Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supplementary Material: The value of ammonia towards integrated power and heat system decarbonisation

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Introduction

This supplementary material presents in detail the mathematical model of the power system planning snapshot problem as well as the accompanied data which particularly pertain to the power system of the UK. Thus, in Section 1 the mathematical snapshot model for the power system planning and operation problem is presented in detail. Then, in Section 2 insights regrading the power and heat demands (subsection 2.1), the used climate data (subsection 2.2) and all necessary techno-economic data (subsection 2.3) are supplied. Finally, nomenclature is provided in Section 3.

1 Mathematical Modelling - LP Snapshot model

A part of the model's constraints is presented in the main manuscript and all equations are presented in this section. Since for the model a chronological time-period clustering (NPCTPC) approach is employed, the formulation is presented in a time-adaptive version where $h \in H$ are the clusters and t_h their corresponding duration.

The presented snapshot model aims to optimise the planning and operation of the integrated power & heat system in a future target year. The presented model determines:

- regarding planning, investments for: (i) capacity expansion of generation and storage technologies and (ii) transmission expansion of electricity network, for a target year , while using initial infrastructure as a starting point.
- regarding operation, decisions for optimisation of resources: (i) generation/production, (ii) transmission/transportation, (iii) storage, throughout the time horizon of the target year.

Objective function:

As the problem aims at planning and operational optimisation, the objective of the problem is to minimise the summation of annualised capital and operational costs. The objective of the problem is to minimise the total system's cost (TSC) which is comprised of: (i) the capital costs ($TotCAPEX$) and (ii) the operating costs ($TotOPEX$). eq. (1) is the objective function of the problem for a certain future target year.

$$minimise \qquad TSC = TotCAPEX + TotOPEX \tag{1}$$

As indicated by eq. (2) fixed costs include investments on generation and storage technologies as well as investments on the transmission and transportation infrastructure of the considered resources.

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These costs are discounted by the capital recovery factors of each technology $j \in J$ or transportation modes $r \in R$.

$$
\begin{aligned}
TotCAPEX = & \sum_{g \in G} \sum_{j \in J} CRF_j^{tech} \cdot C_j^{fix} \cdot Cap_{jg}^{new} \\
& + \sum_{(a,r,g,g') \in TG_{argg'}} CRF_r^{tr} \cdot C_r^{tr} \cdot TR_{argg'}^{new} \cdot \frac{DIS_{gg'}}{2}
\end{aligned} \tag{2}
$$

In particular, the costs regarding the pipeline infrastructure, even though must be modelled using binary variables to indicate decision on pipeline installation, are added to the model to take account for an approximated levelised cost of DEC transportation in the future. Capital recovery factors of each technology $j \in J$, CRF_j^{tech}, depend on the inflation rate, IR, and the corresponding economic lifetime, TP_j^{tech}, as in eq. (3). Similarly, capacity recovery factor of transmission/transportation expansion investments, CRF_r^{tr}, is defined in eq. (4).

$$
CRF_j^{tech} = \frac{IR \cdot (1+IR)^{TP_j^{tech}}}{(1+IR)^{TP_j^{tech}} - 1} \qquad \forall j \in J \tag{3}
$$

$$
CRF_r^{tr} = \frac{IR \cdot (1+IR)^{TP_r^{tr}}}{(1+IR)^{TP_r^{tr}} - 1} \qquad \forall r \in R \tag{4}
$$

The operating costs in eq. (5) include the variable costs of generation and storage charging (C_j^{var}), storing energy carriers (C_j^{stor}), fuel consumption (C_f^{fuel}), interconnection imports (or exports as earning for the system) (C_{ih}^{ic}), curtailment costs (C^{curt}) and the value of the lost load (VoLL) (C^{VoLL}). Moreover, annual costs regarding the carbon tax (C^{CO_2}) and the fixed operation and maintenance cost (O&M) of infrastructure are included as follows:

$$
\begin{aligned}
TotOPEX = \sum_{h \in H} t_h \cdot \Bigg[& \sum_{g \in G} \sum_{j \in J^{pr}} C_j^{var} \cdot P_{jgh} C_j^{var} \cdot ST_{ajgh}^{ch} + \sum_{g \in G} \sum_{(a,j) \in ST_{aj}} C_j^{stor} \cdot ST_{ajgh} \\
& + \sum_{g \in G} \sum_{j \in J^{pr}} \sum_{f:(f,j) \in FJ_{fj}} C_f^{fuel} \cdot V_{fjgh}^{elec} + \sum_{g \in G} \sum_{j \in J^{hs}} \sum_{a:(a,j) \in FJ_{fj}} C_f^{fuel} \cdot V_{fjgh}^{heat} \\
& + \sum_{(i,g) \in IG_{ig}} C_{ih}^{ic} \cdot IC_{igh} + \sum_{g \in G} C^{curt} \cdot LC_{gh} + \sum_{g \in G} C^{VoLL} \cdot LS_{gh} \Bigg] \\
& + \sum_{g \in G} \sum_{j \in J} C_j^{OM,tech} \cdot Cap_{jg} + C^{CO_2} \cdot \left(CO2^{elec} + CO2^{heat} \right)
\end{aligned} \tag{5}
$$

Heat supply chain demand:

Total heat requirement profiles are available for the wide system, $\overline{D}_{gh}^{heat}$ and can be satisfied by available heat fuels/resources. These resources are electricity, hydrogen and natural gas ($A^{hs} =$

$\{Elec, H_2, NG\}$). Thus, the breakdown of the heat requirements is determined by eq. (6):

$$\overline{D}_{gh}^{heat} = \sum_{a \in A^{hs}} \sum_{j:(a,j) \in AJ_{aj}} Q_{ajgh} \qquad \forall g \in G h \in H \tag{6}$$

The efficiencies of the end-use heat technologies determine the required net demands for the corresponding resources. For instance, efficiency of natural gas fueled or for future hydrogen-fueled technologies (η_j^{heat}) are assumed constant and equal to 90%. In contrast, the efficiency of heat pumps (COP_{gh}), which consume electricity, can be estimated beforehand based on real-world data of the ambient temperature (AT_{gh} in °C) using eq. (7) obtained by Vorushylo *et al.* [1]:

$$COP_{gh} = 0.0541 \cdot AT_{gh} + 2.6674 \qquad \forall g \in G h \in H \tag{7}$$

Fuels consumption for end-use heat technologies:

Among the considered heat fuels, consumption (V_{fjgh}^{heat}) is estimated only for the natural gas technologies as the related hydrogen and electricity-related consumption are determined internally by the model. Fuel consumption depends on the heat requirements and the technological efficiency as in eq. (8):

$$V_{fjgh}^{heat} = \frac{Q_{ajgh}}{\eta_j^{heat}} \qquad \forall a \in \{NG\}, j \in J^{hs}, f : (f,j) \in FJ_{fj}, g \in G, h \in H \tag{8}$$

Spatially explicit resource balances:

Electricity and DECs (i.e., H_2 and NH_3 for this case study) constitute the energy vectors of the supply chain. Thus, balances are defined for electricity and DECs (included in the subset $A^{ps} = \{Elec, H_2, NH_3\}$). These balances must respect both the defined temporal and spatial resolution. Towards an optimal operation of the system the goal is to satisfy energy carriers demands (D_{agh}) while considering all operation options:

1. Production/Generation: energy content of a resource is produced/generated (P_{jgh}) by appropriate technologies or can be consumed by other technologies towards their conversion to other resources,
2. Storage: a resource can be charged into the appropriate storage tank (ST_{ajgh}^{ch}) and be discharged out of it (ST_{ajgh}^{dis}),
3. Distribution: Bidirectional transmission or transportation of resources between the geographical regions ($TR_{argg'h}$) is modelled. Interconnections to third countries (IC_{igh}) are also considered only for electricity transmission.

Moreover, options such RES load curtailment (LC_{gh}) and load shedding (LS_{gh}) are taken into consideration for the power system towards electricity demand satisfaction. Hence, a generalised formulation for the energy carriers' balances is presented in eq. (9):

$$
\begin{aligned}
D_{agh} = & \sum_{j:(a,j)\in PR_{aj}} P_{jgh}\cdot\left(1-PL_j\right) - \sum_{j:(a,j)\in CON_{aj}} \frac{P_{jgh}}{\eta_j^{conv}} \\
& + \sum_{j:(a,j)\in ST_{aj}} ST_{ajgh}^{dis} - \sum_{j:(a,j)\in ST_{aj}} ST_{ajgh}^{ch} \\
& + \sum_{(r,g'):(a,r,g,g')\in TG_{argg'}} TR_{arg'gh}\cdot\left(1-DIS_{g'g}\cdot Loss_{ar}^{tr}\right) \\
& - \sum_{(r,g'):(a,r,g,g')\in TG_{argg'}} TR_{argg'h} \\
& + \left[LS_{gh}-LC_{gh}+\sum_{i:(i,g)\in IG_{ig}} IC_{igh}\cdot\left(1-Loss_{ig}^{int}\right)\right]\Bigg|_{a=\{elec\}} \\
& \forall\ a\in A^{ps}\ g\in G h\in H
\end{aligned}
\tag{9}
$$

Particularly, sets PR_{aj} and CON_{aj} contain the information regarding the production or consumption of a resource $a\in A^{ps}$ from a process $j\in J^{ps}$ respectively. A visualisation of the process network is provided in Fig S.1.

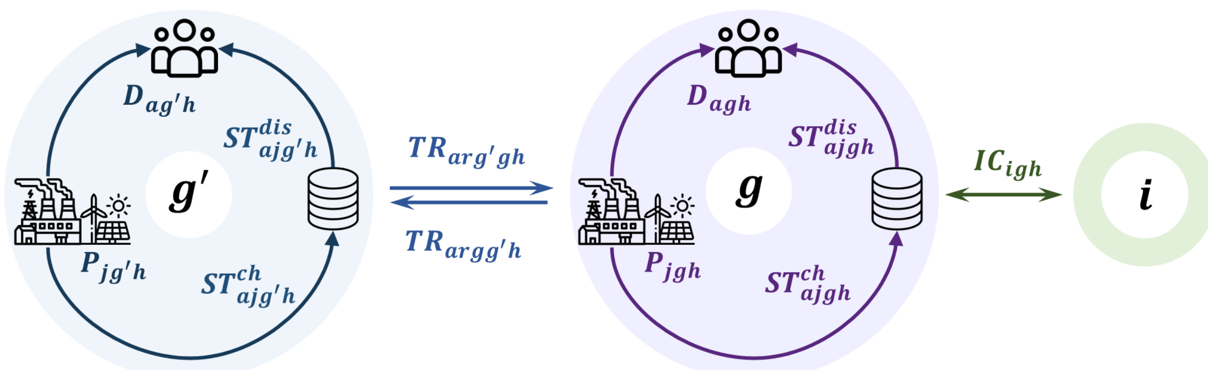


Fig. S.1 Overview of spatially explicit energy balance between regions g, g' and interconnected country i.

Energy carriers demands:

Total demands on electricity and DECs include both the net demands and the heat requirements by eq. (6). In particular, electricity constitutes the most crucial resource for the investigated system and includes the net power demand ($\overline{D}_{gh}^{elec}$) and the electricity towards heat requirements (Q_{ajgh}). Total demand is further increased by a fraction of distribution losses (DL), which quantifies the intrinsic losses in the distribution system. So, the net demand is defined in eq. (10):

$$
D_{agh} = \left[\overline{D}_{gh}^{elec} + \sum_{j\in AJ_{aj}} \left(\frac{Q_{ajgh}}{COP_{gh}}\right)\right]\cdot\left(1+DL\right) \qquad \forall\ a\in\{Elec\}, g\in G h\in H \tag{10}
$$

As solely heat requirements (Q_{ajgh}) may be satisfied by hydrogen, hydrogen's demand is defined by eq. (11). Nonetheless, zero demand is defined for ammonia (eq. (12)), as its role pertains to assist system's optimal operation as an energy storage and transportation alternative.

$$D_{agh} = \sum_{j \in AJ_{aj}} \frac{Q_{ajgh}}{\eta_j^{heat}} \qquad \forall\, a \in \{H_2\}, g \in G h \in H \tag{11}$$

$$D_{agh} = 0 \qquad \forall\, a \in \{NH_3\}, g \in G h \in H \tag{12}$$

Capacity allocation constraints:

Firstly, the installation of a technology/process $j \in J$ in region $g \in G$ is constrained to be lower than a maximum allowable bound (a minimum bound is not considered). As a simplified LP snapshot model is formulated, all technologies' capacities are determined by continuous variables ($Cap_{jg}, j \in J$) and maximum bounds are set by eq. (13):

$$Cap_{jg} \leq Cap_{jg}^{max} \qquad \forall j \in J, g \in G \tag{13}$$

Then, total newly installed capacity of a certain technology in the wide system have to be constrained by the maximum bounds that are imposed by assumed build rates (BR_j) as indicated by eq. (14)[2].

$$\sum_{g \in G} Cap_{jg}^{new} \leq BR_j \qquad \forall j \in J \tag{14}$$

In particular, capacity of renewable technologies are further constrained by land availability data (LA_{jg}) which are available in[3]:

$$Cap_{jg} \leq Cap_{jg}^{ini} + LA_{jg} \qquad \forall j \in J^{res}, g \in G \tag{15}$$

Note that maximum capacities of technologies per region (Cap_{jg}^{max}) are estimated by multiplying the building rates with penetration factors of each technology for a certain region, PF_j (e.g. $Cap_{jg}^{max} = PF_j \cdot BR_j$). Finally, eq. (16) estimates the installed capacity of each technology $j \in J$ per region $g \in G$ accounting for the initially installed, newly installed and planned decommissioned plants.

$$Cap_{jg} = Cap_{jg}^{ini} - Cap_{jg}^{dec} + Cap_{jg}^{new} \qquad \forall j \in J, g \in G \tag{16}$$

Renewable energy generation:

Generated renewable energy strongly depends on the intermittent wind speed and solar irradiation. Hence, the former is estimated using temporal and spatial data of renewable availability (AV_{jgh}) as a rate of the installed capacity in eq. (17). However, a fraction of the generated load may be curtailed (LC_{gh}). Thus, eq. (18) constraints the curtailed amount to be at most equal to the total renewable power generated.

$$P_{jgh} = AV_{jgh} \cdot Cap_{gj} \qquad \forall j \in J^{res}, g \in G, h \in H \tag{17}$$

$$LC_{gh} \leq \sum_{j \in J^{res}} P_{jgh} \qquad \forall g \in G, h \in H \tag{18}$$

Fuel consumption & availability:

Fuel consumption on power system (V^{elec}_{fjgh}) is estimated using the production/generation levels (P_{jgh}) and the efficiencies of the technologies (η^{tech}_j) as in eq. (19):

$$V^{elec}_{fjgh} = \frac{P_{jgh}}{\eta^{tech}_j} \qquad \forall j \in J^{ps}, f : (f, j) \in FJ_{fj}, g \in G, h \in H \tag{19}$$

The availability of biomass fuels in the future can be considered limited (BA). Biomass feedstock availability is modelled through eq. (20).

$$\sum_{j \in J^{bio}} \sum_{g \in G} \sum_{h \in H} \frac{t_h \cdot P_{jgh}}{\eta^{tech}_j} \leq BA \tag{20}$$

Generation and Production limits:

Generation bounds enforce the maximum allowable rates of operation (P^{max}_j) of each technology $j \in J$. As the technologies' capacities are continuous variables, bounds are defined on their total capacity as in eq. (21):

$$P^{min}_j \cdot Cap_{jg} \leq P_{jgh} \leq P^{max}_j \cdot Cap_{jg} \qquad \forall j \in \left(J^{pr} \cup J^{con}\right), g \in G, h \in H \tag{21}$$

However, strict implementation of the minimum bounds (P^{min}_j) in eq. (21) impose hard constraints for the minimum operation level of the processes.

Ramping limits:

Ramping up and down limits (RU_j & RD_j) are defined for the generation or production processes. In this way, the production rates are enforced to obey to maximum allowable changes from their state in the previous time period. Time adaptive constraints for the allowable ramping rates are estimated as in Eqs. (22) - (23).

$$P_{jgh} - P_{jg,h-1} \leq min\left\{t_h \cdot RU_j, P^{max}_j\right\} \cdot Cap_{jg} \qquad \forall j \in J^{pr}, g \in G, h \in H \tag{22}$$

$$P_{jg,h-1} - P_{jgh} \leq min\left\{t_h \cdot RD_j, P^{max}_j\right\} \cdot Cap_{jg} \qquad \forall j \in J^{pr}, g \in G, h \in H \tag{23}$$

As detailed unit commitment is not covered in this work. Eqs. (22) - (23) are sufficient to set the ramping limits considering one state of operation.

Transmission, Transportation, and Interconnections constraints:

Electricity transmission and DECs transportation between geographical regions using transportation modes $r \in R$ is constrained by the corresponding capacity ($TR^{cap}_{argg'}$) as in eq. (24). Especially, expansion of the existing infrastructures $TR^{ini}_{argg'}$ is modelled through new investment variables $TR^{new}_{argg'}$.

Capacity estimations are enforced through Eqs. (25) - (26).

$$TR_{argg'h} \leq TR^{cap}_{argg'} \qquad \forall (a,r,g,g\prime) \in TG_{argg'}, h \in H \tag{24}$$

$$TR^{cap}_{argg'} = TR^{ini}_{argg'} + TR^{new}_{argg'} \qquad \forall (a,r,g,g\prime) \in TG_{argg'} \tag{25}$$

$$TR^{cap}_{argg'} = TR^{cap}_{arg'g} \qquad \forall (a,r,g,g\prime) \in TG_{argg'} \tag{26}$$

Upper bounds on transmission/transportation capabilities differs for the DECs. On the one hand, for electricity an expansion of existing lines can be considered through the continuous variables $TR^{new}_{argg'}$. DECs pipeline infrastructure investments are modelled through discrete variables which indicate decisions regarding the installation of pipelines between two regions. However, such binary variables could increase significantly the computational burden. In this model, in order to approximate the transportation cost for the DECs and to evaluate the usefulness of transportation capabilities for DECs we model them through continuous variables. This simplification allows the formulation of a simplified LP problem and an approximated levelised cost regarding the DEC transportation is estimated. Eq. (27) defines the transmission expansion constraints.

$$TR^{new}_{argg'} \leq TR^{max}_{argg'} \qquad \forall a \in A^{ps}, (r,g,g\prime) : (a,r,g,g\prime) \in TG_{argg'} \tag{27}$$

Finally, regarding interconnections, the variable (IC_{igh}) is employed to model the bi-directional transmission of electricity between LDZs of Great Britain and the interconnected countries in eq. (28).

$$-IC^{cap}_{ig} \leq IC_{igh} \leq IC^{cap}_{ig} \qquad \forall (i,g) \in IG_{ig}, h \in H \tag{28}$$

Storage constraints:

The proposed model considers available storage for all energy carriers $a \in A^{ps}$. Storage level for each resource is estimated by eq. (29):

$$\begin{aligned} ST_{ajgh} = {} & ST^{ini}_{ajg} \big|_{h=1} + \left(1 - t_h \cdot \eta^{loss}_{aj}\right) \cdot ST_{ajg,h-1}\Big|_{h>1} \\ & + \left(t_h \cdot \eta^{ch}_{aj}\right) \cdot ST^{ch}_{ajgh} - \left(\frac{t_h}{\eta^{dis}_{aj}}\right) \cdot ST^{dis}_{ajgh} \\ & \forall (a,j) \in ST_{aj}, g \in G, h \in H \end{aligned} \tag{29}$$

As storage technologies' capital costs can practically be evaluated based on either their power rating or their capacity (in MW or MWh respectively), different approaches are implemented for electricity storage and the storage of DECs. BESS modelling data regarding the energy to power ratio (EP_{aj}, alternatively mentioned as storage duration) are used (Eqs. (30)-(32)).

$$ST_{ajgh} \leq EP_{aj} \cdot Cap_{jg} \qquad \forall a \in \{Elec\}, j : (a,j) \in ST_{aj}, g \in G, h \in H \tag{30}$$

$$ST^{ch}_{ajgh} \leq Cap_{jg} \qquad \forall a \in \{Elec\}, j : (a, j) \in ST_{aj}, g \in G, h \in H \tag{31}$$

$$ST^{dis}_{ajgh} \leq Cap_{jg} \qquad \forall a \in \{Elec\}, j : (a, j) \in ST_{aj}, g \in G, h \in H \tag{32}$$

DECs storage investment costs are evaluated based on their capacity, Cap_{jg}, and consequently storage constraints in Eqs. (33)-(35) are defined using data for their maximum charging and discharging fractions.

$$ST_{ajgh} \leq Cap_{jg} \qquad \forall a \in \{H_2, NH_3\}, j : (a, j) \in ST_{aj}, g \in G, h \in H \tag{33}$$

$$ST^{ch}_{ajgh} \leq ST^{ch,max}_{aj} \cdot Cap_{jg} \qquad \forall a \in \{H_2, NH_3\}, j : (a, j) \in ST_{aj}, g \in G, h \in H \tag{34}$$

$$ST^{dis}_{ajgh} \leq ST^{dis,max}_{aj} \cdot Cap_{jg} \qquad \forall a \in \{H_2, NH_3\}, j : (a, j) \in ST_{aj}, g \in G, h \in H \tag{35}$$

An interesting aspect of storage modelling concerns the initial storage levels of the resources (ST^{ini}_{ajg}). Especially, ammonia's role for seasonal storage is to be evaluated and consequently its initial level is aimed to be optimally determined by the model. In contrast, electricity and hydrogen are assumed beforehand to be suitable for short- or mid-term storage. Hence, initial levels are trivially fixed equal to 50% of the capacity. Finally, the storage level at the end of the time horizon is enforced to be equal to the initial storage level for all resources in eq. (38).

$$ST^{ini}_{ajg} \leq Cap_{jg} \qquad \forall a \in \{NH_3\}, j : (a, j) \in ST_{aj}, g \in G \tag{36}$$

$$ST^{ini}_{ajg} = 0.5 \cdot Cap_{jg} \qquad \forall a \in \{A^{ps}\}, j : (a, j) \in ST_{aj}, g \in G \tag{37}$$

$$ST_{ajgh}\big|_{h=H} = ST^{ini}_{ajg} \qquad \forall (a, j) \in ST_{aj}, g \in G \tag{38}$$

System-wide peak demand:

Constraints in this part secure the adequacy of the system. Towards this goal the system-wide peak demand of electricity, D^{peak}, must be estimated for the integrated system as shown in eq. (39).

$$D^{peak} \geq \sum_{g \in G} D_{agh} \qquad \forall h \in H, a \in \{Elec\} \tag{39}$$

Considering the de-rating factors of interconnection lines (DF^{inter}_i), and generation and storage technologies (DF_j) the total de-rated capacity must exceed system's peak increased by a capacity reserve margin factor (RM) as in eq. (40). In this work, as operating reserve modelling is neglected, a higher de-rated capacity margin equal to 7% is adopted.

$$D^{peak}(1+RM) \leq \sum_{g\in G, j:(a,j)\in\left(ST_{a,j}\cup PR_{a,j}\right)} DF_j \cdot Cap_{gj} + \sum_{(i,g)\in IG_{ig}} DF_i^{inter} \cdot IC_{ig}^{cap} \qquad a \in \{Elec\} \tag{40}$$

Carbon emissions constraints:

Power sector's emissions include fuel consumption for both electricity generation and DECs production, which introduce pathways for excessive energy storage. These are estimated accounting for the fuel consumption (V_{fjgh}^{elec}), carbon capture rates (CCS_j) and the fuels' emission factors (ε_f). Similarly for the heat sector, only the natural gas supplied to heat sector is consider to emit CO_2. Moreover, negative carbon budget is defined and an emission factor for the CO_2 equivalent amount captured in fuels is set (ε_f^{neg}). All constraints are defined in Eqs. (41) - (44).

$$CO2^{elec} = \sum_{j\in J^{pr}} \sum_{f:(f,j)\in FJ_{fj}} \left[\varepsilon_f \cdot \left(1-CCS_j\right) \cdot \sum_{g\in G}\sum_{h\in H} t_h \cdot V_{fjgh}^{elec}\right] \tag{41}$$

$$CO2^{heat} = \sum_{j\in J^{hs}} \sum_{f:(f,j)\in FJ_{fj}} \left(\varepsilon_f \cdot \sum_{g\in G}\sum_{h\in H} t_h \cdot V_{fjgh}^{heat}\right) \tag{42}$$

$$CO2^{neg} = \sum_{j\in J^{neg}} \sum_{f:(f,j)\in FJ_{fj}} \left(\varepsilon_f^{neg} \cdot CCS_j \cdot \sum_{g\in G}\sum_{h\in H} t_h \cdot V_{fjgh}^{elec}\right) \tag{43}$$

$$CO2^{elec} + CO2^{heat} - CO2^{neg} \leq \overline{CO2} \tag{44}$$

2 Supplementary data

In this section the data and further assumptions for the implementation of the proposed model are reported. Initially, some insights regarding the power and heat demand in GB are presented in subsection 2.1. Moreover, climate data for the UK are given in subsection 2.2. Then, all techno-economic data for the implementation of the model are reported in subsection 2.3

2.1 Demand data

The total annual electricity annual demand is predicted for 2040 to 345 TWh according to "System Transformation" scenario of the Future Energy Scenarios by National Grid ESO[4]. It is mentioned that the historical data from National Grid cover the whole Great Britain. In Fig. S.2 is visualised the profile of the total daily electricity demand for Great Britain throughout the year. In this figure the seasonality of the power demand can be noticed, as power demand is crucially increased during the winter months. Moreover the minimum, median and maximum values of total daily demand indicate the range of power demand variation throughout the year.

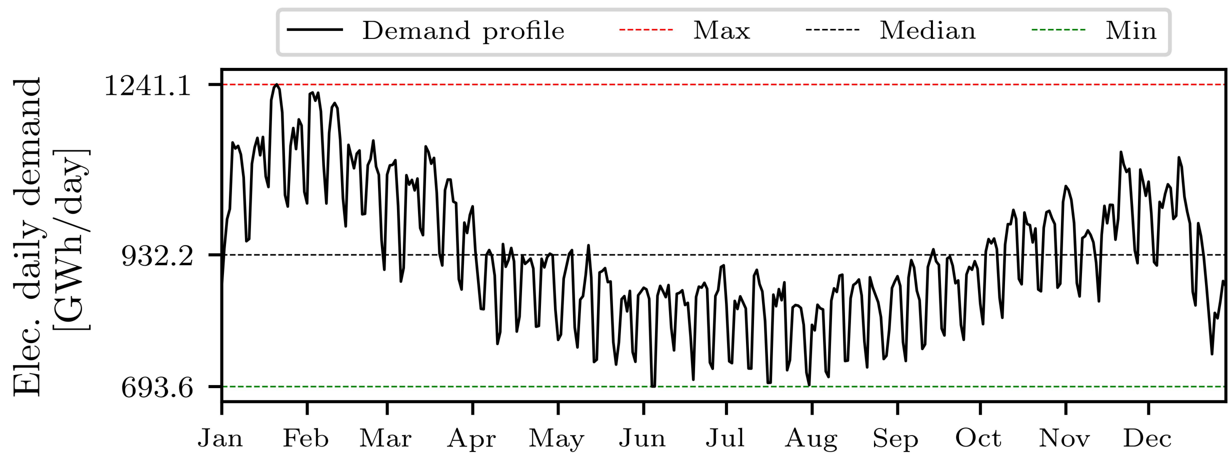


Fig. S.2 Profile of predicted total daily electricity demand for GB in 2040 based on 2015 historical data.

As the original historical data concern the total demand in GB, statistical data from DUKES of BEIS are used to estimate the demand allocation to the Local Distribution Zones[5,6]. These data are reported in Table S.1.

Table S.1 Electricity demand allocation per region[5].

LDZ	**EA**	**EM**	**NE**	**NO**	**NT**	**NW**	**SC**	**SE**	**SO**	**SW**	**WM**	**WN**	**WS**
Share [%]	9.6	7.5	6.5	5.0	13.9	12.1	8.9	2.9	10.9	8.6	8.7	1.5	3.9

Regarding heat demand, the total annual heat requirements are estimated for 2040 to 526 TWh according to data by National Grid ESO[4], CCC[7],[8] while the original hourly spatial profiles regarding the heat demand are adapted from the gas distribution companies and the work by Charitopoulos *et al.*[9]. In Fig. S.3 is visualised a heatmap of the daily heat demand in the LDZs throughout the year. From this heatmap, a big decline in heat demand is observed during the summer months in all LDZs. Even though heat demand data present similar seasonality pattern to the power demand data, the reduction of heat demand is even more steep and very low heat demand exists during the summer months. During the winter months, the demand is high in the more populated regions (e.g., NT, NW, WM) and a correlation between high heat demands and the electricity demand's allocation rates can be observed. In other words, regions with high electricity demand have also high heat requirements.

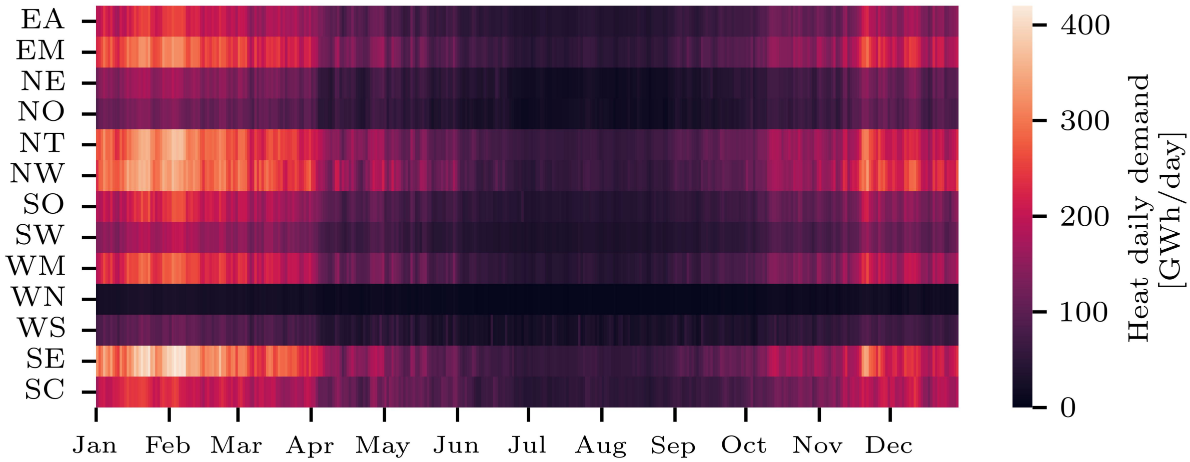


Fig. S.3 Profile of predicted daily heat demand for the LDZs of GB in 2040 based on 2015 historical data.

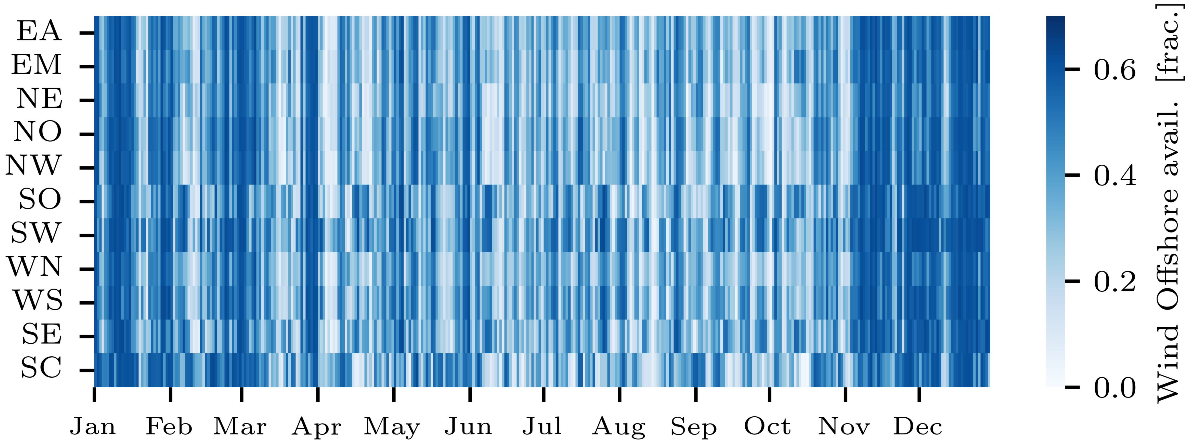
2.2 Climate data

Regarding renewable energy sources (RES) availability (e.g., wind and solar profiles), data from Renewables.Ninja platform is exploited to obtain specific profiles for each LDZ[10]. Then, year 2015 is adopted as the climate basis year and the proposed model is calibrated to the real operation of year 2015. In this context, the proposed model is implemented for year 2015 taking account of the aforementioned datasets on the real GB power system with 2015 infrastructure data estimated by BEIS[5]. The calibration of the model assists the correction of parameters towards a flawless simulation of the real operation of 2015's power system. Thus, RES availability and interconnection availability are calibrated towards a perfect simulation of 2015 power system operation. In Fig. S.4 are visualised the daily average profiles of RES availability for the LDZs of GB for 2015.

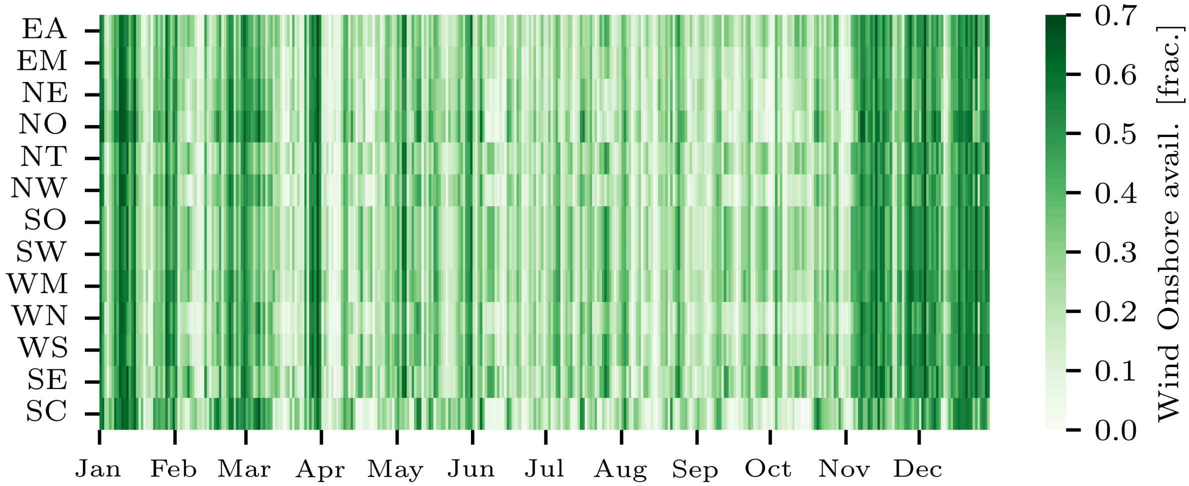
Regarding the availability of wind technologies, a correlation between the variation of availability for onshore and offshore farms can be observed (in Figs. S.4a-S.4b). However, the load factors of the historical data indicate that wind offshore farms can lead to significantly higher load factors (approximately 28% & 41% annual load factors for onshore and offshore wind technologies for 2015). Moreover, the spatial details are of particular interest as indicate the competency of the regions to offer high availability. Regarding offshore wind availability, Scotland (SC) and South West (SW) can achieve slightly higher annual load factors than the other regions (approximately 42% for 2015). Moreover, for onshore wind availability the southern regions (e.g., SE, SW, WS) lead to the highest annual load factors (approximately 31% for 2015). Finally, wind availability also presents seasonality as for the winter months higher availability is observed, while during the summer months a slight decline is observed.

Regarding the availability of solar technologies, the seasonality pattern is more intense. In particular, solar availability is much lower during the winter months and it significantly increases during the summer months. Overall, an annual load factor of approximately 10% is achieved for 2015. Similarly to onshore wind availability, the southern regions (e.g., SE, SW, SO) offer significantly availability. On contrary, Scotland (SC) offers the lowest solar availability, which can be also observed in the heatmap of Fig. S.4c.

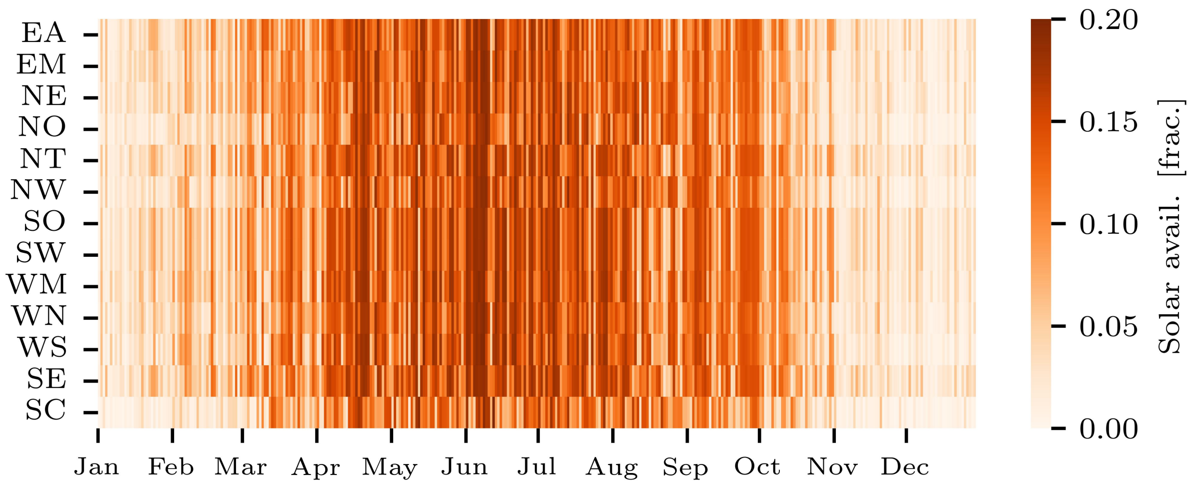
Finally, the ambient temperature is another important climate parameter as COP of heat pumps



(a) Daily mean availability of offshore wind farms.



(b) Daily mean availability of onshore wind farms.



(c) Daily mean availability of solar farms.

Fig. S.4 Heatmaps of the daily mean availability of RES in the LDZs throughout year 2015.

depends on the temperature through Eq. (7). So the profiles of average COP values for the LDZs in 2015 are presented in S.5. Regarding COP there is also a seasonal pattern for the values ans during the cold winter months COP values are reduced. Another important outcome regards the spatial detail: southern regions tend to report higher values of COP, while northern regions consistently lower values of COP with Scotland to be a typical example of this pattern.

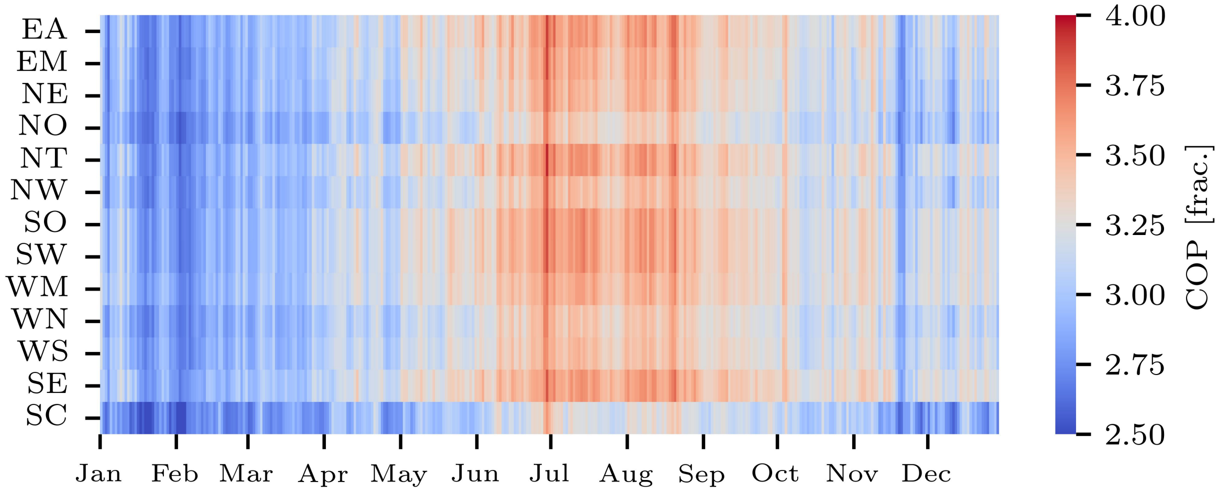


Fig. S.5 Heatmaps of the daily mean COP values in the LDZs throughout year 2015.

2.3 Techno-economic data

It is mentioned that all energy-related data given, are calculated for the Lower Heating Values (LHV) and are based on the output of the technologies. As the case study examines the energy system of Great Britain, the intention of the authors was to use as many data as possible from sources specialised for the UK. For instance, future predictions on CAPEX prices are taken from UK-based sources by governmental sources [11,12]. Moreover, an inflation rate of 7% (IR=0.07) is adopted for the UK.

Moreover, calculations on CCC [13] data the carbon goal in 2040 according to Net Zero trajectory is set to 7.875 $MtCO_2$, while the carbon tax is set equal to 118.75 £/tCO_2. Finally the cost of curtailed energy is set 220 £/MWh and the Value of Lost Load (VoLL) is equal to 17,500 £/MWh [14,15]

Regarding renewable generation technologies, techno-economic data include the capital and operating cost as well as historical data regarding their availability (de-rating factors) and performance (load factor) in the system. In particular, renewable technologies generation is calibrated to much the historical values. Some indicative historical mean values for the load factors are also reported in Table S.2.

Table S.2 Techno-economic specifications of renewable technologies[5,12,16].

Specification	Offshore Wind	Onshore Wind	Solar PV	Hydro
CAPEX [£K/MW][12]	1594	1304	610	-
Lifetime [years][12]	30	25	30	-
O&M cost [£K/MW-year][12]	89.2	31.3	7.7	-
Variable cost [£/MWh][12]	0	0	0	-
De-rating factor [%][16]	8.3	6.7	5.0	91.1
Mean UK load factor [%][5]	38.4	26.6	10.7	36.4

Regarding the conventional generation technologies the data on Table S.3 contain all the necessary information for the implementation of the proposed mathematical model and the operational optimisation.

Table S.3 Techno-economic specifications of conventional electricity generation technologies[12,17,18]

Specification	Nuclear	CCGT	CCGTCCS	Biomass	BECCS
Fuel	Uranium	Gas	Gas	Biomass	Biomass
Efficiency [% LHV]	40.0	58.7	52.0	36.0	29.0
Parasitic load [%]	9.2	1.7	12.0	5.1	20.0
Min load [%]	50	35	50	40	50
Max load [%]	88	87	80	80	80
Committed ramp up[%/h]	10	100	100	30	30
Committed ramp down[%/h]	10	100	100	30	30
CO_2 capture [%]	-	-	90	-	90
Capital cost [£K/MW]	4,343	624	1,425	2,698	5,885
Lifetime [years]	60	25	25	25	25
O&M cost [£K/MW-year]	83.40	20.20	28.30	102.9	150.3
Variable cost [£/MWh]	5	2	5	7	4

As detailed data regarding H_2 or NH_3-fueled generation technologies are limited, we follow the assumptions from the literature. For instance, CAPEX is estimated considering a 10% increase from conventional CCGT price. This is adopted for both H_2- or NH_3-CCGT based on the works by Fasihi *et al.*[19] and Cesaro *et al.*[20], respectively. Moreover, it is assumed that the aforementioned technologies have the same HHV efficiency ratio to the conventional CCGT. The rest techno-economic parameters are assumed the same as for CCGT.

Table S.4 Techno-economic specifications of H_2 or NH_3 - fueled electricity generation technologies[19,20]. Characteristics not mentioned are assumed same as for conventional CCGT.

Specification	H_2-CCGT	NH_3-CCGT	Notes
Fuel	H_2	NH_3	
Efficiency [% LHV]	62.6	63.1	Assumed same HHV as CCGT
Capital cost [£K/MW]	686	686	Assumed 10% increased

Moreover, the data regarding the DEC production technologies are crucial towards the solution of the problem. These technologies are not yet built at large scale and so specific data regarding their operation are limited. All aforementioned technologies are assumed to produce H_2 at 3 MPa[21]. This is an important assumption for the calculation of variable cost regarding NH_3 production and storage which require H_2 at a higher pressure.

Finally, Haber-Bosch (HB) process for ammonia production is a well-established process and techno-economic data are available in literature sources[22]. Here, the Haber-Bosch process values are assumed to contain the costs and electricity consumption for the accompanying air separation units (ASU) for nitrogen (N_2) production which is necessary for the ammonia production. We consider 100% conversion of raw materials to NH_3 which leads to a process efficiency of 87.8% of the H_2 energy input, i.e. 87.8% of the energy of the input H_2 is converted to ammonia energy (all values LHV). . However, the electricity consumption is also significant in the HB process. HB and ASU combined require 0.64 kWh/kg$_{NH_3}$ and pre-compression of H_2 to requires 0.26 kWh/kg$_{NH_3}$. These constitute the 12.4% of the LHV of the output. So this information can be incorporated in the model with two ways: either (i) introduce the necessary electricity consumption in the electricity balance to be accounted as region-specific demand or (ii) estimate the variable operational cost considering a firm-up electricity cost of 90 £/MWh. As the expected necessary power amount is proven to be insignificant to the total system's demand, the second way is selected to approximate the electricity cost. Through this way, it is achieved to not computationally burden the model and a variable operational cost of £10.1/MWh of output is set.

Table S.5 Techno-economic specifications of DEC production technologies.

Specification	SMRCCS [11,21]	BGCCS [11,21]	WE [11,21]	HB [22]
Fuel	Gas	Biomass	Electricity	H_2
Product	H_2	H_2	H_2	NH_3
Efficiency/Conversion [% LHV]	69.5	61.0	71.0	87.8
Min load [%]	50	50	10	40
Max load [%]	100	100	100	100
Committed ramp up[%/h]	10	30	100	20
Committed ramp down[%/h]	10	30	100	20
CO_2 capture [%]	90	90	-	-
Capital cost [£K/MW]	571	1,295	553	687
Lifetime [years]	40	25	30	30
O&M cost [£K/MW-year]	33.1	48.0	33.91	13.74
Variable cost [£/MWh]	0.11	8.52	3.31	10.1*

All aforementioned technologies are considered to consume certain type of fuel. Fuels' characteristics are very important for both economic evaluation and the considerations of decarbonisation. In the Table S.6 predictions for the prices and the emission factors for the calculation of the CO_2 emissions depending on the generation levels are reported. Regarding H_2 and NH_3 neither price nor additional emission are considered. While the former is correct because DEC are produced within the system, the latter is correct by assuming that the DEC consuming technologies are accompanied by Selective Catalytic Reduction (SCR) systems which will efficiently handle the particularly harmful nitrogen oxides (NO_x)[23]. However, it is noted that the assumption for zero emissions for hydrogen or ammonia combustion may be optimistic simplification as a life cycle assessment is out of the scope of this work[24]. Finally limited availability is assumed for the biomass fuels, and a scenario analysis is conducted[13].

Table S.6 Techno-economic specifications of fuels[4,25].

Specification	Uranium	Natural Gas	Biomass	H_2	NH_3
Price [£/MWh]	5	22.5	25	-	-
Emission factor [tCO_2/MWh]	0	0.2038	0.0105	0	0
Negative emission's factor [tCO_2/MWh]	0	0.2038	0.3500	0	0
Availability [TWh]	∞	∞	Limited	-	-

One storage technology is adopted for each of the studied resources. As mentioned during the model description, electricity storage (BESS) is evaluated based on the power rating (in MW), while DEC storage is evaluated based on the total energy storage capacity (in MWh). For the latter, variable operational costs are imposed on both the charging - due to compression as DEC are assumed to be produced at 3 MPa - and the storage of DEC - due to refrigeration of the stored amounts. Electricity consumption for these tasks can be found in the work by Wang *et al.*[26] and Bartels[27]. As proposed for the HB operational costs, such consumption is interpreted to the variable operational cost assuming a firm-up electricity cost of 90 £/MWh. The values are reported in the Table S.7.

Table S.7 Techno-economic specifications of storage technologies.

Specification	BESS[28]	Liquid H_2[26,29,30]	Liquid NH_3[26,29–31]
Round-trip efficiency [%]	85	100	100
Charging efficiency [%]	92.2	100	100
Discharging efficiency [%]	92.2	100	100
Self-discharge [%/day]	0.3	0.1	0.03
Energy to power ratio [h]	4	-	-
Max charge [% Capacity / h]	-	10	10
Max discharge [% Capacity / h]	-	10	10
Capital cost [£K/MW]	614	-	-
Capital cost [£K/MWh]	-	21	0.12
Lifetime [years]	15	30	30
O&M cost [£K/MW-year]	6.7	-	-
O&M cost [£K/MWh-year]	-	0.84	0.0036
Variable cost (charging) [£/MW]	2	15	0.05
Variable cost (stored level) [£/MWh]	-	10^{-4}	10^{-5}

Focusing on the resources' transmission and transportation infrastructure, this work determines the transmission expansion for the future target year. In particular, for electricity transmission the existing network of transmission lines between the LDZs is taken into consideration as initial infrastructure[32]. Then, regarding the investments on transmission and transportation infrastructure, Tables S.8 and S.9 contain data concerning the transmission expansion of the electricity grid and DEC transportation infrastructure between the regions, respectively.

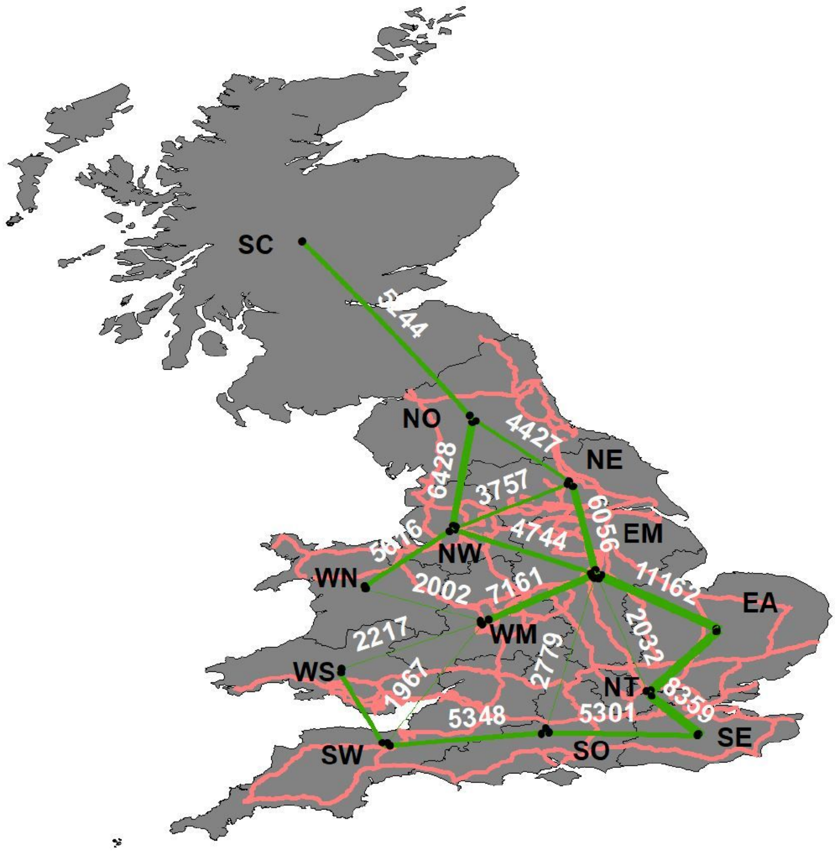


Fig. S.6 Initial network for electricity transmission between LDZs: (i) green lines represent the transmission lines between the centroids of the LDZs in 2020 and their corresponding capacities in MW[32], (ii) red lines indicate the gas distribution network.

Table S.8 Interregional electricity transmission & expansion[33].

Transmission Specifications	Value
CAPEX [£/MW/km]	247
Transmission losses [% /100km]	1
Lifetime [years]	40

Table S.9 Interregional DEC transportation.

Specifications	H_2 [34]	NH_3 [31]
Mode	Pipelines	Pipelines
Maximum flow [MW]	2294	400
CAPEX [10^6£/km]	1.60	0.10
Lifetime [years]	50	50

Finally, data on the structure of interconnections of GB for the year 2040 are presented in Table S.10.

Table S.10 GB interconnections data[16,35,36].

Interconnection	Market connected	LDZ connected	Capacity [GW]	De-rating factor [%]	Thermal losses [%]
IFA	France	SE	2.0	66	1.17
Moyle	Irish SEM	SC	0.5	54	2.36
BritNed	Netherlands	SE	1.0	61	3.45
EWIC	Irish SEM	WN	0.5	54	4.68
NEMO	Belgium	SE	1.0	64	2.67
Eleclink	France	SE	1.0	66	2.08
IFA2	France	SO	0.5	66	4.68
NSS	Norway	NO	1.5	83	7.98
Greenlink	Irish SEM	WS	0.5	54	3.30
Fablink	France	SW	1.4	66	4.68
Vikinglink	Denmark	EM	1.0	55	6.90
Northconnect	Norway	SC	1.4	83	7.35

Apart form the techno-economic specification for the solution of the model, the specific data regarding the construction of scenarios are additionally provided. The limits on build rates and biomass availability are reported in Table S.11 and the cases on the predicted load factors are reported in S.12. The load factors are imposed into modelling using appropriate calibration factors and thus the precise resulted load factor value may vary due to planning decisions.

Table S.11 Assumptions on build rates and biomass availability for the defined scenarios[2,13].

Scenarios	Balanced	RES Innovation	NonRES Innovation	CCS Slow Progression	Biomass Shortage
			BR_j [GW]		
BECCS	7.5	6.0	10.0	5.0	7.5
BGCCS	7.5	6.0	10.0	5.0	7.5
Biomass	9.8	9.8	9.8	9.8	9.8
CCGT	15.0	15.0	15.0	15.0	15.0
CCGTCCS	15.0	10.0	20.0	7.5	15.0
H_2CCGT	10.0	7.5	12.5	12.5	10.0
Haber-Bosch	10.0	7.5	12.5	12.5	10.0
NH_3CCGT	10.0	7.5	12.5	12.5	10.0
Nuclear	10.8	7.8	13.8	13.8	10.8
SMRCCS	12.5	7.5	16.0	7.5	12.5
WE	10.0	7.5	12.5	12.5	10.0
Solar	60.0	80.0	40.0	80.0	60.0
Offshore Wind	60.0	80.0	80.0	80.0	60.0
Onshore Wind	60.0	80.0	40.0	80.0	60.0
BESS	60.0	80.0	45.0	80.0	60.0
Total Thermal	58.1	48.6	68.6	51.1	58.1
			BA [TWh]		
Biomass	134.35	134.35	134.35	134.35	61.39

Table S.12 Assumptions for renewable technologies future load factors cases[37].

Load factors [%]	L - case	M - case	H - case
Solar	11.0	11.0	11.0
Offshore Wind	47.5	55.4	63.4
Onshore Wind	31.9	36.9	42.1

3 Nomenclature

Indices

a	power and heat system resources
f	fossil fuels
g,g'	geographical regions
h,h'	time periods/clusters
i	interconnected countries

j	technologies/processes
n	clustering parameters
r	transportation modes

Sets

A	set of power system resources
F	set of fossil fuels
G	set of geographical regions
H, H'	set of time periods
I	set of interconnected countries
J	set of technologies/processes
N	set of parameters of original time series
R	set of transportation modes
A^{ps}	subset of resources for the power system
A^{hs}	subset of resources for the heat system
J^{hs}	subset of end-use heat system technologies
J^{neg}	subset of technologies/processes, which contribute to negative carbon budgets
J^{pr}	subset of production technologies/processes
J^{st}	subset of storage technologies/processes
J^{th}	subset of thermal generation technologies/processes
AJ_{aj}	subset of heat fuels $a \in A^{hs}$ that are consumed in process j
CON_{aj}	subset of processes j that consume power supplied by the system of resource a
FJ_{fj}	subset of fuels f that are consumed in process j
IG_{ig}	subset of connections between interconnected countries i and regions g for electricity transmission
PR_{aj}	subset of technologies j which contribute power on the system as resource a
SA_{aj}	subset of storage technologies j which can store resource a
$TG_{argg'}$	subset of transportation modes r which are available for transmission/transportation of resource a between regions g, g'

Parameters

AT_{gh}	Ambient temperature in region g during time period h [$^{\circ}C$]
AV_{gjh}	Availability of renewable sources regarding technology j at region g in hour h
BA	Availability of biomass fuel feedstock [MWh (LHV)]
BR_j	Capacity bound for technology $j \in J^{con}$ due to building rates [MW]
C^{CO_2}	Carbon emission tax [£/MtCO_2]
C^{curt}	Cost regarding curtailment of renewable energy [£/MWh]
C_j^{fix}	Fixed capital cost of investment of technology j [£/MW or £/MWh]
C_j^{fuel}	Cost of fuel f [£/MWh]

C_j^{int}	Price of electricity transmission from/to interconnected countries i in time period h [£/MWh]
C_r^{tr}	Capital cost of transmission/transportation infrastructure investment regarding transportation mode r [£/MW]
$C_j^{OM,tech}$	Operation and Maintenance (O&M) cost of installed technology j [£/MW]
C_j^{var}	Variable operational cost of production/storage technology j [£/MW]
C^{VoLL}	Value of Lost Load (VoLL) regarding electricity shedding [£/MWh]
Cap_j^{dec}	Capacity of technology j to have been decommissioned till study year [MW]
Cap_{jg}^{ini}	Capacity of technology j initially installed [MW]
Cap_{jg}^{max}	Maximum capacity of technology j in region g [MW]
COP_{gh}	Coefficient of performance for heat pumps in region g during time period h [-]
$\overline{CO2}$	CO_2 emissions goal [MtCO_2]
CCS_j	Fraction of CO_2 removed by emissions of technology j [%]
CRF_j^{tech}	Capacity recovery factor regarding investments of technology j [%CAPEX/year]
CRF_r^{tr}	Capacity recovery factor regarding investments of infrastructure of mode r [%CAPEX/year]
$\overline{D}_{gh}^{elec}$	Electricity demand in region g during time period h [MW]
$\overline{D}_{gh}^{heat}$	Heat demand in region g during time period h [MW]
$DIS_{gg'}$	Distance between the centroids of two regions g, g' [km]
DL	Distribution losses on the electricity network as a fraction of total electricity demand [%]
DF_j	De-rating factor of technology j [%]
DM_h	Dissimilarity measure of cluster h [%]
EP_{aj}	Energy to power ratio for power storage [hours]
h_{min}	Index of cluster with the minimum dissimilarity measure between it and its successive cluster
h_{rem}	Index of cluster with the minimum dissimilarity measure between it and its precedent cluster
IC_{ig}^{cap}	Capacity of interconnection line from/to country i to/from region g
IR	Interest rate [%]
LA_{jg}	Capacity bound of technology $j \in J^{res}$ in region g due to land availability [MW]
$Loss_{ar}^{tr}$	Losses during transportation of resource a using mode a [%/km]
$Loss_{ig}^{int}$	Losses during interconnection between country i and region g [%]
NC	Number of clusters in clustering algorithm
P_j^{max}	Maximum level of production/generation of technology $j \in J^{pr}$ [%]
P_j^{min}	Minimum level of production/generation of technology $j \in J^{pr}$ [%]
PL_{nh}	Priority levels for each parameter n at time period h
PF_{jg}	Capacity allocation factor of technology $j \in J$ in region g [%]
RD_j	Ramping down rate of technology j [%]
RM	Reserve margin for total capacity of power supply chain [%]
RU_j	Ramping up rate of technology j [%]

$ST_{aj}^{ch,max}$	Maximum charging rate of storage technology j of resource a [%]
$ST_{aj}^{dis,max}$	Maximum discharging rate of storage technology j of resource a [%]
t_h	Duration of time period/cluster h [hours]
TP_j^{tech}	Economical lifetime of investment of technology j [years]
TP_r^{tr}	Economical lifetime of infrastructure investment of mode r [years]
$TR_{argg'}^{ini}$	Initially installed transmission/transportation capacity of mode r for resource a between regions g, g' [MW]
$TR_{argg'}^{max}$	Maximum bound on investments to transmission/transportation capacity of mode r for resource a between regions g, g' [MW]
ε_f	Emission factor of fuel f for estimation of carbon budget [MtCO_2/MWh]
ε_f^{neg}	Emission factor of fuel f for estimation of negative carbon budget [MtCO_2/MWh]
η_{aj}^{ch}	Efficiency factor of charging storage technology j of resource a [%]
η_j^{conv}	Conversion factor of technology $j \in J^{pr}$ [MWh in to MWh out]
η_{aj}^{dis}	Efficiency factor of discharging storage technology j of resource a [%]
η_j^{heat}	Net efficiency of heat technology $j \in J^{hs}$ [%]
η_j^{tech}	Net efficiency of production/generation technology $j \in J^{pr}$ [%]

Free Variables

IC_{igh}	Electricity transmitted from/to interconnected country i to/from region g in time period h [MW]
TSC	Total system's annualised cost [£/year]
$TotCAPEX$	Total annualised capital expenditures [£/year]
$TotOPEX$	Total annualised operational expenditures [£/year]

Positive Variables

Cap_{jg}	Total installed capacity of technology $j \in J^{con}$ in region g [MW]
Cap_{jg}^{new}	Newly installed capacity of technology $j \in J^{con}$ in region g [MW]
$CO2^{elec}$	Total CO_2 emissions by power generation technologies [MtCO_2]
$CO2^{heat}$	Total CO_2 emissions by end-use heat technologies [MtCO_2]
$CO2^{net}$	Total negative CO_2 emissions [MtCO_2]
D_{agh}	Demand of resource a in region g during time period h [MW]
D^{peak}	Electricity system-wide peak demand of the coupled system [MW]
LC_{gh}	Load curtailment of renewable energy in region g during time period h [MW]
LS_{gh}	Load shedding in region g during time period h [MW]
P_{jgh}	Generation/production load of technology j at region g during time period h [MW]
ST_{ajgh}	Stored level of resource a using technology j in region g during time period h [MW]
ST_{ajgh}^{ch}	Storage charging of resource a using technology j in region g during time period h [MW]
ST_{ajgh}^{dis}	Storage discharging of resource a of technology j in region g during time period h [MW]

$TR_{argg'}$	Transmitted/transported level of resource a using transportation mode r between regions g, g' [MW]
$TR^{cap}_{argg'}$	Total transmission/transportation capacity for resource a using transportation mode r between regions g, g' [MW]
$TR^{new}_{argg'}$	Newly expanded transmission/transportation capacity for resource a using transportation mode r between regions g, g' [MW]
V^{elec}_{fjgh}	Consumption of fuel f using technology j in power supply chain in region g during time period h [MW]
V^{heat}_{fjgh}	Consumption of fuel f using technology j in heat supply chain in region g during time period h [MW]
Q_{ajgh}	Heat requirement of resource a using end-use heat technology j in region g during time period h [MW]

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