourced (ASHPs) or ground-sourced (GSHPs), resistive heating (RH) and direct heating (radiators).

The key benefits of electrifying heat is the flexibility opportunity it provides to the power system for better integration of renewable energy sources (RES) as well as the technology readiness levels of end-use options[2]. A number of studies have indicated that electricity-fuelled district heat networks coupled with thermal energy storage and demand side response measures can result in reduction of RES curtailment [3, 4]. For the decentralised scenario where individual heat pumps are deployed, the effect of heat pumps on the flexible integration within the power sector was found positive under assumptions on energy efficiency measures and thermal storage [5, 6].

Munuera et al. [7] investigated the role of energy efficiency in the electrification of heat. Utilising data from the Energy Saving Trust's heat pump field trial the effect of the building stock's energy efficiency on the correct sizing of the required HP as well as the contribution to the peak load was examined. Results from this field trial concluded that the COP for ASHPs was between 1.6-2.2 while for GSHPs 1.8-3.0 [8]. A technical feasibility study on electrifying heat in rural off-grid areas was reported in [9]. The study concludes that bigger energy savings can be realised using HPs rather than RH. Without energy efficiency improvements, 84% of homes can efficiently adopt electrified heat while the share rises to 93% with loft & wall insulation. However, the authors identified that the technical feasibility can be endangered under their 1-in-20 winter peak scenario for which only 41% to 63% (depending on the type of HP) of the homes could electrified.

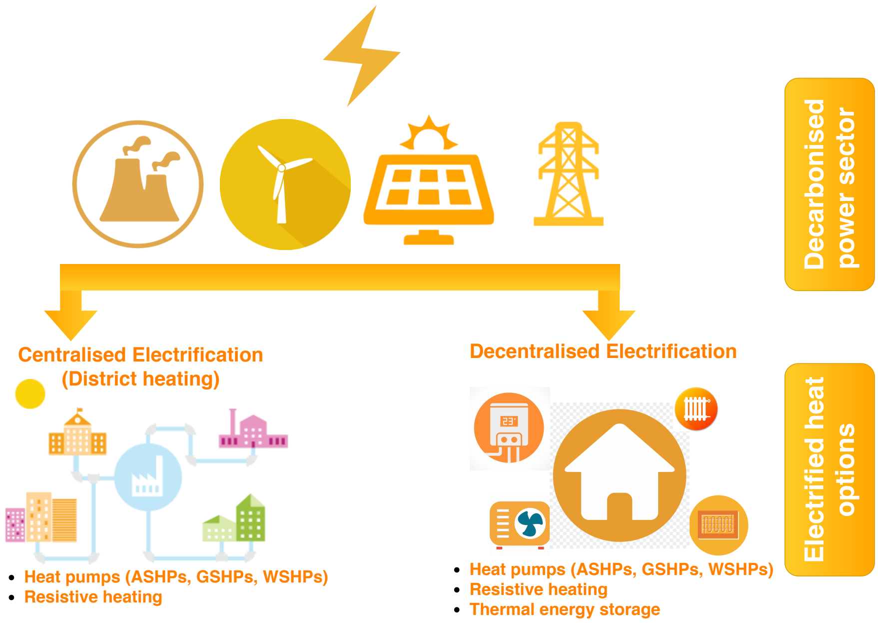


Figure 2: Categorisation of heat electrification options

Peak heat demand in the UK can reach up to four times the peak demand from the current electricity system [10]. Owing to the existing gas storage system in the UK, balancing between the demand and supply sides can be achieved without excessive capacity investments. However, for the electricity system this is not the case since instantaneous balancing is required to avoid power outages.

Another implication that arises from high deployment of renewable variable energy sources is the energy system's dependence on weather conditions. This issue is further exacerbated in cases such as winter cold days with low solar and wind generation when the need for domestic heat is likely to peak and endanger the system's balancing mechanisms [11]. Failing to account for such cases in energy planning scenarios can lead to human exposure for lengthy periods in cold indoor environments which in turn can result in health risks [12]. Nonetheless, the electrification of heat offers the advantage of improved energy usage, when heat pumps are considered, since on average their efficiency is 2-3 times higher compared to the currently used gas boilers. In a recent study on the electrification of the heating sector in the EU, it was identified that based on incumbent generation capacity twelve member states can readily achieve full electrification [13].

Electrifying heat raises also concerns about the future of the gas infrastructure in the UK as well as the amount of investments needed. In terms of economic cost, heat electrification is characterised by high-capital and low-operational costs due to the increased efficiency of heat pumps. The main drivers from the high-capital expenditure are: (i) investments in generation capacity expansion, (ii) investments in transmission's network reinforcement and (iii) high up-front costs from the consumers for HPs [14].

Hydrogen conversion

Among the different decarbonisation pathways in the literature, the potential of a "Hydrogen Economy" has constituted a notable alternative towards clean energy for the heat and transportation sectors in the UK [15]. and a conceptual overview of this pathway is given by Fig.3. Unlike natural gas, hydrogen does not result in GHG emissions upon combustion. Nonetheless production of hydrogen in scale is reliant on processes which result in emissions and thus its low-carbon potential is bounded with extensive investments on carbon capture and storage (CCS) [16].

Hydrogen can be produced through a variety of processes, involving renewable and non-renewable energy sources, and as such can be adopted through the different potential phases for energy decarbonisation. Nonetheless, its potential as a successor to the incumbent gas system has been met with scepticism since there exist many social, economical and safety barriers that need to be addressed before this option is realised. The main production routes for hydrogen production include:

- Coal or biomass gasification
- Steam methane reforming
- Water electrolysis

In order to avoid emissions during the production process, the aforementioned technologies are considered in conjunction with CCS while for water electrolysis electricity from renewables can be utilised. Hydrogen can also be supplied as a by-product from chlor alkali and refineries processes. In the latest report on hydrogen by the Committee on Climate Change, coal gasification is not considered a viable option due to its high cost and limited emissions savings to the incumbent natural gas system. The only production route of hydrogen that does not require investment in CCS is water electrolysis using curtailed RES. The viability of such option was briefly examined and as indicated in [17] if wind curtailment reaches the level of 75TWh by 2050, then hydrogen produced by water electrolysis would only satisfy 14% of UK's domestic heat demand.

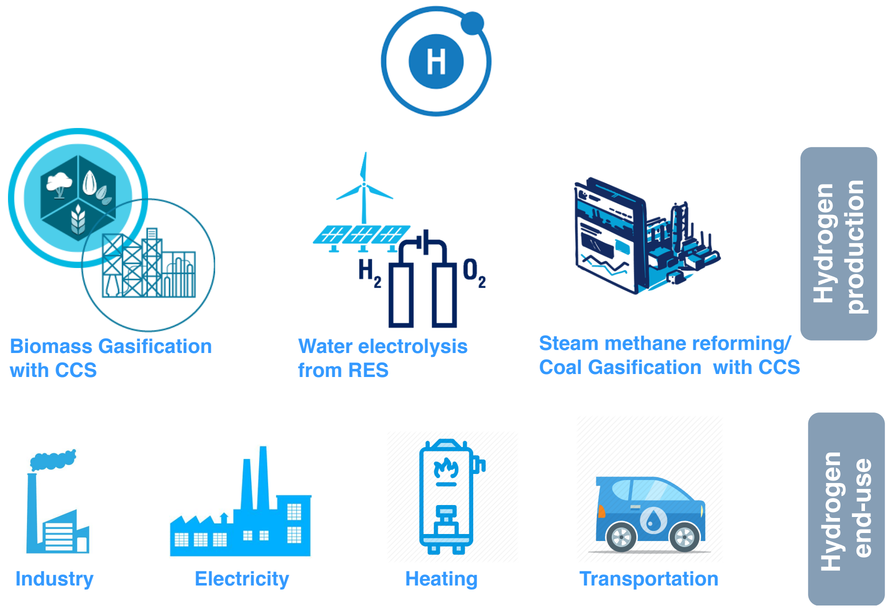


Figure 3: Conceptual representation of hydrogen economy production and end-use pathways

Hydrogen's decarbonisation pathway is characterised by significant uncertainties with regards to technology deployment and resulting end-costs. Shifting from natural gas to hydrogen would require considerable investments in adjusting the existing gas grid to secure safe and efficient transmission on top of replacing existing domestic end-use appliances. Dodds and Demoullin [18], interviewed specialists from industry, government and academia and conducted a simulation study on the cost-optimal conversion of the existing UK gas system to transport hydrogen. The key findings indicated that the current high-pressure transmission gas system would need to be modified to safely transport hydrogen while the low-pressure system does not need any modifications. Another issue was found to be the resulting reduced capacity and linepack storage compared to natural gas due to different energy volumetric densities of the two fuels. The future of the UK gas system was the focus of [19]. The authors using a revised version of the UK MARKAL model to compare the scenarios of injecting biomethane to the gas grid or converting it for hydrogen concluded that the cost-optimal choice is the hydrogen solution.

Cost estimates for infrastructure and appliance conversion have been presented in the H21 Leeds city gate and North of England report [20]. Apart from the costs attributed to generation and transmission infrastructure, inter-seasonal storage costs via salt cavers need to be considered as a way of reducing capacity investments [16]. Recent studies focusing on the energy systems planning [21] and the use of hydrogen as energy carrier for inter seasonal energy storage [22].

Hybrid pathways

The heat electrification and hydrogen conversion pathways suffer from potentially excessive capital investments and high-levels of uncertainty respectively. To this end, a number of pathways have been proposed by hybridising "low-regret" options with components of the aforementioned pathways [23]. As illustrated in Fig.4, the hybrid pathways involve low-carbon district heat networks, hybrid boiler configurations and partial electrification of heat.

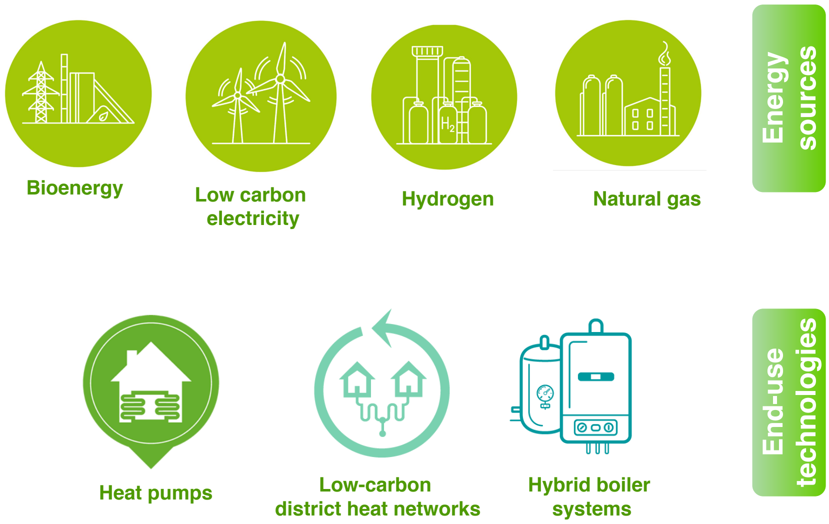


Figure 4: Conceptual representation of hybrid pathways for heat decarbonisation.

The contribution of bioenergy towards decarbonisation of the heat sector is dependent on: (i) availability and type of feedstocks and (ii) the lifecycle emissions of the resulting bioenergy production and transportation. In general, biomethane is considered a low-carbon energy carrier due to the CO_2 captured during the growth of the feedstock [24]. A key advantage of biomethane is that it can be injected safely into the existing gas grid without the need of modifications. Researchers have investigated the potential of emission savings and cost efficiency of biomass in the context of district heat networks [25, 26]. Following the government's Renewable Heat Incentive (RHI) programme the amount of bioenergy for heating purposes has increased. In 2016, UK injected 2TWh of biomethane into the gas grid while currently more than 13,000 biomass boiler operate mostly in off gas grid areas [27].

Another alternative constitutes the deployment of hybrid configurations of electric heat technologies with gas components so as to mitigate the impact of heat demand's seasonality on the future energy infrastructure [28]. Hybrid heat pumps constitute such as solution where the gas component, either hydrogen, biogas or natural gas, is utilised to meet excessive heat demand during peak seasons [29]. The rationale is to preserve the flexibility electrified heat offers to the power sector, reduce the emissions but prevent excessive investments into the capacity generation and transmission networks [23]. A question that arises however is with respect the economic viability of preserving a gas system that will be underutilised and further research is required on that front.

Existing literature on modelling of decarbonisation pathways for the heat sector

Electrification of domestic heat is likely to result in excessive electricity infrastructure expansion given that hot water and space heating account for almost 80% of the energy use of the buildings sector in Europe and 60% in the US. In the literature a variety of strategies have been proposed for the decarbonisation of heat which can be broadly categorised as follows: (i) electrification of heat, (ii) low/zero-carbon gases, e.g. hydrogen or biomethane, (iii) district heating networks that supply heat from low-carbon sources, (iv) efficiency measures and (v) behavioural change related approaches.

A spatially-explicit, multi-period MILP model was developed by Jalil-Vega and Hawkes to investigate the heat supply and network infrastructure trade-offs in the City of Bristol [30]. The authors considered both domestic and commercial demand while a number of different end-user technologies were involved including heat pumps and district heating networks. Gas, electricity and heating network infrastructure costs were also considered. The same authors later on examined the role of hydrogen towards the decarbonisation of heating [31]. They revised their model to account for hydrogen demand however infrastructure decisions were only made on a aggregate network level. In their results, heating demand was primarily satisfied using district level heat pumps with hydrogen boilers being the second technology in demand satisfaction, under a flat heat demand assumption. Quiggin and Buswell presented a model for estimating the impact of heat electrification in the UK from a demand-supply viewpoint [32]. Six published scenarios for the decarbonisation of heat were investigated and underlined the role of demand side management and heating demand reduction measures for securing supply. In [29], the impact of exploiting thermal building inertia and the effect of weather events on heat demand was studied. The authors integrated a "resistance-capacitance" representation in their energy planning model for the case of Ireland and showed that thermal building inertia can reduce operational and capital costs for both the demand and supply side while also contribute to more flexible deployment of RES.

An analysis of the gas and electricity demand profiles in the UK is conducted identifying the variable component for heating. The authors used data available from the National Grid and examined the scenario where 30% of the NMD from gas is transferred to electrification either with resistive heating or heat pumps. The role of domestic energy efficiency, seasonal storage, biomass heating were briefly discussed.

In [33], an overview of the key technological and economic uncertainties related with the decarbonisation of heat in the UK is given. The authors provided a high-level analysis on the affect different uncertainties, such as fuel price or efficiencies, have on the final energy system costs and carbon emissions.

The impact of hybrid heating devices towards decarbonisation of heat in Ireland was studied in [34]. In this work, an investment model was formulated as linear program and the least-cost option was found to be the hybrid ASHPs-gas boilers under different scenarios on future gas prices and building energy efficiency measures.

Heinen et al. (2016) investigated the economic and operational performance of different hybrid heating technologies and concluded that the combination of gas-boilers and electric heat

Table 1: Overview of modelling methods for the examination of heat decarbonisation pathways

Model	Purpose	Approach	Spatial resolution	Temporal resolution	Heat demand	Heat technologies	Unit commitment constraints
FESA [35]	Scenario analysis	Grid balancing with merit-order generation	Single node	Hourly steps over one year	Hourly average constant heat demand	CHPs, HPs, RH	NaN
SHED [32]	Scenario analysis, hybrid bottom-up/top-down	Grid balancing	Single node	Hourly steps over one year	HDDs and Economy 7 hourly demand patterns	HPs, Solar thermal, CHPs	NaN
EnergyPLAN [36]	Exploration	Optimisation, simulation	National, regional	Hourly steps over one year	HDDs and daily cycle profiles	Biomass/ Gas Boilers, H_2 $^{-}$−CHPs, HPs, RH, DHN	NaN
ESME [37]	Exploration	LP least-cost optimisation	12 UK regions	5-year steps until 2050 with 10 time slices	HDDs and hourly consumption data	Biomass/ Gas Boilers, $^{-}$−CHPs, HPs, RH, DHN	NaN
HIT [30]	Investment	MILP least-cost optimisation	City of Bristol, 55 regions	5-year steps until 2050 with 16 time slices	Hourly average constant heat demand	DHNs, HPs, HP-B	NaN
IWES [38]	Scenario analysis, investment	MILP least-cost optimisation	5 UK regions	Hourly steps over one year with 3 additional extreme days	Hourly heat demand data from [39]	HPs, DHN, HP-B	NaN
Heinen et al. [34]	Investment	LP least-cost optimisation	Single node	Hourly steps over one year	Hourly heat demand from smart meter data	HPs, RH, Gas Boilers, RH-B, HP-B, HP-RH	NaN
MARKAL/ TIMES [40]	Exploration	LP least-cost optimisation	National, regional	5-year steps until 2050 with 16 time slices	Daily heat demand profiles	Solar Thermal, HPs, RH, DHN, $^{-}$−CHPs	NaN

pumps provide significant advantages over the other options such as resistive heating and gas boilers. Heat demand density has been reported as a determining indicator for the suitability of region to benefit from distributed heat networks. McKenna and Norman (2010) investigated the potential of energy recovery from industrial heat loads for Great Britain in a spatially-explicit manner [41].

The opportunity of harnessing heat content from industrial activity in order to satisfy domestic space and water heating demand was also highlighted for the US case by the work of Rattner and Garimella [42]. Zhang et al. presented a whole-system study on the decarbonisation of heat in GB to optimally decide on the end-use heat generation system design involving heat-pumps, district heat networks (DHN) and hybrid deployment of heat-pumps with gas boilers (HP-B) [38]. The authors concluded that the HP-B pathway presents economic and operational benefits over the other alternatives, due to the lower capital cost of decommissioning existing domestic gas-boilers and the avoidance of reinforcing the electricity network because of heat peak demand. The deployment of DHN was found to be beneficial to some extent only in urban areas due to high heat density but always in conjunction with HP-B.

Bloess et al. [43] presented a literature review on the topic of heat electrification with emphasis on Europe and concluded that, up to an extent, electrifying heat together with flexible thermal storage technologies can prove to be beneficial for higher integration of renewables into the energy mix.

Qadrdan et al. presented a linear programming model with electricity dispatch consideration to study the impact of heat electrification on the GB gas and electricity system [44]. In their approach GB is represented by a single node and a one-year operation with half-hourly resolution was employed to model the impact of electrifying heat on the low- and high-pressure gas network of the GB. The authors concluded that even though the total gas demand for the low-pressure network is likely to decrease the peak-load demand in future scenarios was found to be increasing posing economic implications as far as maintenance and utilisation of the network were concerned. Love et al. using operational data of heat pumps in 696 domestic sites from the Renewable Heat Premium Payment scheme, investigated the impact on peak demand and ramp rates for the electricity system [45]. Scenarios with national heat pumps uptake up to 20% were examined and the authors concluded that: (i) maximum ramp rate is likely to increase by 0.3 (GW/half hour) compared to its current value, (ii) shift of the peak demand from the evening hours (17:00-18:00) to early morning (06:00-08:00) and (iii) increase of the peak demand by 7.5 GW. Dodds [40] using the UK MARKAL model investigated future scenarios for the residential heat sector under the 80% decarbonisation target by 2050. In his study, gas boilers remained predominant until 2030 providing around 90% of the heat demand while by 2050 around 60% of heat demand was provided by HPs. A more refined disaggregation of the domestic sector in the UK MARKAL model was employed in order to study changes in the fuel consumption and technology selection for heating. The results indicated that the disaggregation (36 house categories), does not change the overall fuel consumption however different policy insights can be generated due to selection of technologies in different house types.

With heat decarbonisation being a key priority area, the government and its independent bodies have published a number of reports, a timeline of which can be envisaged in Fig.5.

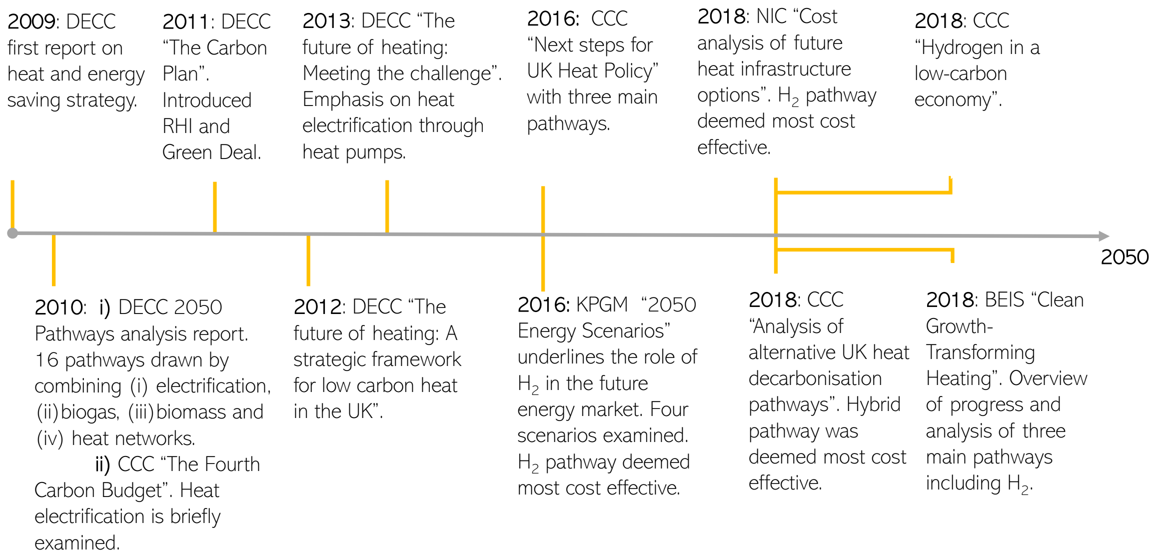


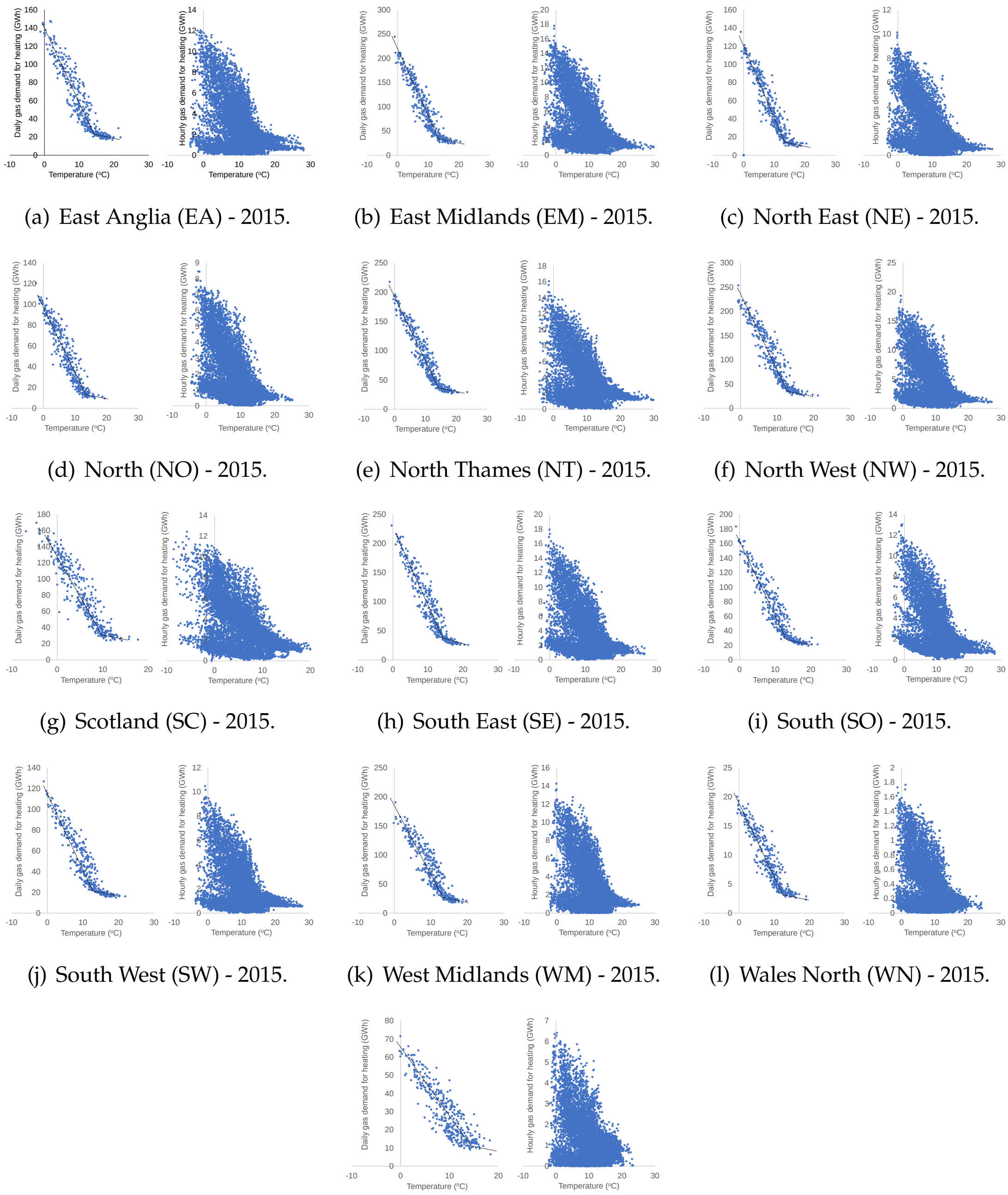
Figure 5: Indicative timeline of key policy and technical reports on heat decarbonisation for the UK.

In a report for the National Infrastructure Commission by Element Energy and E4tech, the cost of future decarbonisation pathways was examined [46]. Among the key findings was that regardless of the pathway, the heating cost is increased compared to the current heat infrastructure system with the annual average cost increase per household to be £100-300 in 2050. Deep electrification was reported to lead to additional peak demand of at least 45GW and the least-cost option was found to be the hydrogen pathway which however suffers from uncertainty in terms of safety and technology costs. A hybrid gas-electricity infrastructure was found to be the second least-cost pathway while heat electrification with heat pumps was the most costly with the cumulative cost until 2050 reaching £270bn. The role of biomass gasification and biogas injection to the gas grid were also found to be low-regret options in some of the scenarios.

The cost of three heat decarbonisation pathways was also investigated by Imperial College London in their report for the Committee on Climate Change [47]. A variety of decarbonisation scenarios was considered with emission targets by 2050 ranging from 30-0 Mt/year. The hybrid gas-electric pathway was found to be the least-cost option under all scenarios while the hydrogen pathway was the most costly and most sensitive to variations in emission targets.

In contrast to the aforementioned works, a report published by the Energy Networks Association found that the decarbonisation pathway of hydrogen is the one resulting in the least capital and operational costs under the 2050 targets [48]. In this work, KPMG employed a top-down approach to evaluate four alternative scenarios including full electrification, two alternative hybrid pathways and the switch to hydrogen. Heat electrification was reported as the most expensive pathway with almost double the cost incurred by the hydrogen pathway. For the heat electrification scenario, the increased costs were attributed to the investments for nuclear and renewables energy sources as well as the reinforcement of the transmission network.

Supplementary note 2: Heat demand analysis



(a) East Anglia (EA) - 2015.

(b) East Midlands (EM) - 2015.

(c) North East (NE) - 2015.

(d) North (NO) - 2015.

(e) North Thames (NT) - 2015.

(f) North West (NW) - 2015.

(g) Scotland (SC) - 2015.

(h) South East (SE) - 2015.

(i) South (SO) - 2015.

(j) South West (SW) - 2015.

(k) West Midlands (WM) - 2015.

(l) Wales North (WN) - 2015.

(m) Wales South (WS) - 2015.

Figure 6: Temperature dependence on daily (right graph) and hourly (left graph) domestic heat-related gas demand. Despite the temperature being one of the key factors that determine heat demand, the relationship on finer timescales (hourly) seems to be highly nonlinear. On the other hand, when the same data set is aggregated on a daily level the dependence between heat demand and temperature can be explained clearly via segmented linear regression.

Fig. 6 indicates the nonlinear nature of the correlation between heat-related gas demand and ambient temperature. While on a hourly level, the relationship between the two can be accurately modelled following a piecewise linear regression, when examining the same data on a finer half-hourly scale, a nonlinear trend is observed. In Fig. 7, a heat map that indicates the timings of regional peak demand during the so-called "Beast from the East" in GB during the period 28th of February - 1st of March 2018 is shown. While the GB-wide peak gas demand was on the 1st of March at 6pm from a regional perspective the peak gas consumption varied with regions like NT and SC having their peak demand on the 28th of February between 6-7pm.

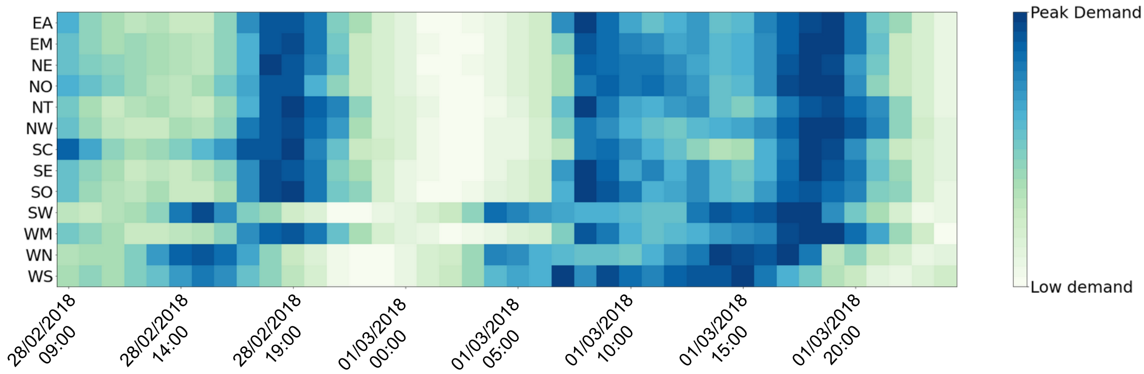


Figure 7: Heat map of regional heat demand during the period 28th of February - 1st of March 2018.

Supplementary note 3: OPHELIA model overview

OPHELIA is formulated as a multiperiod spatially explicit mixed integer linear program which seeks to optimise simultaneously strategic and operational decisions by explicitly considering the electricity and heat sectors in Great Britain. The key assumptions of the model can be summarised as follows:

- Deterministic operational, cost and demand data;
- Centralised least-cost decision making;
- Electricity and gas demand are inelastic. Prices for interconnection are provided exogenously and future price projections are based on the European Network of Transmission System Operators' Electricity ten-year network development plan [49];
- Gas demand data are used as a proxy for the proportion of gas consumption that accounts for domestic heat demand [50];
- The model considers demand on a regional level for heat and electricity;
- Unmet electricity demand is penalised with a cost equal to the Value of Lost Load (VoLL) which is 6,000£/MWh [51];
- Unmet short term operating reserve requirements are penalised at 75£/MWh and 25 £/MWh for the cases of upward and downward reserve respectively while we assume an average cost of renewable generation curtailment of 47£/MWh [51];
- Regional distribution networks are not modelled and their respective losses are accounted by a factor proportional to the regional electricity demand [52];
- Transmission distances are calculated as the distance between the centroids of each region;
- Power plants' efficiencies are considered deterministic and heat rate curves for part-load are not considered;

- The regional allocation of Solar & Onshore Wind power plants is not constrained by land-availability restrictions;
- The allocation of nuclear & hydro power plants as well as new capacity of pumped hydro storage is restricted to regions where existing capacity is present;
- For generation capacity expansion we consider future projections of build rates over five-year planning steps based on [53].

Table 2: Modelling characteristics of the proposed approach.

Model Details	**Description**	**Comments**
Modelled area	Great Britain	
Spatial resolution	13 regions	GB is spatially disaggregated following the gas network LDZs.
Temporal resolution	Dual: 5-year strategic time steps with N_D representative days with hourly steps	Time-ordered statistical clustering of 24 hour intervals into representative days
Electricity demand	Non-heat and heat-driven demand	The heat-driven demand is optimised by the model
Heat demand	Hourly demand profiles by region	It is assumed that heat demand is derived by the corresponding gas consumption.

Mathematical formulation

Objective function

OPHELIA's objective function is the minimisation of the total system's cost (TSC) comprising of: (i) total operating costs and (ii) total capital costs accounting for generation and transmission capacity expansion for the power sector and generation and storage capacity costs for the heat sector. Eq.(1) provides the summary of the terms comprising the TSC discounted by DFC_t.

$$min\,TSC = \sum_{t} DFC_t(TotCAPEX_t + TotOPEX_t) \tag{1}$$

$$\begin{aligned} TotCAPEX_t = &\sum_{g,j \in J_{th}} C_j^{fix} Cap_j^{Unit} CUnits_{g,j,t} + \sum_{g,j \in J_{rew} \cap J_{es}} C_j^{fix} Cap_{g,j,t}^{New} \\ &+ \sum_{g,j \in JR_h \cap J_{h_s}} C_j^{fix} hcu_j CUnits_{g,j,r,t}^{heat} + \sum_{g,g' \in NG_{g,g'}} C_{tr}^{fix} LDD_{g,g'} TRI_{g,g',t}/2 \quad \forall t \end{aligned} \tag{2}$$

Eq. (2) summarises the total capital expenditure that accounts for investments for: (i) new power generation capacity, (ii) new grid-level storage capacity, (iii) new heat end-use technologies and

(iv) new transmission grid capacity between regions.

$$
\begin{aligned}
TotOPEX_t = \sum_{c,h} WD_c \,(\sum_{g,j \in J_{th} \cap J_{rew}} C_j^{var} P_{g,j,c,h,t} + \sum_{j,f \in Jf_{j,f}} C_{f,t}^{fuel} V_{g,j,f,c,h,t}^{elec} \\
+ \sum_{g,j \in J_{es}} C_j^{var} DC_{g,j,c,h,t} + \sum_{g,j \in J_{th}} (C_j^{start} Cap_j^{Unit} v_{g,j,c,h,t} + C_j^{shut} Cap_j^{Unit} w_{g,j,c,h,t}) \\
+ \sum_{g,j \in J_{th}} C_j^{OM} Cap_j^{Unit} NUnits_{g,j,t} + \sum_{g,j \in J_{rew} \cap J_{es}} C_j^{OM} Cap_{g,j,t} \\
+ \sum_{i,g \in IG,c,h,t} C_{i,g,c,h,t}^{INCX} PIM_{i,g,c,h,t} + C_t^{CO_2} (CO_{2t}^{elec} + CO_{2t}^{heat} - CO_2^{elec_{neg}}) \\
+ C^{VoLL} \sum_g LShed_{g,c,h,t} + C^{CRTL} \sum_g LCurtail_{g,c,h,t} \\
+ C^{STORdn} l_{c,h,t}^{OPRES_{down}} + C^{STORup} l_{c,h,t}^{OPRES_{up}} + \\
\sum_{g,j,r \in JR_h \cap J_{h_s}} C_j^{OM} hcu_j NUnits_{g,j,r,t}^{heat} + \sum_{f \in Jf_{j_h,f}} C_{f,t}^{fuel} V_{g,j,f,c,h,t}^{heat}) \quad \forall t \quad (3)
\end{aligned}
$$

Eq. (3) represents the total operating costs of the power and heat system and accounts for: variable costs for generation and storage (C_j^{var}) (which comprise of marginal OPEX and cost of CO_2 transport and storage where applicable); fuel consumption costs (C^{fuel}); fixed O&M costs (C_j^{OM}) for power and heat generation and storage; cost of interconnection ($C_{i,g,c,h,t}^{INCX}$), which depending on the flow of electricity may reflect revenue or expenditure, cost of net CO_2 emissions from both sectors ($C_t^{CO_2}$) and finally penalties for shedding upward (C^{STORup}) or downward (C^{STORdn}) short term operating reserve, electricity demand (C^{VoLL}) or curtailing renewable generation (C^{CRTL}).

Heat supply chain

In this section the key constraints used to model the heat demand and generation components of the model are detailed.

Heat balance

Eq.(4) represents the regional heat balance. In each region (g), on-gas or off-gas grid regional area (r), cluster (c), time-slice (h) and time-step (t) the heat demand and storage should be satisfied by the generation from different end-use technologies and the heat discharged.

$$
HDem_{g,r,c,h,t} = \sum_{j \in JR_h} Q_{g,r,j,c,h,t}^{heat} + Q_{g,r,c,h,t}^{dheat} - Q_{g,r,c,h,t}^{sheat} \quad \forall g,r,c,h,t \quad (4)
$$

The set JR_h is employed to allow for heat-end use technologies depending on whether the referred regional demand is connected to the gas grid. That is, off-gas grid regional demand is allowed to be served by heat electrification technologies only while on-grid demand can be satisfied by gas boilers or ASHPs, subject to emissions constraints.

Heat related power demand calculation

Eq.(5) calculates the resulting electricity demand due to heat electrification.

$$P^{heat}_{g,r,c,h,t} = \sum_{j\in\{ASHPs\}} \frac{Q^{heat}_{g,r,j,c,h,t}}{COP_{g,c,h,t}} \quad \forall g, r, c, h, t \tag{5}$$

The main modelling approaches for simulating the energy consumption and heat generation of ASHPs is through their coefficient of performance (COP). Despite COP being strongly dependent on the temperature of the energy source and the target temperature and thus time-varying, in some research works for the sake of simplicity it has been assumed as constant. Considering the COP of HPs as constant can lead to underestimation of the power required to meet the related heat demand and to this end a more elaborate calculation of the COP is pursued. Heinen et al. [34] proposed to calculate the COP of HPs as a linear function of the ambient temperature while piecewise linear functions have also been proposed in the literature [54, 55]. We should note, that for the case of centralised systems, such as DHN, the COP is assumed to be constant given that large-scale HPs are typically sourced from temperature-stable energy sources. Bach et al. [56] argued that the same assumption can be valid for the case of water-sourced heat pumps since the ambient temperature of the HP does not vary significantly throughout the year. To allow for time-varying and regional COPs we employ eq.(6) which has been reported to preserve good accuracy over the performance range [55] whilst still being a linear function of the ambient temperature ($T^a_{g,c,h,t}$).

$$COP_{g,c,h,t} = 0.0541T^a_{g,c,h,t} + 2.6674 \quad \forall g, c, h, t \tag{6}$$

Heat technologies capacity constraints

Eq.(7) imposes that the heat generated by a specific end-use technology at any time should not exceed the existing installed capacity, while eq. (8) imposes that the number of installed units should be equal to the number of properties in each region (nH_g).

$$Q^{heat}_{g,j,r,c,h} \leq hcu_{j,g} NUnits^{heat}_{g,j,r,t} \quad \forall g, r, j \in JR_h, c, h, t \tag{7}$$

$$\sum_{j\in JR_h} NUnits^{heat}_{g,j,r,t} \leq nH_{g,r} \quad \forall g, j, r, t \tag{8}$$

The overall balance on heating technologies is given by eq. (9).

$$\begin{aligned} NUnits^{heat}_{g,j,r,t} = NUnits^{heat}_{g,j,r,t-1} + CUnits^{heat}_{g,j,r,t} - DUnits^{heat}_{g,j,r,t} \\ - CUnits^{heat}_{g,j,r,t-tp_j} \quad \forall g, r, j \in J_h, t \end{aligned} \tag{9}$$

Thermal energy storage constraints

We consider generic hot water tanks as thermal energy storage (TES). Eq. (10) is the heat storage balance where we consider a 5% self-discharge [57] for every hour. Eqs. (11)-(13) represent the allowable upper bounds on heat storage level ($S^{heat}_{g,j,r,c,h,t}$), charging ($Q^{sheat}_{g,j,r,c,h,t}$) and discharging ($Q^{dheat}_{g,j,r,c,h,t}$) amounts and related data are given in Table 8.

$$S^{heat}_{g,j,r,c,h,t} = S^{heat}_{g,j,r,c,h-1,t}(1-\eta^{heat}_{storage}) - Q^{dheat}_{g,j,r,c,h,t} + Q^{sheat}_{g,j,r,c,h,t} \quad \forall g, j \in J_{hs}, r, c, h, t \tag{10}$$
$$S^{heat}_{g,j,r,c,h,t} \leq hcu_j Tes_j NUnits^{heat}_{g,j,r,t} \quad \forall g, j \in J_{hs}, r, c, h, t \tag{11}$$
$$Q^{dheat}_{g,j,r,c,h,t} \leq hcu_j NUnits^{heat}_{g,j,r,t} \quad \forall g, j \in J_{hs}, r, c, h, t \tag{12}$$
$$Q^{sheat}_{g,j,r,c,h,t} \leq hcu_j NUnits^{heat}_{g,j,r,t} \quad \forall g, j \in J_{hs}, r, c, h, t \tag{13}$$
$$NUnits^{heat}_{g,j,r,t} \leq \sum_{j \in J_{h_e}} NUnits^{heat}_{g,j,r,t} \quad \forall g, j \in J_{h_s}, t \tag{14}$$
$$S^{heat}_{g,j,r,c,h,t} = 0 \quad \forall g, j \in J_{h_s}, c, h = H, t \tag{15}$$

We only allow for deployment of TES in properties that have installed ASHPs and this is achieved by eq. (14) while in order to avoid energy cross-overs between representative days, eq. (15) imposes that the TES level empties at the end of each day.

Heating fuel consumption

The demand of heating fuel, i.e. natural gas, in the model is considered as endogenous. More specifically, demand of natural gas is related to the consumption by gas condensing boilers as shown by eq.(16).

$$V^{heat}_{g,j,r,f,c,h} = \frac{Q^{heat}_{g,r,c,h,t}}{\eta^{tech}_{g,j,c,h,t}} \quad \forall g, j \in J_h \wedge JF_{j,f}, f, c, h, r =' On - grid' \tag{16}$$

Power supply chain

Spatially explicit power balance

Eq.(17) presents the overall energy balance of the energy system on a temporal (c,h,t) and spatial granularity (g,g'). More specifically, the left-hand side of the equation refers to energy sources including: power produced ($P_{g,j,c,h,t}$), energy storage discharge ($DC_{g,j,c,h,t}$), power transmitted among neighbouring regions ($TR_{g',g,c,h,t}$) and for the regions who are interconnected the related power imports or exports ($PIM_{i,g,c,h,t}$). The right-hand side represents energy sinks for the system including: energy demand ($D_{g,c,h,t}$), energy storage charge ($CH_{g,j,c,h,t}$), transmission to neighbouring regions ($TR_{g,g',c,h,t}$), renewables' curtailment ($LCurtail_{g,c,h,t}$), power shedding

$(LShed_{g,c,h,t})$.

$$\sum_{j\in J_e} P_{g,j,c,h,t}(1-PL_j) + \sum_{j\in J_{es}} DC_{g,j,c,h,t} + \sum_{g'\in NG_{g,g'}} TR_{g',g,c,h,t}(1-TL_{g',g}LDD_{g',g})$$
$$+\sum_{i\in IG_{i,g}} PIM_{i,g,c,h,t}(1-InterLoss_{i,g}) = D_{g,c,h,t}(1+DL) - LShed_{g,c,h,t} + LCurtail_{g,c,h,t}$$
$$+\sum_{g'\in NG_{g,g'}} TR_{g,g',c,h,t} + \sum_{j\in J_{es}} CH_{g,j,c,h,t} \quad \forall g,c,h,t \quad (17)$$

Notice that the electricity demand $(D_{g,c,h,t})$ further comprises of non-heat demand $(P^{elec}_{g,c,h,t})$ and demand resulting from electrification of heat $(P^{heat}_{g,r,c,h,t})$ as shown by eq.(18).

$$D_{g,c,h,t} = \sum_r P^{heat}_{g,r,c,h,t} + P^{elec}_{g,c,h,t} \quad \forall g,c,h,t \quad (18)$$

while the resulting system-wide peak demand $(PeakD_t)$ for each planning time step is computed through eq. (19).

$$PeakD_t \geq \sum_g D_{g,c,h,t} \quad \forall t \quad (19)$$

Finally the fuel consumption for power generation of thermal power plants is computed by eq.(20).

$$V^{elec}_{g,j,f,c,h,t} = \frac{P_{g,j,c,h,t}}{\eta^{tech}_{g,j,c,h,t}} \quad \forall g, j\in J_{th}, f\in Jf_{j,f}, c,h,t \quad (20)$$

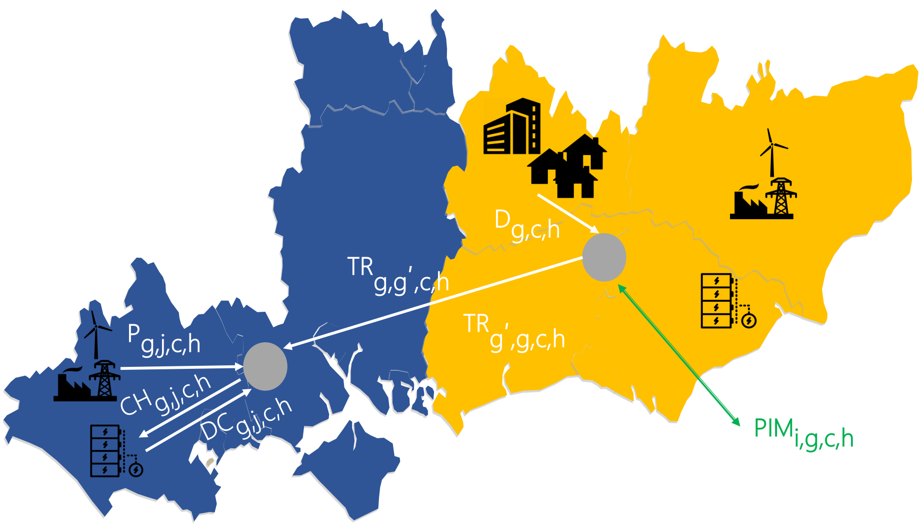


Figure 8: Spatially explicit energy balance for regions g and g′ and a fixed year t.

Transmission and interconnection

In the case that a region cannot meet its power demand from its regional power generation, electricity can be transmitted between regions. The amount of electricity transmitted between regions is limited by the capacity of the transmission network ($TRC_{g,g'}$) as shown by eq. (21).

$$TR_{g,g',c,h,t} \leq TRC_{g,g',t} \quad \forall (g,g') \in NG_{g,g'}, c, h, t \tag{21}$$

$$TRC_{g,g',t} = TRC_{g,g',t-1} + TRI_{g,g',t} \quad \forall (g,g') \in NG_{g,g'}, t \tag{22}$$

$$TRC_{g,g',t} = TRC_{g',g,t} \quad \forall (g,g') \in NG_{g,g'}, t \tag{23}$$

$$TRI_{g,g',t} \leq TRI^{up} \quad \forall (g,g') \in NG_{g,g'}, t \tag{24}$$

Overall, eqs. (21)-(24) model transmission corridors between regions with existing transmission capacity as well as transmission capacity expansion balance and investment limits (TRI^{up}). For the case of interconnection, interconnection capacities are considered deterministic and as model inputs based on the data given in Table 9. Eqs. (25)-(26), impose upper and lower limits on the bi-directional flow of electricity ($PIM_{i,g,c,h,t}$).

$$PIM_{i,g,c,h,t} \leq ICap_{i,g,t} \quad \forall (i,g) \in IG_{i,g}, c, h, t \tag{25}$$

$$PIM_{i,g,c,h,t} \geq -ICap_{i,g,t} \quad \forall (i,g) \in IG_{i,g}, c, h, t \tag{26}$$

Unit commitment

On the operational level of the model, decisions are modelled following the unit commitment (UC) formulation [58–60]. In order to rigorously model normal operation, start-ups and shut-downs of the generation plants the variables $u_{g,j,h}$, $v_{g,j,h}$, $w_{g,j,h}$ are accordingly employed.

$$u_{g,j,c,h,t} = u_{g,j,c,h-1,t} + v_{g,j,c,h,t} - w_{g,j,c,h,t} \quad \forall g, j \in J_{th}, c, h, t \tag{27}$$

$$\sum_{h'=h-UT_j}^{h} v_{g,j,c,h',t} \leq u_{g,j,c,h,t} \quad \forall g, j \in J_{th}, c, h \in [UT_j + 1, H], t \tag{28}$$

$$u_{g,j,c,h,t} \leq NUnits_{g,j,t} \quad \forall g, j \in J_{th}, c, h, t \tag{29}$$

$$\sum_{h'=h-DTj}^{h} w_{g,j,c,h',t} \leq NUnits_{g,j,t} - u_{g,j,c,h,t} \quad \forall g, j \in J_{th}, c, h \in [DT_j + 1, H], t \tag{30}$$

Eqs.(27)-(30) are employed to model the operational status of the generators clusters as well as the related start-up and shut-down events. Notice that eqs.(28)-(30) mathematically represent the polytope of the minimum up/down constraints and constitute the most computationally efficient formulation [61, 62].

Power generation limits

Each thermal generation plant has specified minimum (P_j^{min}) and maximum (P_j^{max}) stable thermal generation limits to model this, we employ eqs.(31)-(32).

$$P_j^{min} Cap_j^{Unit} u_{g,j,c,h,t} \leq P_{g,j,c,h,t} + r_{g,j,c,h,t}^{down} \quad \forall g, j \in J_{th}, c, h, t \tag{31}$$

$$P_{g,j,c,h,t} + r_{g,j,c,h,t}^{up} \leq P_j^{max} Cap_j^{Unit} u_{g,j,c,h,t} \quad \forall g, j \in J_{th}, c, h, t \tag{32}$$

Notice that in case that no generator is committed, i.e. $u_{g,j,h} = 0$, then the power generated is forced to be zero as well. The variables $r_{g,j,c,h}^{down}$ and $r_{g,j,c,h}^{up}$ refer to the participation in downward and upward operating reserve market respectively.

On the other hand, intermittent renewables energy sources ($j \in J_{rew}$) most of the times are not dispatchable immediately when required and their power production in depended weather factors such as solar irradiation and wind speed. To account for this issue eq.(33) is used and the parameter $AV_{g,j,h}$ defines the availability of the renewable source as a fraction of the installed capacity.

$$P_{g,j,c,h,t} = AV_{g,j,c,h,t} Cap_{g,j,t} \quad \forall g, j \in J_{rew}, c, h, t \tag{33}$$

$$LCurtail_{g,c,h,t} \leq \sum_{j \in J_{rew}} P_{g,j,c,h,t} \quad \forall g, c, h, t \tag{34}$$

Eq.(34) secures that the amount of curtailed power at any time and region should be less or equal to the amount of power generated by renewable sources.

Thermal generation ramping limits

Operations of conventional thermal generation plants are restricted by their hourly ramp-up and ramp-down capabilities. To model this, eq. (35) is used for the case of ramp-up rates with consideration of different capabilities during the start-up (SU_j) and the committed phase (RU_j).

$$\begin{aligned} P_{g,j,c,h,t} - P_{g,j,c,h-1,t} \leq\ & SU_j Cap_j^{Unit} v_{g,j,c,h,t} \\ & + RU_j Cap_j^{Unit} (u_{g,j,c,h,t} - v_{g,j,c,h,t}) - r_{g,j,c,h,t}^{up} \quad \forall g, j \in J_{th}, c, h, t \end{aligned} \tag{35}$$

Equivalently, to model ramp-down restrictions of thermal generation plants eq.(36) is employed and similarly to above we model different capabilities during the shut-down (SD_j) and the committed phase (RD_j).

$$\begin{aligned} P_{g,j,c,h-1,t} - P_{g,j,c,h,t} \leq\ & max[SD_j, P_j^{min}] Cap_j^{Unit} w_{g,j,c,h,t} \\ & + RD_j Cap_{g,j} (u_{g,j,c,h,t} - v_{g,j,c,h,t}) - r_{g,j,c,h,t}^{down} \quad \forall g, j \in J_{th}, c, h, t \end{aligned} \tag{36}$$

Operating reserve modelling & requirements

In order to account for upward and downward operating reserve requirement eq.(37)-(39) are used.

$$\sum_{j \in J_{th}, g} (r^{up}_{g,j,c,h,t} + r^{up_{nonsync}}_{g,j,c,h,t}) + \sum_{j \in J_{es}, g} r^{up_{nonsync}}_{g,j,c,h,t} = OPRES^{up}_{c,h,t} - l^{OPRES_{up}}_{c,h,t} \quad \forall c, h, t \quad (37)$$

$$\sum_{j \in J_{th}, g} r^{down}_{g,j,c,h,t} = (OPRES^{down}_{c,h,t} - l^{OPRES_{down}}_{c,h,t}) \quad \forall c, h, t \quad (38)$$

$$r^{up_{nonsync}}_{g,j,c,h,t} \leq (NUnits_{g,j,t} - u_{g,j,c,h,t}) * max(P^{min}_j, SU_j) Cap^{Unit}_j \quad \forall g, j \in J_{th}, c, h, t \quad (39)$$

In eq.(37) the variable $OPRES^{up}_{c,h,t}$ represents the system-wide requirement for upward operating reserve while the decision variable $l^{OPRES_{up}}_{g,c,h,t}$ stands for the amount of load shedding for upward operating reserve. Similar quantities were introduced in eq.(38). We also account for non-synchronous participation ($r^{up_{nonsync}}_{g,j,c,h,t}$) in the reserve markets for thermal generators that are not committed, via eq. (39) and for grid-level storage units. The upward ($OPRES^{up}_{g,c,h,t}$) and downward ($OPRES^{down}_{g,c,h,t}$) reserve requirements are computed endogenously by OPHELIA based on eqs. (40)-(41).

$$OPRES^{up}_{g,c,h,t} = D^{error}_{c,h} \sum_g D_{g,c,h,t} + Res^{Error}_{c,h} \sum_{g, j \in J_{res}} AV_{g,j,c,h,t} Cap_{g,j,t} + SCap^{N-1} \quad \forall c, h, t \quad (40)$$

$$OPRES^{down}_{g,c,h,t} = 0.5 (D^{error}_{c,h} \sum_g D_{g,c,h,t} + Res^{Error}_{c,h} \sum_{g, j \in J_{res}} AV_{g,j,c,h,t} Cap_{g,j,t} + SCap^{N-1}) \quad \forall c, h, t \quad (41)$$

As shown by eqs. (40)-(41) the short term operating reserve is a function of the demand error and generation output error of renewable energy sources along with the N-1 security consideration ($SCap^{N-1}$). The downward operating reserve is parameterised as 50% of the upward reserve requirement.

Energy storage constraints

Energy storage is modelled using eqs.(42)-(45). Charging (eq. (42)) and discharging (eq. (43)) is restricted by the installed capacity. The total energy volume stored cannot exceed storage volume capacity (which is defined as its storage capacity times maximum output hours at that capacity, eq. (44)). Finally, eq. (45) makes sure that total energy discharging cannot exceed the energy volume that was stored before ($ST^{init}_{g,j,t}$) and total net charging during the modelling horizon.

$$CH_{g,j,c,h,t} \leq Cap_{g,j,t} \quad \forall g, j \in J_{es}, c, h, t \tag{42}$$

$$DC_{g,j,c,h,t} \leq Cap_{g,j,t} \quad \forall g, j \in J_{es}, c, h, t \tag{43}$$

$$\sum_{h'|h' \leq h} (\eta_j CH_{g,j,c,h',t} - DC_{g,j,c,h',t}) + ST^{init}_{g,j,t} \leq Cap_{g,j,t} ST^{out}_j \quad \forall g, j \in J_{es}, c, h, t \tag{44}$$

$$\sum_{h'|h' \leq h} (DC_{g,j,c,h',t} - \eta_j CH_{g,j,c,h',t} + r^{up_{nonsync}}_{g,j,c,h,t}) \leq ST^{init}_{g,j,t} \quad \forall g, j \in J_{es}, c, h, t \tag{45}$$

$$ST^{init}_{g,j,t} = 0.5 Cap_{g,j,t} \quad \forall g, j \in J_{es}, t \tag{46}$$

Capacity expansion constraints

We consider capacity expansion of power generation units over five-year time steps (t) along with the initially available generation fleet and their projected decommissioning timings at the end of their operating lifetime. In summary the constraints employed are given by eqs. (47)-(51).

$$\begin{aligned} NUnits_{g,j,t} = NUnits_{g,j,t-1} + CUnits_{g,j,t} - DUnits_{g,j,t} \\ - CUnits_{g,j,t-tp_j} \quad \forall g, j \in J_{th}, t \end{aligned} \tag{47}$$

$$\begin{aligned} Cap_{g,j,t} = Cap_{g,j,t-1} + Cap^{New}_{g,j,t} - DCap_{g,j,t} \\ - Cap^{New}_{g,j,t-tp_j} \quad \forall g, j \in J_{rew} \cup J_{es}, t \end{aligned} \tag{48}$$

$$\sum_{g,j \in J_{th}} DF_j Cap^{Unit}_j NUnits_{g,j,t} + \sum_{g,j \in (J_{rew} \cup J_{es})} DF_j Cap_{g,j,t} \geq (1 + RM) PeakD_t \quad \forall t \tag{49}$$

$$CUnits_{g,j,t} \leq BR_{j,t} \Delta t \quad \forall g, j \in J_{th}, t \tag{50}$$

$$Cap^{New}_{g,j,t} \leq BR_{j,t} \Delta t \quad \forall g, j \in J_{rew} \cup J_{es}, t \tag{51}$$

Eqs. (47)-(48) represent the capacity balances for thermal and renewables/energy storage units respectively. While for the case of thermal generation we consider integer number of identical units ($NUnits_{g,j,t}$) with fixed unit capacity (Cap^{Unit}_j) for the case of RES and energy storage we allow the capacity to be a continuous variable ($Cap_{g,j,t}$) owing to the flexibility in capacity sizes. Eq. (49) reflects the planning reserve requirement which indicates that the system's installed capacity, after considering for technology-specific de-rating factors [63], should be at least equal to the peak demand plus a reserve margin factor which in our case is taken to be 13%. Finally, eqs. (50)-(51) impose new capacity deployment restrictions based on build rates ($BR_{j,t}$) over the five-year time steps (Δt).

Carbon emissions constraint

We consider separate carbon emissions targets for the electricity and the heat sectors. For the power sector carbon emissions targets are set as carbon budgets as advised by the UK Committee on Climate Change [64]. For the heat sector we linearly extrapolate from 2018 to 2053 towards gross zero heat emissions as we do not allow for negative emissions to be allocated for the heat carbon budgets. Eqs. (52)-(53) are used to monitor the emissions from the heat sector while eqs. (54)-(56) are employed for the power sector.

$$CO_{2t}^{heat} \leq \overline{CO_2^{heat}}_t \quad \forall t \tag{52}$$

$$CO_{2t}^{heat} = \sum_{g,j \in J_h, f \in JF_{j,f}} \varepsilon_f \sum_{c,h} WD_c V_{g,j,f,r,c,h,t}^{heat} \quad \forall t \tag{53}$$

$$CO_{2t}^{elec} - CO_{2t}^{elec_{neg}} \leq \overline{CO_2^{elec}}_t \quad \forall t \tag{54}$$

$$CO_{2t}^{elec} = \sum_{g,j \in J_{th}, f \in JF_{j,f}} \varepsilon_f \sum_{c,h} WD_c (1 - CCS_j^{rem}) V_{g,j,f,c,h,t}^{elec} \quad \forall t \tag{55}$$

$$CO_{2t}^{elec_{neg}} = - \sum_{g,j \in J_{neg}, f \in JF_{j,f}} \varepsilon_f \sum_{c,h} WD_c CCS_j^{rem} V_{g,j,f,c,h,t}^{elec} \quad \forall t \tag{56}$$

Model implementation and solution procedure

The overall OPHELIA model is formulated as a mixed integer linear program (MILP) and is implemented in GAMS 31.2 and solved with CPLEX 12.1 on a computer cluster composed of 32 machines with a total of 384 GB RAM (24 threads). Solving the model in a monolithic fashion, is computationally prohibitive as the for perfect foresight and 12 representative days the model comprises of 3.8 million equations, 6 million constraints and 500,000 discrete variables. To this end, we employ a myopic rolling horizon procedure in which the we decompose the planning periods in bins of two adjacent periods and each time one bin is solved. Then all the design decisions are fixed and the planning horizon is shifted by two time steps and the procedure is repeated until the entire horizon is covered. Following this procedure the model is solved to optimality gap of 3% in 22-26 hours depending on the scenario and input data.

Supplementary note 4: OPHELIA summary of data

Electricity demand data

Electricity demand data for GB are publicly available on a half-hourly and nation-wide basis [65]. First, aggregate and average out the half-hourly data to hourly resolution. Then in order to disaggregate the data regionally we use the sub-national electricity consumption statistics [66] and compute the regional demand shares for its LDZ as shown in Table 3.

Table 3: Electricity demand allocation per region

Local Distribution Zone (LDZ)	Share (%)
EA	9.6
EM	7.5
NE	6.5
NO	5.0
NT	13.9
NW	12.1
SC	8.9
SE	2.90
SO	10.9
SW	8.6
WM	8.7
WN	1.5
WS	3.9

Transmission grid assumptions and data

To model the transmission capability of the system across the different regions, the system technical data from the ten-year grid statement are used [67]. Due to the scope of the present to model simultaneously the UK electricity and gas system we aggregate the transmission line capacities into the 13 regions considered in the model. To do so, the line capacities of the National Grid's ten year statement technical data are employed. In the technical data the seasonal line capacities are detailed with the summer being around 80% of the winter's rating [67]. Aggregating all the line capacities that cross a local distribution zone's borders using the 2018 data and assuming that transmission is done between the centroids of the regions we calculate the linear distance (LDD) and transmission capacities between LDZs ($TRC_{g,g',t}$) as shown in Table 4. Transmission losses are assumed to be 1% per 100km [68]. A graphical representation is given in Fig.9. UK security standards require the transmission system to endure failure of up to two circuits (N-2 security rule). Other models such as highRES [68] and ELMOD[69] impose a security margin between 20-25% on the nominal transmission capabilities to simulate a more realistic operation of the system. Nonetheless, the proposed model can be easily modified to account for such parametrisation. Finally, in Table 4 the techno-economic data of the transmission system are given.

Table 4: Cross-regional transmission data (Overground 75 km 400kV (AC)).

Transmission Characteristics	Value	Source
Marginal CAPEX (£/MVA/km)	247	[68]
Transmission losses (%/100km)	1	[68]
Lifetime (years)	40	[68]

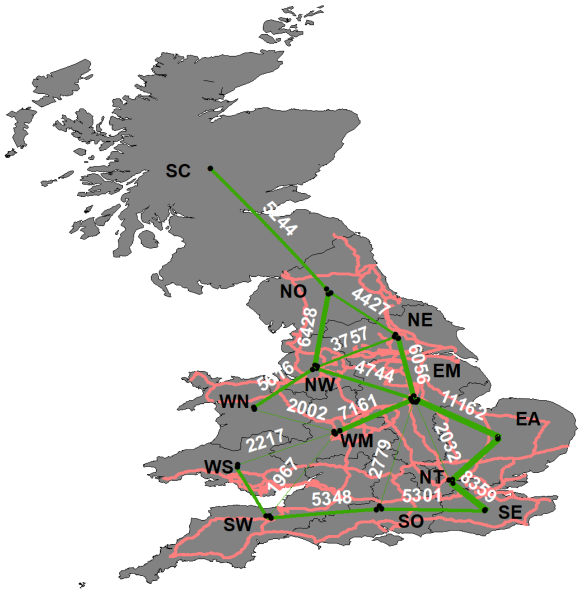


Figure 9: Initial cross-regional transmission capacities

Power generation technology data

OPHELIA considers existing power plant's capacities across the regions along with their decommissioning at the end of their lifetime based on the data available from BEIS [70]. A summary of the techno-economic characteristics for the thermal generation technologies is given in Table 5 while for renewable energy sources the relevant data are summarised in Table 6.

Table 5: Techno-economic specifications of thermal generation technologies.

	Nuclear	Coal	CCGT	CCGTCCS	OCGT	Biomass	BECCS	Sources
Net efficiency (LHV) (%)	0.391	0.356	0.515	0.49	0.39	0.35	0.28	[71–73]
Min uptime (h)	12	8	2	4	1	4	8	[71–73]
Min downtime (h)	12	8	2	4	1	4	8	[71–73]
Min load (%)	0.5	0.35	0.35	0.5	0.3	0.4	0.5	[71, 72]
Max load (%)	0.88	0.8	0.87	0.8	0.94	0.8	0.8	[71–73]
Parasitic load (%)	0.0917	0.0513	0.0171	0.12	0.0171	0.0513	0.2	[71–73]
Committed Ramp up (%)	0.1	0.3	1	1	1	0.3	0.3	[71, 72]
Committed Ramp down (%)	0.1	0.3	1	1	1	0.3	0.3	[71, 72]
Start-up Ramp up (%)	0.3	0.3	1	1	1	0.3	0.3	[71, 72]
Shut-down Ramp down (%)	0.3	0.3	1	1	1	0.3	0.3	[71, 72]
Start-up cost (£/MW-start-up)	22.4	72.4	54.2	22.06	64.5	65.2	44.9	[71, 72, 74]
Fixed O & M (£'000/MW-year)	72.94	56.4	11.44	30.98	4.57	65.5	139.14	[71, 72, 75]
Capital cost (£'000/MW)	4435.5	1237	583.5	2100	750	3075	5885.5	[71, 72, 75]
CO_2 capture (%)	-	-	-	0.9	-	-	0.9	[71, 76]
Variable cost (£/MWh)	2.62	2.2	1.43	2.5	1.91	4	7.86	[71, 72, 75]

Table 6: Techno-economic specifications of RES technologies.

	Onshore Wind	Offshore Wind	Solar PV	Source
Fixed O & M (£'000/MW-year)	23.5	28	6.7	[77]
Capital cost (£'000/MW)	1400	2100	750	[77]
Variable cost (£/MWh)	0	0	0	[77]
Lifetime (years)	25	30	30	[77]
De-rating factor (%)	0.25	0.36	0.14	[77]

Table 7: Energy storage technologies characteristics. As a generic grid-level storage technology we consider NaS (sodium-sulfur) battery. For pumped hydro storage we consider the medium cost estimates from [71]. For domestic thermal energy storage we consider hot water tanks.

Storage Characteristics	Pumped storage	Grid-level storage	Thermal storage	Source
Marginal CAPEX (10^3£/MW)	1032	612	35	[57, 71, 78]
Variable OPEX (£/MWh)	10	2	8	[38, 57, 78]
Fixed O&M (£/kW-year)	11.2	3.6	incl. in Capex	[57, 71, 78]
Round-trip efficiency (%)	77	86	-	[29, 71, 78]
Power to Energy ratio	8	6	4	[38, 68, 71, 78]
Thermal losses per hour (%)	-	-	5	[34, 57]
Lifetime (years)	50	20	20	[38, 71, 78]

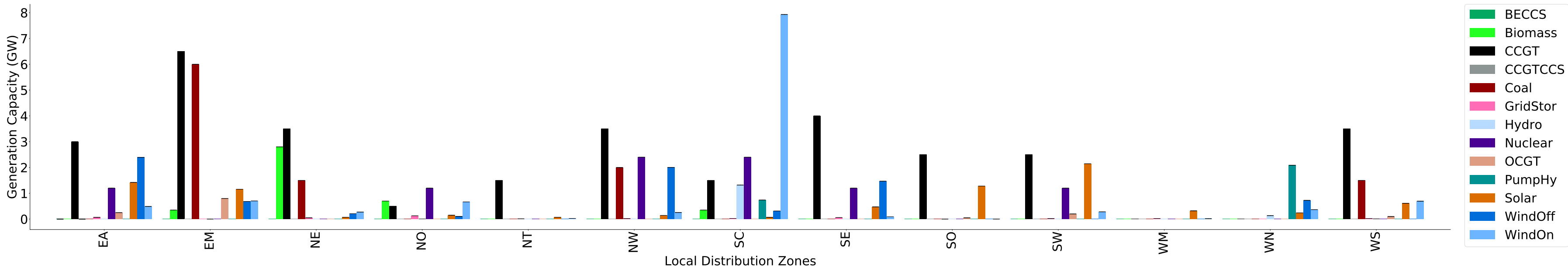
Table 8: Heat end-use technologies data.

Technology Characteristics	Gas boiler	ASHP	Source
Marginal CAPEX (10^3£/MW)	75	612	[47]
Fixed O&M (£/kW$_{th}$-year)	32	20	[34, 38]
Lifetime (years)	15	15	[34, 38]
Efficiency (%)	90	160-350	[34, 38]

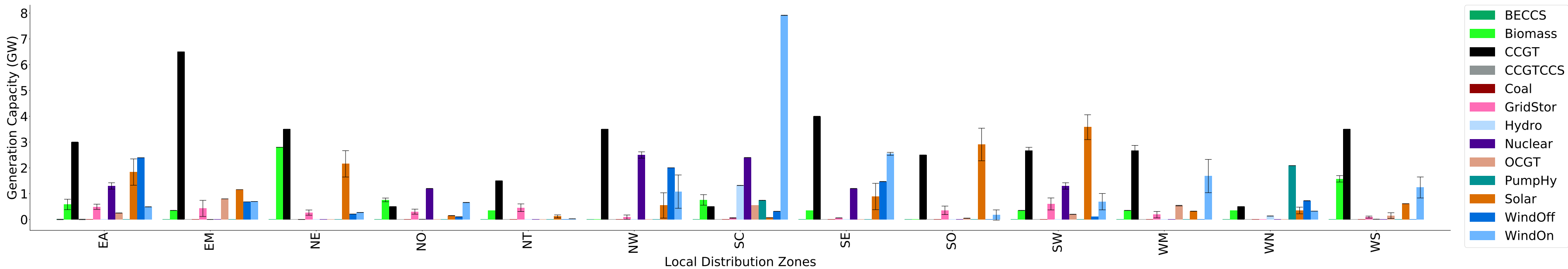
Table 9: Interconnection data [79, 80].

Interconnection	Connected markets	LDZ connection	Capacity (GW)	Thermal losses (%)
IFA	France	SE	2	1.17
MOYLE	Irish SEM	SC	0.5	2.36
BritNed	Netherlands	SE	1	3.45
EWIC	Irish SEM	WN	0.5	4.68
NEMO	Belgium	SE	1	2.67
Eleclink	France	SE	1	2.08
IFA2	France	SO	0.5	4.68
NSS	Norway	NO	1.5	7.98
Greenlink	Irish SEM	WS	0.5	3.30
Fablink	France	SW	1.4	4.68
Vikinglink	Denmark	EM	1	6.90
Northconnect	Norway	SC	1.4	7.35

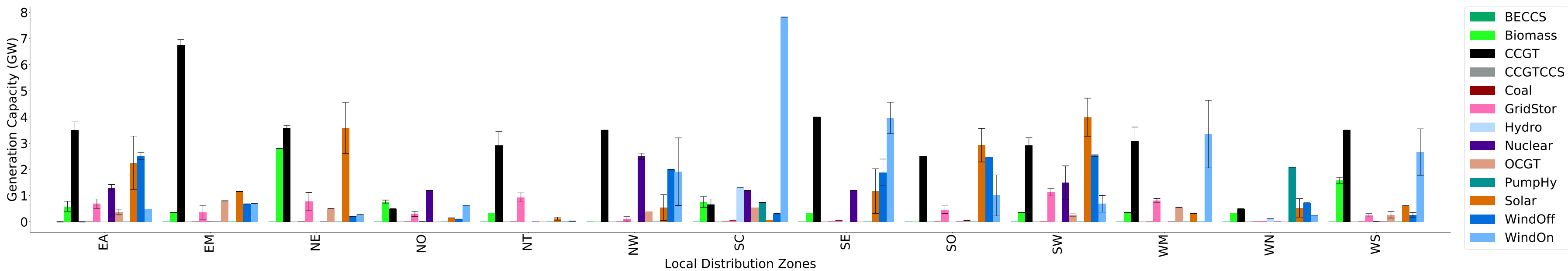
Supplementary note 5: Overview of regional results



(a) Installed generation capacities across LDZs in 2018 (input data).

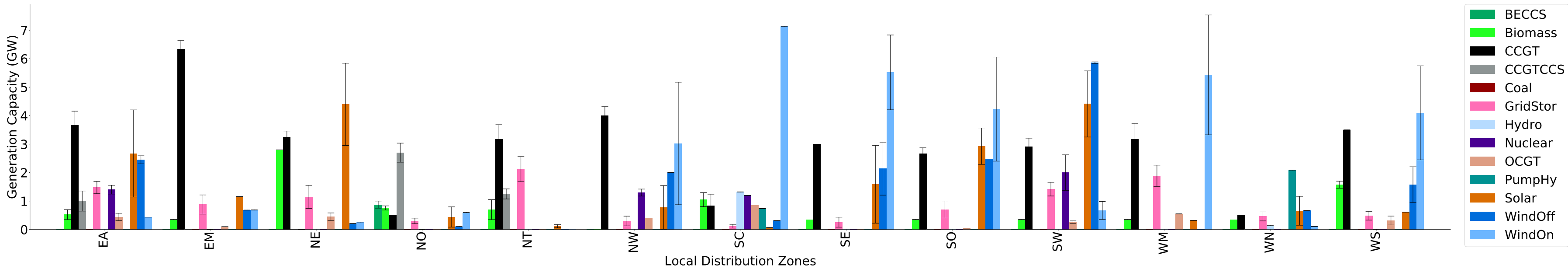


(b) Installed generation capacities across LDZs in 2023 (model output).

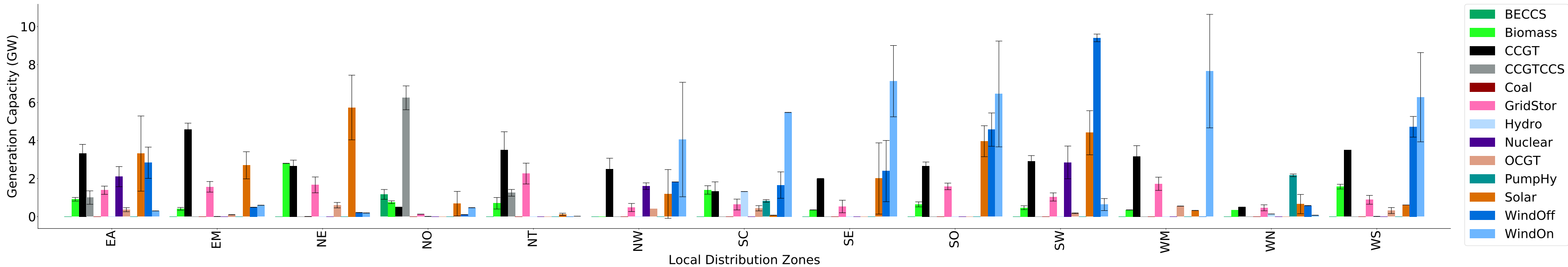


(c) Installed generation capacities across LDZs in 2028 (model output).

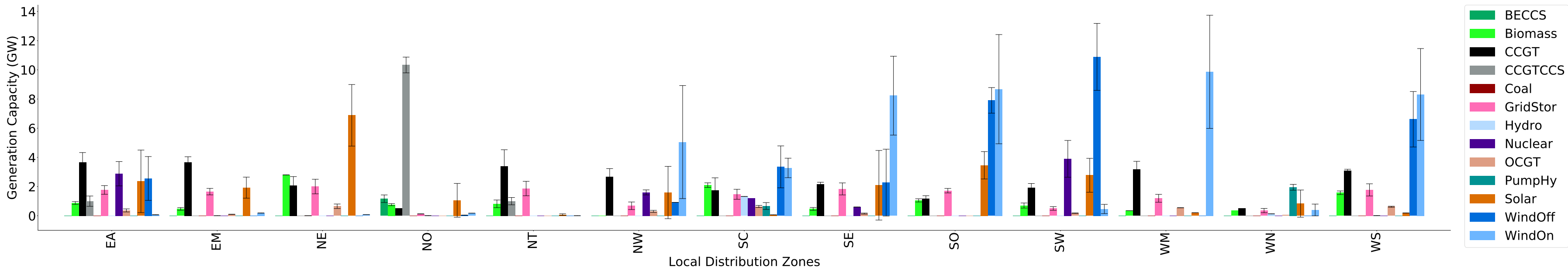
Figure 10: Optimised regional allocation of generation capacities for 2018-2053. The error bars of the individual bars indicate the variation resulting from running the optimisation model with different heat demand data from 2015-2018.



(a) Installed generation capacities across LDZs in 2033 (model output).

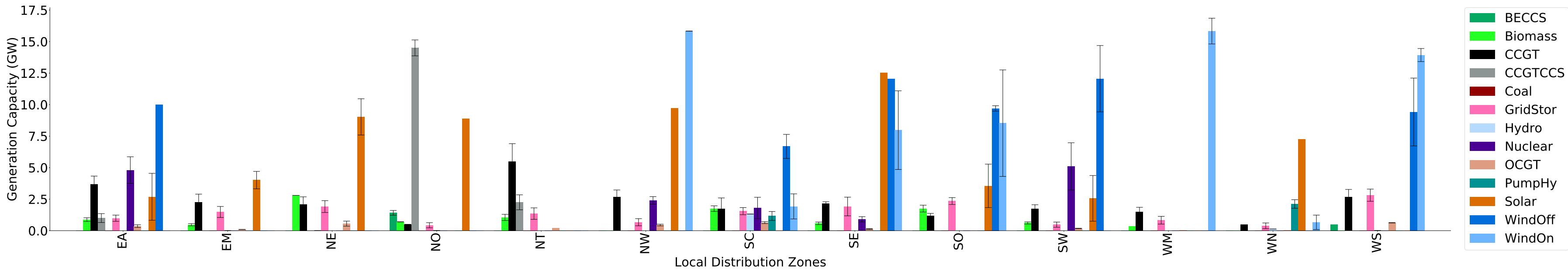


(b) Installed generation capacities across LDZs in 2038 (model output).

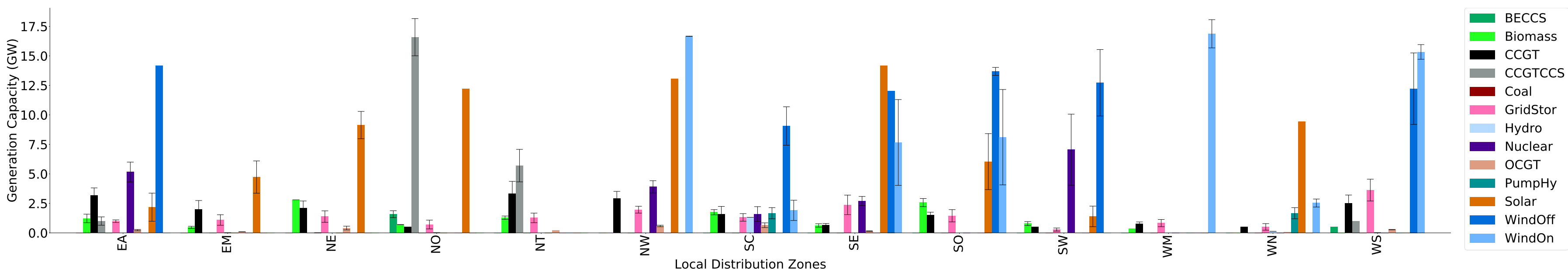


(c) Installed generation capacities across LDZs in 2043 (model output).

Figure 10: (continued) Optimised regional allocation of generation capacities for 2018-2053. The error bars of the individual bars indicate the variation resulting from running the optimisation model with different heat demand data from 2015-2018.

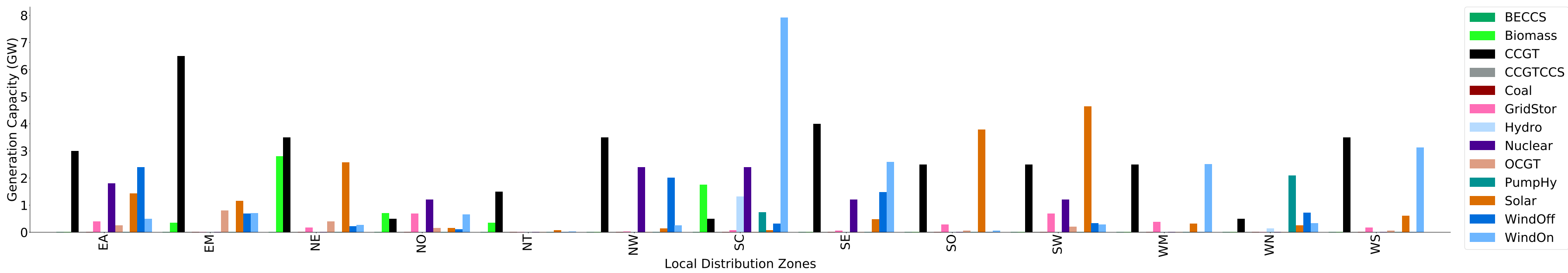


(d) Installed generation capacities across LDZs in 2048 (model output).

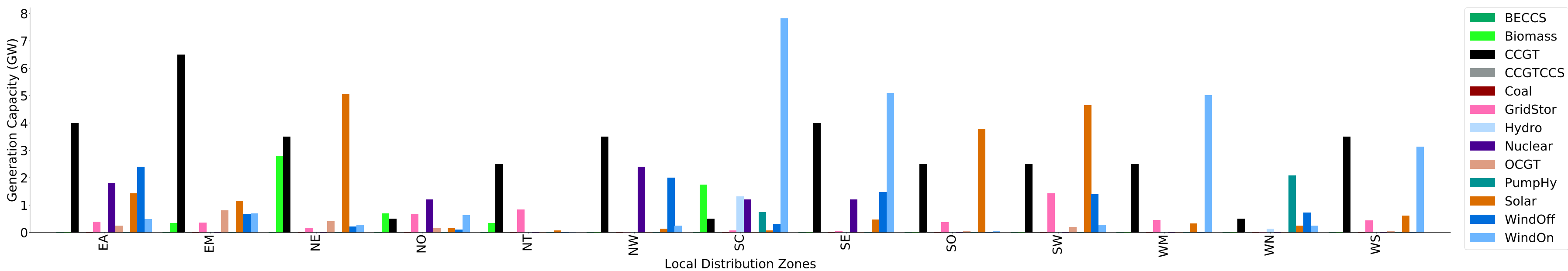


(e) Installed generation capacities across LDZs in 2053 (model output).

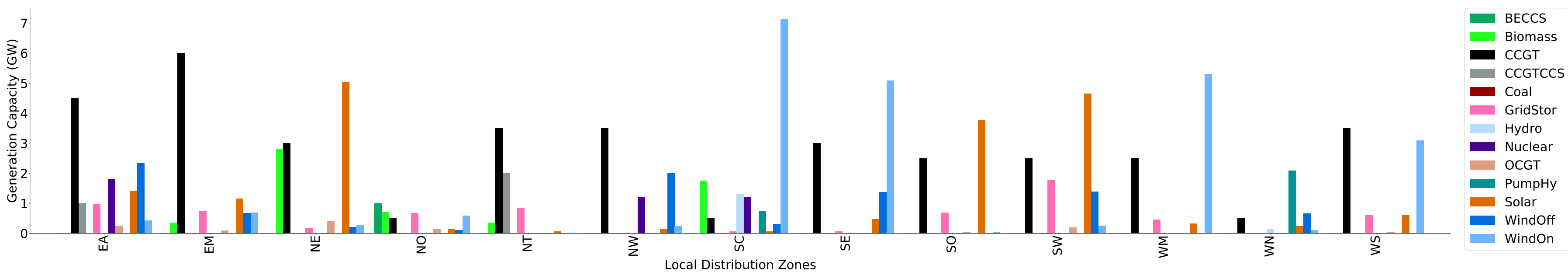
Figure 10: (continued) Optimised regional allocation of generation capacities for 2018-2053. The error bars of the individual bars indicate the variation resulting from running the optimisation model with different heat demand data from 2015-2018.



(f) Installed generation capacities across LDZs in 2023 (model output).

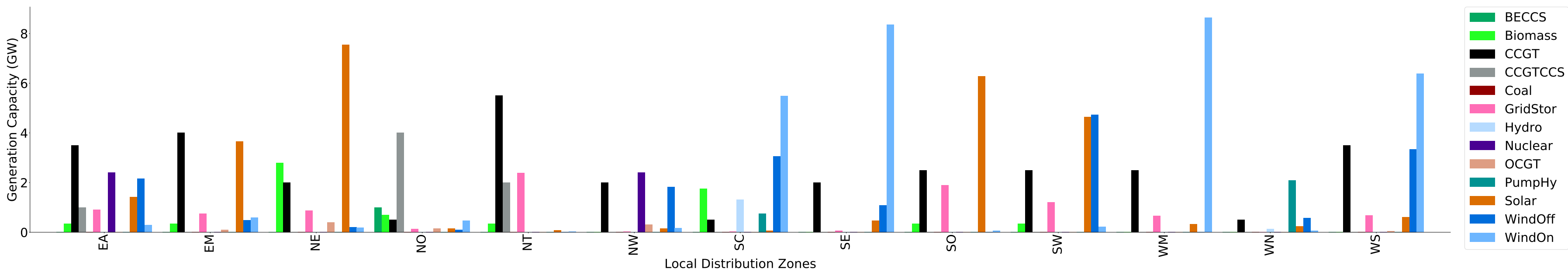


(g) Installed generation capacities across LDZs in 2028 (model output).

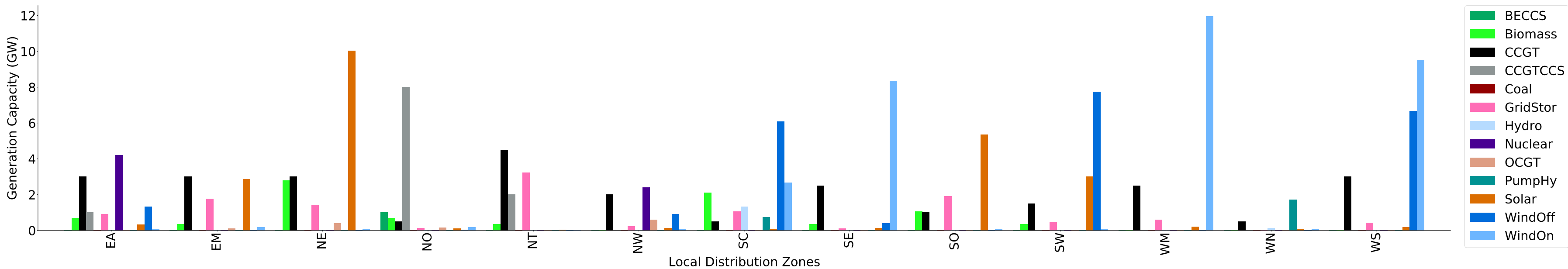


(h) Installed generation capacities across LDZs in 2033 (model output).

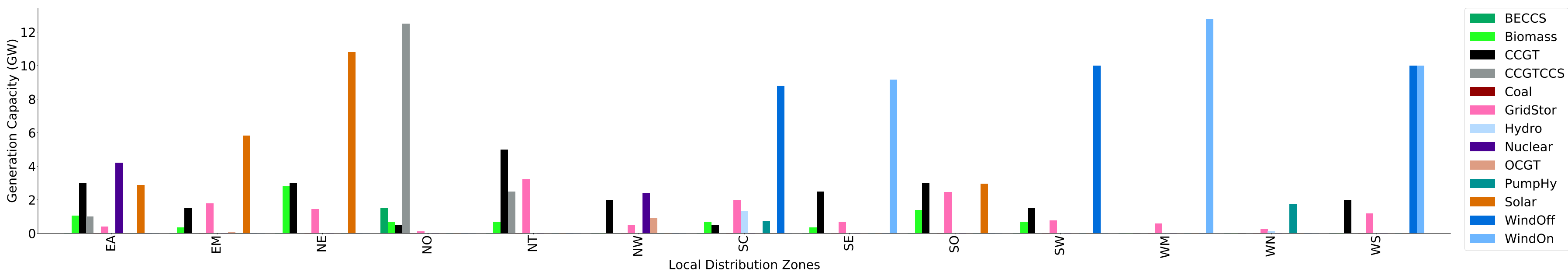
Figure 11: Optimised regional allocation of generation capacities for 2018-2053 for power sector only decarbonisation.



(a) Installed generation capacities across LDZs in 2038 (model output).

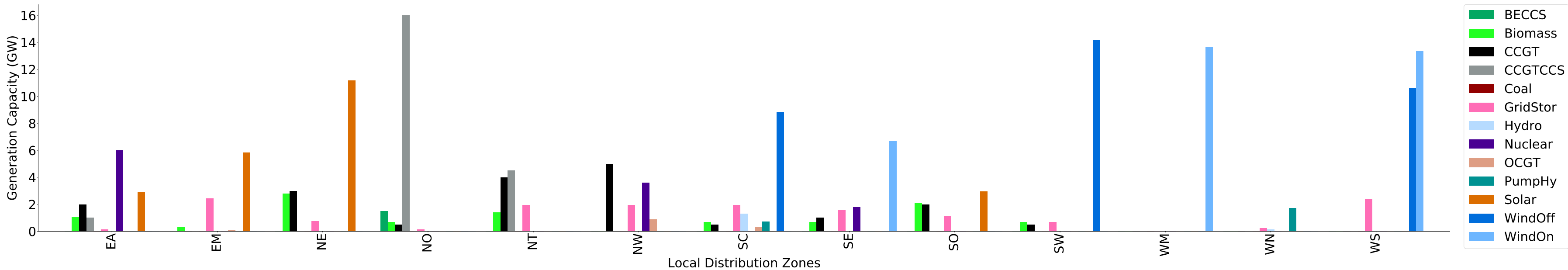


(b) Installed generation capacities across LDZs in 2043 (model output).



(c) Installed generation capacities across LDZs in 2048 (model output).

Figure 11: (continued) Optimised regional allocation of generation capacities for 2018-2053 for power sector only decarbonisation.



(d) Installed generation capacities across LDZs in 2053 (model output).

Figure 11: (continued) Optimised regional allocation of generation capacities for 2018-2053 for power sector only decarbonisation.

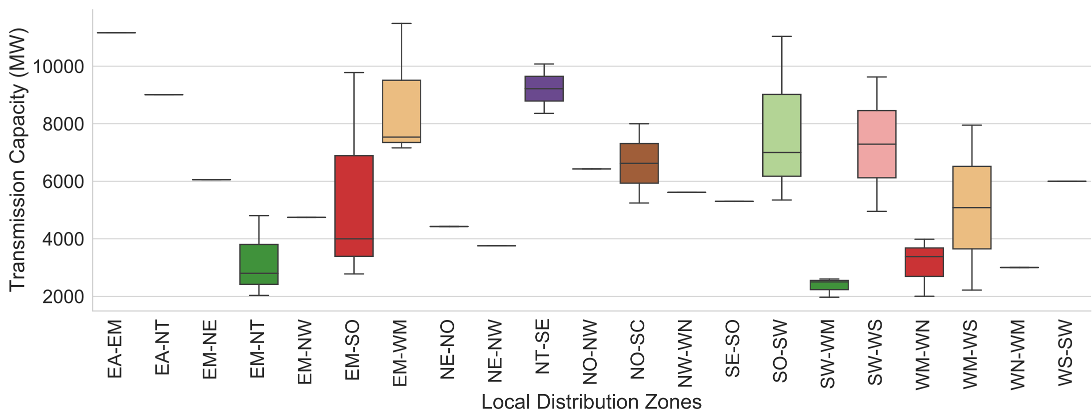
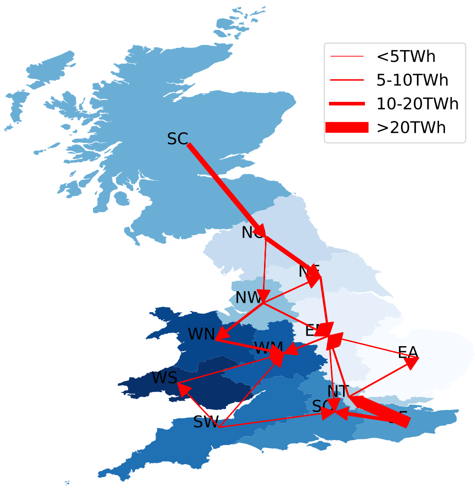
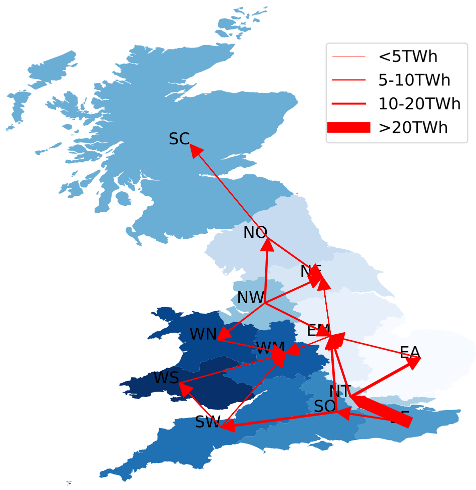


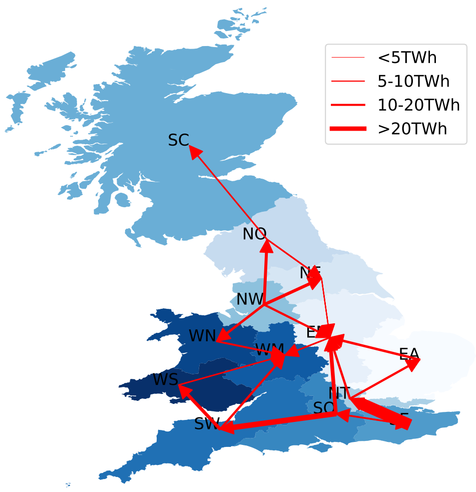
Figure 12: Boxplots of cross-regional transmission capacities in 2053 over different optimisation runs with different heat demand data from 2015-2018.



(a) Net transmission flows in 2028



(b) Net transmission flows in 2038



(c) Net transmission flows in 2053

Figure 13: Regional net transmission flows (TWh/year) with 2015 input data. Consistently the largest amount of transmission is observed from SE to NT. This is attributed to three factors: (i) NT absorbs significant amounts of the intermittent generation from SE (Solar & Onshore Wind) owing to the lack of within region installed capacity (cf. Fig. 10), (ii) increased demand of electricity due to heat electrification in NT and (iii) flexibility due to the presence of interconnection in SE. We also note that SC progressively towards mid-century becomes a net importer from NO mostly because of: (i) increased allocation of CCGT-CCS capacity in NO vs a predominantly intermittent capacity mix in SC & (ii) increased interconnection from SC to Norway.

Nomenclature

Sets

c Cluster of days

f Fuel

g, g' Geographic regions

h, h' Time-slices (hours)

j Technologies

j_e Electricity generation technologies

j_f Dynamic set of technologies j consuming fuel type f

j_h End-use heating technologies

j_s Energy storage technologies

j_{h^s} Thermal storage technologies

j_{rew} Renewable generation plants

j_{th} Thermal generation plants

t Time-steps (years)

Parameters

ϵ_f Fuel f emissions factor [tCO2e/MWh]

$\eta^{tech}_{g,j,c,h,t}$ Performance efficiency for end-use heating technologies [-]

$\overline{CO2}^{elec}_t$ CO2 emissions upper limit for the power sector in year t [tCO2e]

$\overline{CO2}^{heat}_t$ CO2 emissions upper limit for the heat sector in year t [tCO2e]

$Av_{g,j,c,h,t}$ Availability of renewable energy sources $j \in J_{rew}$ [%MW]

$BR_{j,t}$ Build rate of technology j at year t [-/MW]

$C^{CO_2}_t$ Carbon price at year t [£/tCO2e]

C^{CRTL} Unit cost of curtailed renewable power [£/MWh]

C^{fix}_j Fixed capital cost of technology j [£/MW]

C^{fix}_{tr} Fixed capital cost of transmission lines [£/MW]

$C^{fuel}_{f,t}$ Unit consumption cost of fuel f at year t [£/MWh]

$C^{INCX}_{i,g,c,h,t}$ Price of interconnected power from interconnector i to region g at time slice h and year t [£/MW]

C^{OM}_{j} Fixed O&M cost of technology j [£/MW]

$C^{OPRES_{down}}$ Value of loss load for shedding downward operating reserve requirements [£/MWh]

$C^{OPRES_{up}}$ Value of loss load for shedding upward operating reserve requirements [£/MWh]

C^{shut}_{j} Shut-down cost cost of technology j [£/MW]

C^{start}_{j} Start-up cost cost of technology j [£/MW]

$C^{STOR_{dn}}$ Unit cost of downward short term operating reserve [£/MW]

$C^{STOR_{up}}$ Unit cost of upward short term operating reserve [£/MW]

C^{var}_{j} Variable operating cost of technology j [£/MWh]

C^{VoLL} Unit cost of load shedding (Value of Loss Load) [£/MWh]

$CapUnit_j$ Unit capacity of thermal power plants [MW]

CCS^{rem}_{j} Capture rate of CO2 of technology j [%]

$COP_{g,c,h,t}$ Coefficient of performance for ASHPs [-]

$D^{error}_{c,h}$ Forecasting demand error for reserve calculations [%]

DF_j Derating factor of technology j for capacity reserve calculations [%]

DFC_t Discount factor [-]

DL Distribution power losses [%]

DT_j Minimum down-time of generation unit j [hours]

hcu_j Unit capacity of heat-end use technologies [MW]

$ICap_{i,g,t}$ Interconnection capacity between interconnector i, region g at year t [MW]

$InterLoss_{i,g}$ Interconnection transmission losses [%]

$LDD_{g,g'}$ Linear distance between the centroids of two geographic regions [km]

$nHg_{g,r}$ Number of domestic properties at region g and area r [-]

$P^{elec}_{g,c,h,t}$ Electricity demand [MWh]

P^{max}_{j} Maximum stable generation of generation plant [MWh]

P^{min}_{j} Minimum stable generation of generation plant [MWh]

PL_j Parasitic load factor % of gross generation [-]

r Discount rate [-]

RD_j Maximum ramp-down rate of generation unit j when committed [MWh]

$Res^{Error}_{c,h}$ Forecasting renewable generation error for reserve calculations [%]

RM Capacity reserve margin [%]

RU_j Maximum ramp-up rate of generation unit j when committed [MWh]

$SCap^{N-1}$ N-1 security capacity parametrisation for loss of larger power plant or interconnector [MW]

SD_j Maximum ramp-down rate of generation unit j when shutting-down [MWh]

ST^{out}_j Energy to power ratio for power storage [hours]

SU_j Maximum ramp-up rate of generation unit j when starting-up [MWh]

$T^{\alpha}_{g,c,h,t}$ Hourly ambient temperature [°C]

TES_j Energy to power ratio for thermal storage [hours]

$TL_{g,g'}$ Percentage of transmission losses per km of transmission [-]

tp_j Lifetime of technology j [years]

TRI^{up} Upper investment limit in new transmission capacity [MW]

UT_j Minimum up-time of generation unit j [hours]

WD_c Weight of each cluster (number of days) [-]

Integer variables

$CUnits^{heat}_{g,j,r,t}$ Number of new heat-end use units at region g within area r (on/off-gas grid) and year t

$CUnits_{g,j,t}$ Number of new thermal power generation units j in region g and year t

$DUnits^{heat}_{g,j,r,t}$ Number of decommissioned heat-end use units at region g within area r (on/off-gas grid) and year t

$DUnits_{g,j,t}$ Number of decommissioned thermal power generation units j in region g and year t

$NUnits^{heat}_{g,j,r,t}$ Number of installed heat-end use units in region g within area r (on/off-gas grid) and year t

$NUnits_{g,j,t}$ Number of installed thermal power generation units j in region g and year t

$u_{g,j,c,h,t}$ Number of thermal plants j$\in J_{th}$ in region g at time-slice h and year t committed

$v_{g,j,c,h,t}$ Number of thermal plants j$\in J_{th}$ in region g at time-slice h and year t starting-up

$w_{g,j,c,h,t}$ Number of thermal plants j$\in J_{th}$ in region g at time-slice h and year t shutting-down

Continuous variables

$Cap^{New}_{g,j,t}$ New investment capacity of non-thermal generation or storage technologies at region g and year t [MW]

$Cap_{g,j,t}$ Installed capacity of non-thermal generation or storage technologies at region g and year t [MW]

$CH_{g,j,c,h,t}$ Power charger to storage unit j at region g, time-slice h and year t [MWh]

${CO_2^{elec_{neg}}}_t$ Total negative CO2 emissions from the power sector at year t [tCO2e]

${CO_2^{elec}}_t$ Total CO2 emissions from the power sector at year t [tCO2e]

${CO_2^{heat}}_t$ Total CO2 emissions from the heat sector at year t [tCO2e]

$D_{g,c,h,t}$ Power demand (heat and non-heat) at region g, time-slice h and year t [MWh]

$DC_{g,j,c,h,t}$ Power discharged from storage unit j at region g, time-slice h and year t [MWh]

$HDem_{g,r,c,h,t}$ Hourly heat demand at region g and year t [MWh]

$l^{OPRES_{down}}_{c,h,t}$ Load shedding of downward reserve at region g, time-slice h and year t [MWh]

$l^{OPRES_{up}}_{c,h,t}$ Load shedding of upward reserve at region g, time-slice h and year t [MWh]

$LCurtail_{g,c,h,t}$ Curtailment of renewable energy resources connected to transmission at region g, time-slice h and year t [MWh]

$LShed_{g,c,h,t}$ Load shedding of electricity demand at region g, time-slice h and year t [MWh]

$OPRES^{down}_{g,c,h,t}$ Downward operating reserve requirement at region g, representative day c, time-slice h and year t [MWh]

$OPRES^{up}_{g,c,h,t}$ Upward operating reserve requirement at region g, representative day c, time-slice h and year t [MWh]

$P^{heat}_{g,r,c,h,t}$ Electricity load resulting from electrified heat [MWh]

$P_{g,j,c,h,t}$ Power generated at region g, by units j at time-slice h and year t [MWh]

$PeakD_t$ Peak power demand at year t [MWh]

$PIM_{i,g,c,h,t}$ Power imported at region g through interconnector at time-slice h and year t [MWh]

$Q^{dheat}_{g,r,h,t}$ Heat discharged from thermal storage at time-slice h at region g and year t [MWh]

$Q^{heat}_{g,r,j,c,h,t}$ Heat generated at time-slice h at region g and year t from technology j [MWh]

$Q^{sheat}_{g,r,h,t}$ Heat stored to thermal storage at time-slice h at region g and year t [MWh]

$r^{down}_{g,j,c,h,t}$ Downward reserve of thermal unit j at region g, time-slice h and year t [MWh]

$r^{up_{nonsync}}_{g,j,c,h,t}$ Upward nonsynchronous reserve of technology j at region g, time-slice h and year t [MWh]

$r^{up}_{g,j,c,h,t}$ Upward reserve of thermal unit j at region g, time-slice h and year t [MWh]

$S^{heat}_{g,r,c,h,t}$ Heat storage level at region g, grid area r, at time-slice h and year t [MWh]

$ST^{init}g, j, t$ Initial stored energy for technology j at region g and year t [MWh]

$TotCAPEX_t$ NPV of total electricity and heat system's capital costs at year t [£]

$TotOPEX_t$ NPV of total electricity and heat system's operating costs at year t [£]

$TR_{g,g',c,h,t}$ Power transmitted inter-regionally at time-slice h and year t [MWh]

$TRC_{g,g',t}$ Inter-regional transmission capacity [MW]

$TRI_{g,g',t}$ Inter-regional transmission capacity investement [MW]

TSC NPV of total electricity and heat system's costs [£]

$V^{elec}_{g,j,f,c,h,t}$ Fuel consumption of type f at region g by technology j, time-slice h and year t for power generation [MWh]

$V^{heat}_{g,j,f,c,h,t}$ Fuel consumption of type f at region g by technology j, time-slice h and year t for power generation [MWh]

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