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Dynamic knowledge graph approach for modelling the decarbonisation of power systems

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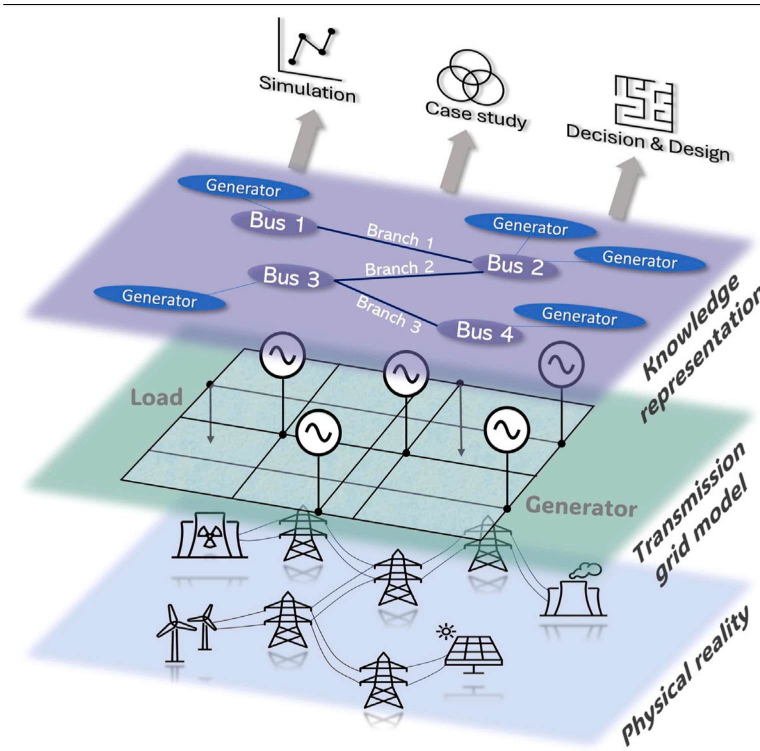
HIGHLIGHTS

- Dynamic knowledge graph approach for modelling power systems.
- Developed domain ontologies to instantiate data relevant to power systems.
- Designed computational agents for automated data processing and simulation.
- Case study investigates decarbonisation trajectories for UK power system.

GRAPHICAL ABSTRACT



ARTICLE INFO

ABSTRACT

This paper presents a dynamic knowledge graph approach that offers a reusable, interoperable, and extensible framework for modelling power systems. Domain ontologies have been developed to support a

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linked data representation of infrastructure data, socio-demographic data, areal attributes like demand, and models describing power systems. The knowledge graph links the data with a hierarchical representation of administrative regions, supporting geospatial queries to retrieve information about the population within the vicinity of a power plant, the number of power plants, total generation capacity, and demand within specific areas. Computational agents were developed to operate on the knowledge graph. The agents performed tasks including data uploading, updating, retrieval, processing, model construction and scenario analysis. A derived information framework was used to track the provenance of information calculated by agents involved in each scenario. The knowledge graph was populated with data describing the UK power system. Two alternative models of the transmission grid with different levels of structural resolution were instantiated, providing the foundation for the power system simulation and optimisation tasks performed by the agents. The application of the dynamic knowledge graph was demonstrated via a case study that investigates clean energy transition trajectories based on the deployment of Small Modular Reactors in the UK.

1. Introduction

Climate change has led to mounting global concerns. These include vulnerabilities in public health [1], food safety [2,3], water supply [4], the frequency of extreme weather events [5] and other prospective hazards. The transition towards a low-carbon future is strongly motivated by the recognition of greenhouse gas emissions as a significant driver of climate change.

Energy-related carbon emissions are the dominant source of anthropogenic emissions. For instance, in the USA and EU, these constitute roughly 80% of total emissions. While electricity accounts for only 20% of final energy consumption, the generation of electricity is responsible for more than 40% of all energy-related emissions [6]. Global emissions resulting from the combustion of fossil fuels for electricity (and heat) generation amounted to roughly 14.5 $GtCO_2e$ in 2021, with the major contributions coming from coal (and peat and oil shale), natural gas and oil respectively [7]. This motivates a pressing requirement to outline a path to clean power systems. The UK government has declared its commitment to achieving complete decarbonisation of all sectors of the national economy by 2050 in order to meet its net zero emissions target [8]. Among these sectors, electric power generation is responsible for approximately 16% of greenhouse gas emissions in the UK, amounting to 53.7 $MtCO_2e$ in 2022 [9]. In order to reach this objective, the recent “Energy White Paper” [10] and the “Ten-Point Plan for a Green Industrial Revolution” [11] both outline a plan for the UK to advance the adoption of alternative energy sources, for example wind and nuclear power, as a means of replacing fossil-fuelled energy generation. The analysis and study of power systems is a critical component of evaluating potential transition pathways and the integration of renewable energy sources.

The comprehensive analysis of power systems requires diverse data encompassing different social and technical domains. This could include details of power plant specifications, statistics describing electricity generation and demand, sociodemographic and geospacial information such as population density, geographic characteristics, and administrative data. Moreover, the study of power networks may also necessitate establishing physical and/or mathematical models to facilitate calculations, simulations, and optimisation processes. Diverse categories of networks exist, including transmission grids (operating at high voltage), distribution grids (functioning at middle/low voltage), microgrids, smart grids, and others [12]. Among these, the transmission grid plays a pivotal role in renewable energy integration, such as variability management [13], grid expansion [14,15], the implementation of energy storage systems [16], as well as in inter-regional, inter-state, and international long-distance power exchange [17–19]. Models that capture the features of the transmission grid, including its nodal topological structure, specifications, and constraints, offer an opportunity for in-depth analyses of many aspects of low-carbon generation technology adoption and the implications for energy policy. For example, it facilitates the examination of strategies for mitigating the disparity between power consumption and generation, thereby contributing to the exploration of generation patterns and the potential for balancing when integrating variable renewable energy [18].

The development of transmission grid models usually involves a collaborative effort, integrating collected data and information with the specialised knowledge of experts in the field [20]. It is conceivable that conducting such a study requires significant manual effort and decision-making, particularly in formulating rules to simplify real-world grids to suit diverse research objectives and scopes. This opens the door to the possibility of having multiple variants of a model to represent the same grid with different levels of resolution and distinct model parameters. It is worth realising that managing these model variants can be prone to errors in the absence of reliable provenance records and appropriate encapsulation measures [21]. The development of the models additionally involves the processing of data from a multitude of sources, often presented in diverse formats. This implies that data processing procedures are pervasive in the assembly of the models.

Power Flow (PF) analysis [22] and Optimal Power Flow (OPF) analysis [23] are fundamental tools in power system engineering. They play a critical role in applications such as grid stability assessment, voltage regulation, network planning, and loss minimisation. With the imperative shift towards power system decarbonisation, PF and OPF analyses are important tools for evaluating the impact of the integration of renewable energy sources.

PF analyses have been improved and applied to tackle the challenges arising from stochastic power injections due to the penetration of renewable energies, such as employing graph neural network (GNN) models trained on historic data to predict power flow outcomes [24], developing a residual-learning-inspired neural network (NN) framework to alleviate the computational load in traditional probabilistic power flow analysis [25]. The integration of charging stations into the grid is imperative to meet the needs of downstream clean electricity consumers, for example, to support the uptake of electric vehicles (EVs). Assessing the impacts on grid operations, including considerations of voltage stability and load fluctuations, as well as evaluating optimal station siting and sizing, can be effectively accomplished through stochastic PF analysis [26].

Stochastic OPF analyses are widely applied in studying hybrid power systems with renewable energy sources, such as wind–solar system [27,28], wind–solar–storage hybrid system [29], and wind–solar–small hydropower system [30–33]. These analyses specifically target challenges associated with the inherent unpredictability and intermittency of renewable energy sources, such as difficulties in maintaining voltage and frequency stability. OPF analysis also finds application in studying integrated energy storage systems [34–36] and optimising the control of energy storage devices in microgrids [37]. Maheshwari et al. [38] offers an overview of the development of OPF in the context of its application with renewable energy sources.

In addition to considering the integration of renewables, current research explores the integration of nuclear power into the power systems of Europe and North Africa [19], the UK [39,40], and the Association of South East Asian Nations (ASEAN) countries [41] to achieve a zero-emission targets. These studies are data-driven, computer-aided, and grid-model-based problems but rely on a relatively traditional and less automated approach. Implementing a “data-tool” methodology, integrating data, models, algorithms, and computational tools, can enhance and streamline the research process.

Therefore, a number of challenges emerge: how to store, process and manage heterogeneous data without introducing domain-specific barriers that inhibit interoperability? Moreover, how to guarantee the self-consistency, traceability of multiple data streams and the absence of human error throughout the research "journey" when exploring pathways for energy system decarbonisation? This "journey" commences with data collection and representation to reflect the scope under consideration. Subsequently, rules and methodologies are employed to construct a model, which is then furnished with input derived from data to execute analysis tasks with different initial conditions and objectives. Ultimately, the analysis results are post-processed and interpreted to yield insights and a deeper understanding of the cases under study.

These challenges have not been fully addressed. This hampers the efficiency of cross-domain studies in energy systems and undermines data management. It introduces difficulties when exploring diverse opportunities via the consideration of multiple scenarios under different "what-if" conditions, each representing different low-carbon transition routes. The World Avatar (TWA) [42], a dynamic knowledge graph (KG) implemented using technology from the Semantic Web stack and integrated with computational agents that perform a wide array of tasks provides a possible way forward.

The ***purpose of the paper*** is to develop an adaptable prototype of a dynamic knowledge graph that can facilitate research within the broad context of power system analysis and decarbonisation. The approach aims to promote data interoperability and overcome the inherent cross-domain challenges described above. We use the UK power system as an example to demonstrate the functionality and application of the prototype to investigate potential trajectories for a clean energy transition while considering the transmission grid characteristics. These capabilities broaden the application of TWA in the domain of power systems by creating new and augmenting existing domain ontologies. By using the concepts and properties specified in these ontologies, the power system components are represented ontologically via a "from reality to model" paradigm that provides a reusable, interoperable and extensible method for conceptually representing power systems to facilitate the research within this field.

The remainder of this paper is organised as follows: The next section summarises key information about the Semantic Web technologies and ontologies relevant to this work. Section 3 describes the methodological developments in the form of the ontologies and computational agents for studying power systems to investigate the potential decarbonisation trajectories. Section 4 introduces a case study that demonstrates the application of the approach by examining the consequences of different strategies for the deployment of Small Modular Reactors (SMRs). Finally, Section 5 draws conclusions and discusses future research directions.

2. Methods

2.1. The semantic web, linked data, ontologies and knowledge graphs

The Semantic Web [43] is an extension of the current World Wide Web that incorporates machine-interpretable metadata to represent data and information in an interlinked manner. In the context of the Semantic Web, the word *semantic* refers to the meaning and interpretation of data, while *web* conveys the idea of a navigable space of interconnected objects. Its ultimate goal is to empower computers for more effective manipulation of information on behalf of humans, thereby encouraging the development of automated applications based on internet technologies.

Linked Data is a specific implementation and a set of best practices within the broader Semantic Web. It is grounded in principles that involve the use of HTTP Uniform Resource Identifiers (URIs) for resource identification, utilising Resource Description Framework (RDF) for data presentation, and linking data to other data sources [44,45]. RDF [46] is a foundational data model for metadata, presenting data through SPO (*subject*, *predicate*, and *object*) triples. It offers a range of syntax notations and data serialisation formats, facilitating the representation of information on the web in the form of a directed graph.

Resources on the Semantic Web are defined as instances of ontological classes identified using Internationalised Resource Identifiers (IRIs) to ensure an unambiguous representation. An ontology defines a common vocabulary to share information within a domain of interest, comprising machine-interpretable definitions of concepts (also known as *classes*), relationships among them (referred to as *object properties* and *data properties*), and restrictions on these relations [47]. An *object property* creates a connection between instances of classes, while a *data property* associates an instance of a class with a specific data element. Ontologies are commonly conveyed and published through ontology languages, with the Web Ontology Language (OWL) [48] being a prevalent example. OWL is a Description Logic-based semantic markup language for authoring and sharing ontologies. It is developed as a vocabulary extension of RDF and originates from the DAML+OIL Web Ontology Language [49], which is widely adopted for its capacity to represent complex knowledge models and support reasoning and inference.

From the perspective of a Description Logic (DL) [50] formalism, ontologies can be alternatively expressed as a TBox (Terminological Component), complemented by the ABox (Assertional Component). The TBox provides the class hierarchy and their associative relations, while the ABox instantiates ("operationalises") the TBox by populating it with individual instances and their attributes. Within the context of DL-based ontologies, a knowledge base (KB) is constituted by an ontology (TBox) and a set of individual instances of classes (ABox). However, the distinction between where an ontology concludes and a knowledge base commences may present a nuanced delineation in practical applications [47]. A knowledge graph (KG), formed by ontologically described data, can be thought of as a KB structured as a directed graph. The graph is a "node-edge" network, where the nodes are concepts or their instances (data items) and the edges are links between related concepts or instances. KGs are usually constructed following the principles of Linked Data, promoting machine readability, resolving inconsistencies, and enhancing discoverability across data sources on the Semantic Web. These practices align with the FAIR (findability, accessibility, interoperability, and reusability) data principles [51].

Knowledge graphs are stored and managed in graph databases, also known as triple stores or RDF stores. Various software solutions are available to cater for diverse needs, including Java-based RDF4J (formerly Sesame) [52], Jena TDB [53], and Lightweight Fuseki [54]. For reasoning-supported large-scale applications, GraphDB [55] and Virtuoso [56] (with virtualisation support) are viable. Blazegraph [57] stands out for its high performance in large-scale scenarios, and AllegroGraph [58] distinguishes itself through its unique SPARQLMotion feature, which allows users to define complex data processing tasks. Triple stores offer access endpoints, referred to as SPARQL endpoints and identified by IRIs, facilitating the querying and updating of data using SPARQL [59]–a World Wide Web Consortium (W3C)-recommended semantic query language.

2.2. The world avatar – a dynamic knowledge graph

The World Avatar (TWA) [42,60] proposes the use of a dynamic knowledge graph – a knowledge graph that is operated on and kept up-to-date by autonomous computational agents – as a universal approach to implement connected digital twins. The vision is of an open digital ecosystem that unlocks the power of data and knowledge to support better decision-making within the context of complex systems of systems.

TWA includes the notion of a *base world* that describes the real world, and *parallel worlds* that act as "exploratory containers" to explore hypothetical scenarios relative to the base world [21]. The design

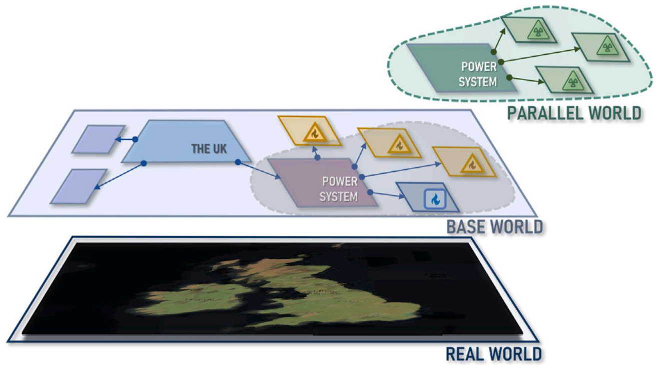

Fig. 1. The "base world" and "parallel worlds" in The World Avatar. The power system of the UK is exemplified. The *base world* describes the current fossil-fired power system in the UK, while *parallel worlds* explore options for decarbonisation via the deployment of SMRs.

intent is that the parallel worlds overlay the base world, where unchanged entities remain connected to the base world and changes to entities exist only in the parallel world, so do not interfere with the base world [42]. This is illustrated in Fig. 1.

TWA is realised using technologies from the Semantic Web stack [61] and implemented as a dynamic knowledge graph operated on by computational agents. This facilitates decentralised hosting and the sharing of data and agents through web-based HTTP services. Ontologies are used to represent and link entities, creating a rich and seamlessly interconnected data network. This interconnectedness transcends domain boundaries, fostering a holistic semantic context and thus promoting interoperability. This facilitates a unified and integrated data management environment, providing a uniform platform for hosting, querying, traversing data, and retrieving related information. The use of ontologies, as opposed to simple mechanical linking of data, ensures that the relationships carry logical significance, enabling the use of reasoning to infer concealed information.

These characteristics collectively enable TWA to address cross-domain applications. Thus far, TWA has been applied across diverse domains including chemistry and laboratory automation [62–69], energy systems [20,70–76], process engineering and eco-industrial parks [77–81], and smart city and disaster evaluation [82–84]. Reusable tools and frameworks have been developed to support these applications. Of particular relevance to the current work is the derived information framework for tracking data provenance and dependencies within a dynamic knowledge graph [85]. Other examples include an agent discovery and composition service [86] and a smart contract system [87] to facilitate the use of combinations of agents to achieve more complex tasks. Zhou et al. [88–90] and more recently Tran et al. [91] and Pascazio et al. [92] have and demonstrated the possibility of knowledge-based intelligent query interfaces to access (chemical) data from dynamic knowledge graphs.

2.3. Domain ontologies for decarbonised power systems

A number of domain ontologies for power systems have been developed. Pradeep et al. [93], introduced a high-level ontology for exchanging event information among interconnected power system operators. Santos et al. [94] proposed an ontology to facilitate integration and communication among multi-agent systems involved in electricity market simulations, while Huang and Zhou [95] presented a detailed ontology for the electrical grid, focusing on the description of grid assets.

More recent contributions include DABGEO [96], a reusable global ontology offering a common representation of energy domains, OntoPowSys [20], a domain ontology designed for formally representing Energy Management Strategies (EMS) in a wide industrial estate, and OntoEIP [80], an ontology addressing concepts relevant to eco-industrial parks, including the energy network. Other notable contributions have been made by Kovalyov and Lukinova [97], who presented an ontology delineating major operational processes in the distribution of heat and electric grids, Schweikert et al. [98], who crafted an ontology tailored for photovoltaic systems in smart grids, and Monaco et al. [99], who proposed an ontology targeting non-functional requirements in industrial energy management systems (IEMS).

3. Dynamic knowledge graph for power systems

3.1. Conceptual representation of a power system

The conceptual architecture of the knowledge graph used to represent power systems is illustrated in Fig. 2, utilising the UK as an illustrative example. The knowledge graph is constructed sequentially. The first step is to represent the tangible elements and entities from the physical world that are relevant to the power system. This includes information regarding power plants and local electricity consumption, population statistics and geospatial information specific to UK administrative areas [100].

The knowledge graph representation includes simplified topological structures that model the power transmission grid. This is illustrated in the central section of Fig. 2. This abstraction bridges the gap between describing the physical reality of the transmission to describing something that is suitable for use by power flow models. The simplified topological representation of the grid includes conceptual elements such as electric buses and branches, and the relationships between them. As different simplification strategies may be applied, multiple variants of the transmission grid models can co-exist in the knowledge graph. Each of these topological models reflects distinct internal structures characterising the transmission grid, tailored to fulfil different modelling needs.

Finally, the knowledge graph specifies which real-world generators and electricity demand data are associated with which nodes in the topological transmission grid models. This is illustrated in the top section of Fig. 2. This provides the information that is required to develop a mathematical representation of the power system to serve various simulation objectives. By constructing the knowledge graph in this manner, the description of the power system uses a principled knowledge-based approach to traverse the continuum from real-world representation to conceptual modelisation, reflecting various levels of conceptualised world existence.

3.2. Ontology development

The first step in creating the knowledge graph is to define the required concepts and relationships. Fig. 3 provides an overview of the employed ontologies and the primary concepts that each ontology offers. The domain ontologies, OntoPowSys [20], OntoEIP [79,80] and OntoCAPE [101] are reused and expanded where needed. A new ontology – *OntoEnergySystem* – is introduced to define the additional concepts and relationships that are required to describe and model the full power system. OntoPowSys, OntoEIP, and OntoEnergySystem are developed by reusing and extending the concepts and relationships from the top-level ontology modules in OntoCAPE. Classes are defined using the Web Ontology Language (OWL), and are linked to broader and more generic classes, known as the "least common subsumers", using the "subclassOf" relationship. This pattern facilitates the creation of hierarchical structures within the ontologies.

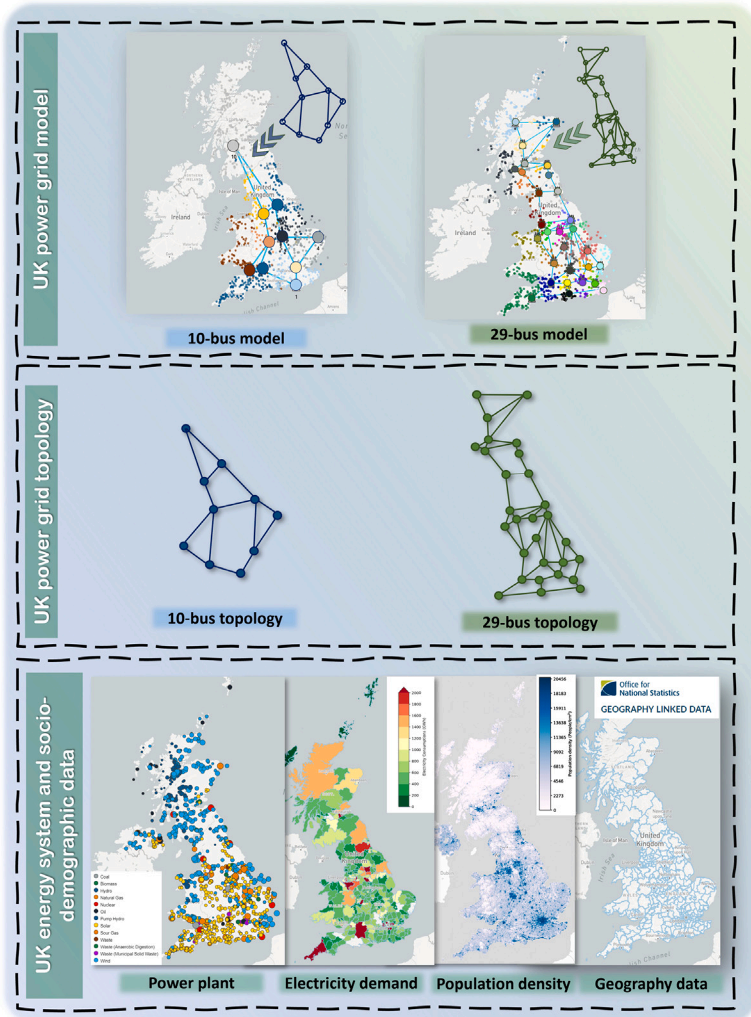

Fig. 2. The conceptual architecture of the knowledge graph representing the UK power system.

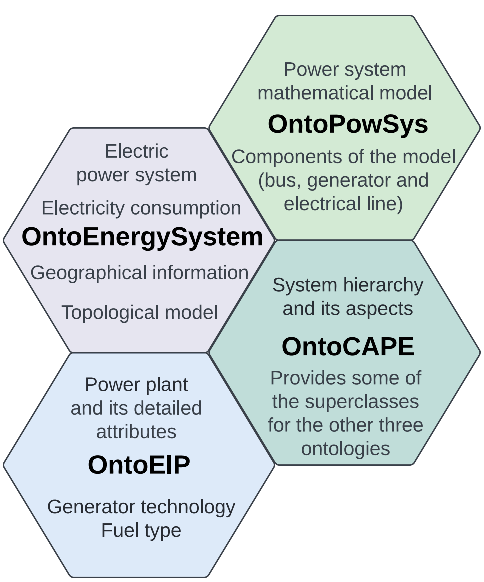

Fig. 3. The applied ontologies and the associated concepts in representing the power system.

3.2.1. *OntoEnergySystem*

OntoEnergySystem (Fig. 4) defines concepts related to physical assets within an energy system, the energy system itself, its properties, corresponding topological models, and associated geographical areas.

The key classes are described below.

- `Asset` class: Physical infrastructure or equipment for generating, transmitting and distributing energy resources.
- `GeographicalArea` class: A demarcated area of the Earth. An *AdministrativeDivision* is a type of `GeographicalArea`.
- `EnergySystem` class: A system that delivers energy services to consumers including households, industries, and commercial facilities.
- `EnergyConsumption` class: The amount of energy consumed by end users in a `GeographicalArea`.
- `ElectricPowerSystem` class: An electrical system composed of `Assets` that generate, transmit, and distribute electricity to meet the demands of the applications and end-users.
- `TotalElectricityConsumption` class: The amount of electricity consumed by end users. This class is divided into the electricity utilised by residential consumers, `DomesticElectricityConsumption`, and that consumed for non-residential purposes, `Non-DomesticElectricityConsumption`, according to the categories used for reporting in the UK [102]. The latter further includes usage for industrial and commercial purposes.

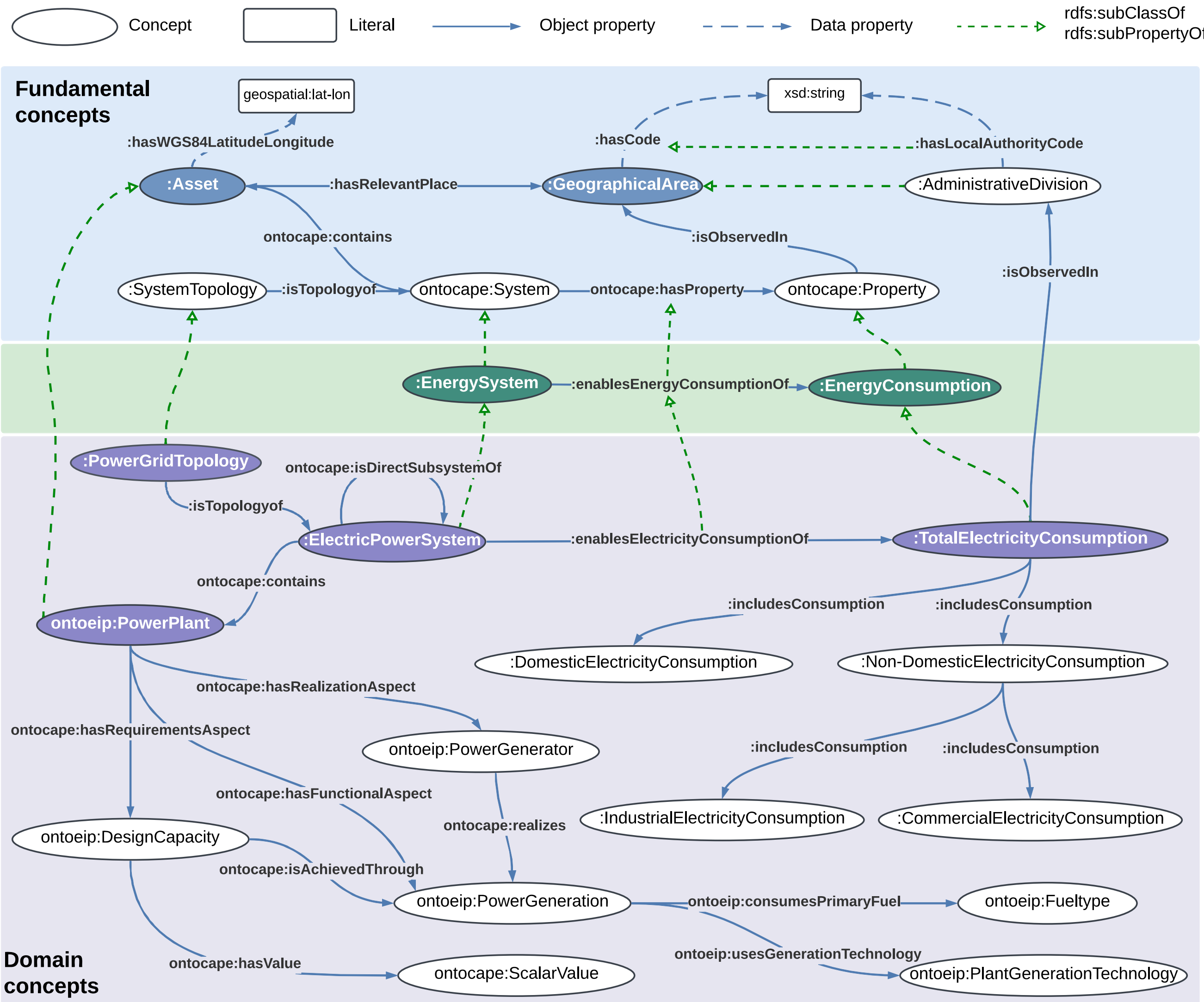

Fig. 4. OntoEnergySystem ontology. Concepts and properties defined in the *OntoEnergySystem* appear without a prefix. The key classes are highlighted with coloured ovals. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

- `PowerPlant` class: An industrial facility that converts energy from sources like fossil fuels, renewables or nuclear reactions into electricity. A power plant typically has a designated capacity and may include one or more generators using specific power generation technologies. It is classified as an `Asset`, and characterised by attributes like `name`, `geolocation`, `owner` and `construction` year.

By defining these concepts, otherwise isolated data associated with the entities illustrated at the bottom of Fig. 2 can be represented and linked in a knowledge graph with embedded semantics. As data interconnects and relationships are made explicit, a deeper context is forged. This elevates the information beyond being a mere collection of individual data points, and distinguishes knowledge graphs from other data formats. The augmented information can be queried and explored to benefit applications reliant on these insights.

3.2.2. OntoPowSys

OntoPowSys [20] defines concepts that are leveraged to represent the topological and mathematical models of the power system, as shown in the middle and upper sections of Fig. 2. *OntoPowSys* was expanded to include concepts that allow entities from the real world to be mapped to their abstract counterparts in the topological and mathematical models. The extended version of *OntoPowSys* is shown in Fig. 5.

The key classes are described below.

- `PowerGridTopology` class: A topological model that provides information about the connections between the bus nodes and different components of power transmission systems.
- `PowerSystemModel` class: A description of an electric power transmission grid system, formulated using a `PowerGrid-Topology`.
- `OptimalPowerFlowModel` class: A description of an electric power transmission grid system designed for initialising optimal power flow analyses.
- `PowerFlowModel` class: A description of an electric power transmission grid system designed for initialising power flow analyses.
- `BusNode` class: A physical point of connection between two electrical devices, playing a crucial role in constructing the electrical network topology.
- `ElectricalLine` class: Cables with specified voltage levels, whether above ground or underground, through which electricity is transmitted to an area or building.

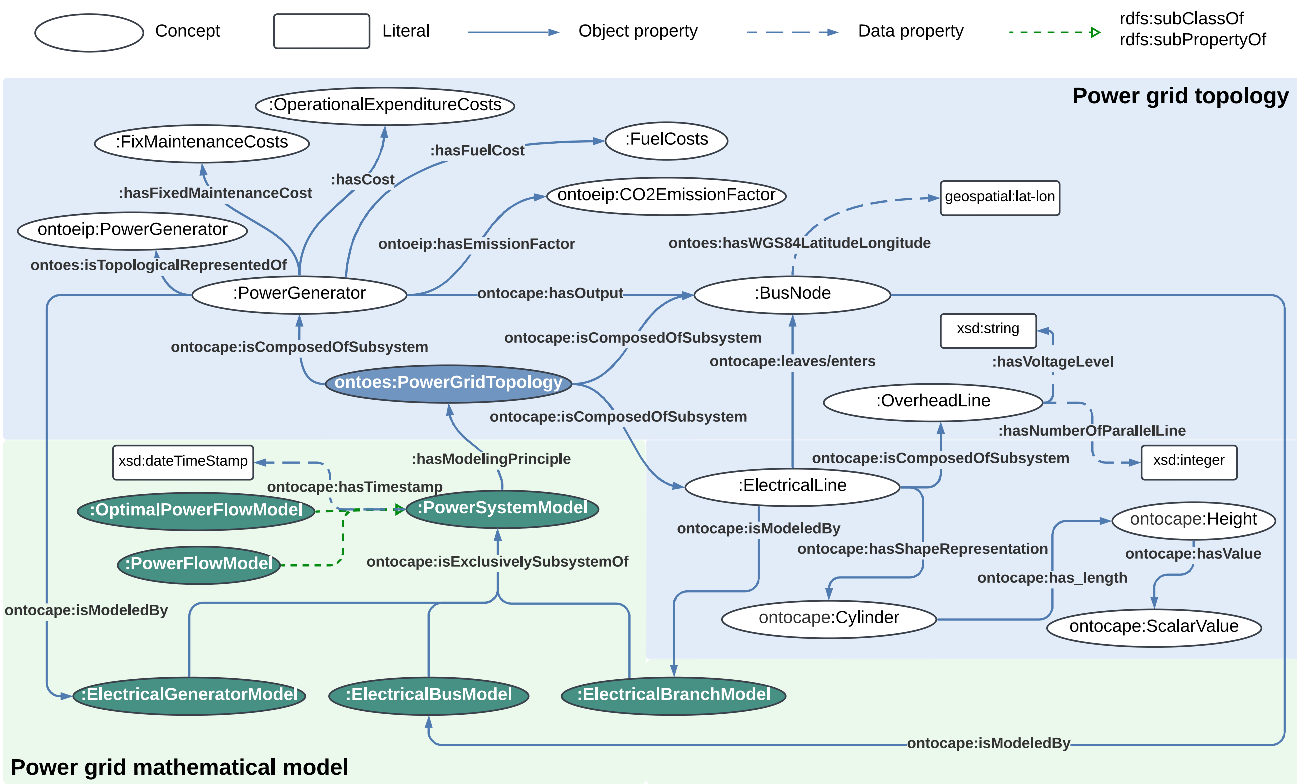

Fig. 5. Extended OntoPowSys ontology. Concepts and properties defined in the extended *OntoPowSys* ontology appear without a prefix. The prefix "ontoes" is short for *OntoEnergySystem*. The key classes are highlighted with coloured ovals. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

- `ElectricalGeneratorModel`, `ElectricalBusModel` and `ElectricalBranchModel` classes: Mathematical model components that represent `PowerGenerator`, `BusNode` and `ElectricalLine` in the topological model.

By using *OntoPowSys*, the provenance of the information used by the models (*i.e.*, which data contribute to which models) is explicitly integrated into the data structure. Using this information, the results of scenario analyses can be traced back to their respective real-world entities for subsequent processing and interpretation.

3.3. Agent development

Agents were developed to perform specific tasks on the knowledge graph. Fig. 6 shows the workflow of the key agents in this study, highlighting that the population of the knowledge graph describing the power system is a sequential process, where the information assembled in previous steps is carried forward for use in subsequent steps. The figure indicates the specific agent(s) responsible for each segment of the knowledge graph, identified by corresponding zones with labels. The activities of each agent are described below.

3.3.1. Initialiser agents

The *PowerSystemInitialiser*, *PowerPlantInitialiser* and *ElectricityDemandInitialiser* agents read data from DUKES [103], sub-national gas consumption data [102] and the UK high-resolution population density data [104] to construct a knowledge graph describing power plants and electricity consumption. The data are represented using the *OntoEnergySystem*, *OntoEIP*, and *OntoCAPE* ontologies. No queries are made to the knowledge graph by these agents at this stage, rather the role of the agents is to ingest new data.

3.3.2. Power grid topology model constructor

The *PowerGridTopologyConstructor* agent uses terms from *OntoEnergySystem* and the extended *OntoPowSys* ontology to represent grid topology models in the knowledge graph. Unlike the initialiser agents, this process entails querying the knowledge graph, as the topology construction relies on information about the power system.

Fig. 7 shows an activity diagram for the *PowerGridTopologyConstructor*. The initial information required by the agent is shown in the *Config* box. The agent proceeds to instantiate the topology components, bus nodes and branches. The primary attributes of bus nodes include their geolocation, while branches are characterised by their interconnections with buses and respective voltage levels.

After the components of the topology model are instantiated, the agent enters a loop in which each real-world power plant (except those in Northern Ireland, which operate on a separate power grid) is represented as a generator that is assigned to a bus node in the topology model. This is depicted in the *Loop* box. Two methods are provided in this agent for bus allocation: `SameRegionMethod` and `ClosetBusMethod`. The former is designed for simple topology models where each region has at most only one bus. The latter method is more capable and is designed to handle any topology model. In this study, two topology models were instantiated: one with 10 buses and 14 branches [71] generated by `SameRegionMethod`, and another with 29 buses and 99 branches [105] created using `ClosetBusMethod`. The structure and specifications of both bus models are detailed in the Appendix.

The activity of the *PowerGridTopologyConstructor* agent concludes after full configuration of a topology model including all bus, branch, and generator components.

3.3.3. Power grid mathematical model constructor

The *PowerGridMathematicalModelConstructor* agent uses terms from the extended *OntoEnergySystem* ontology to represent the information

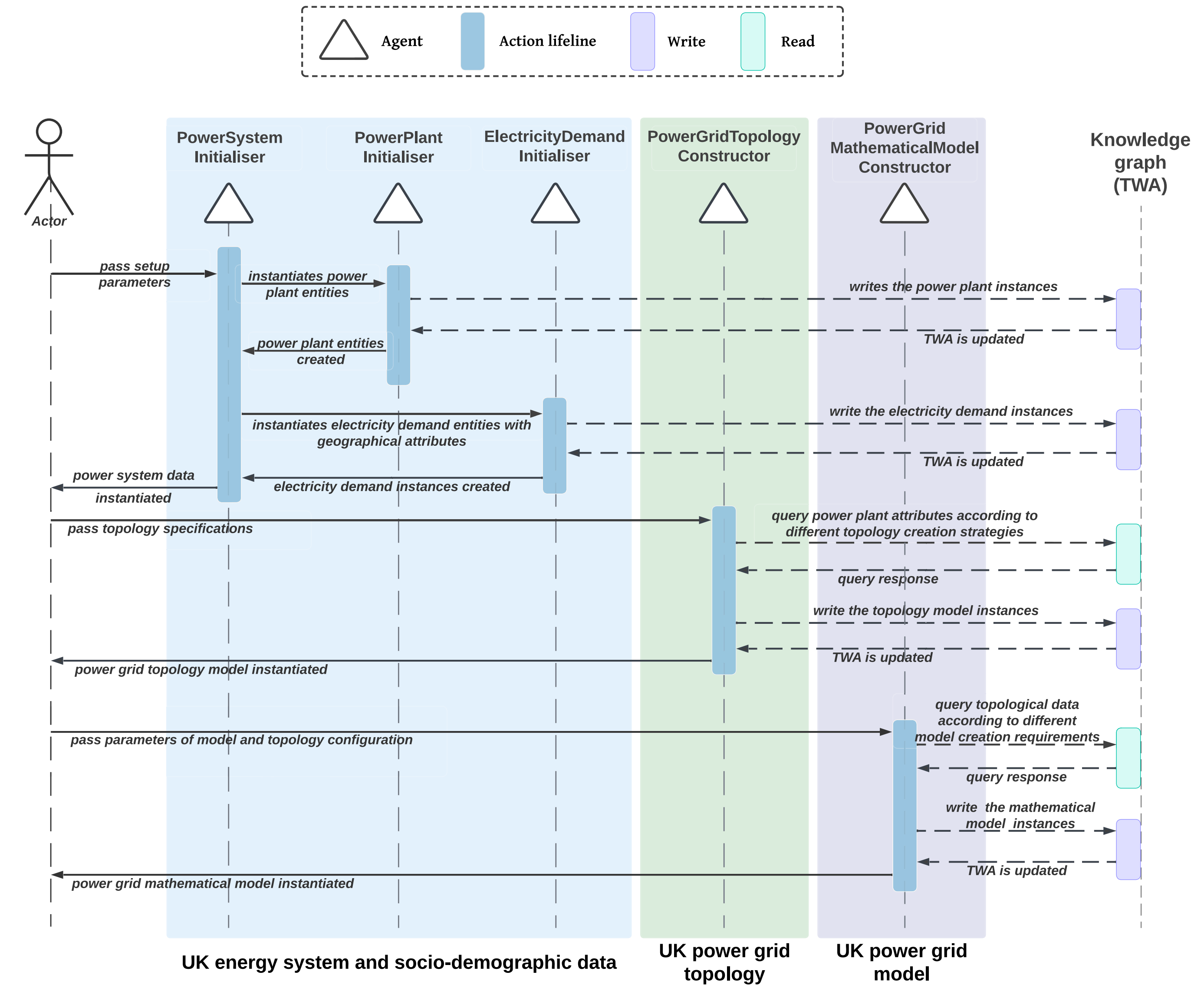

Fig. 6. Sequence diagram showing the agents involved in the creation of the knowledge graph describing the power system.

needed by power flow and optimal power flow analyses. Fig. 8 shows an activity diagram. The agent queries the knowledge graph to retrieve a topology model. This provides the starting point for the subsequent steps. The agent can optionally receive input to specify additional generators, such as newly introduced renewables, or indicate the removal of any generators during mathematical model construction. This boosts the adaptability of model construction for application in diverse scenario analyses.

The agent enters a first loop in which a load is assigned to each bus. This data is used by PF and OPF analyses to determine the power injection required to balance the demand load. Two methods to do this are provided: `AllocateRegionalLoadMethod` and `AllocateClosetAreaLoadMethod`. The former is designed for use with data that specifies demand by region. The latter is designed for data with any level of granularity. After the loop, the agent processes the branch data to instantiate resistance, reactance, and susceptance data. PF and OPF analyses use these data to calculate branch (grid) losses.

The agent now enters a second loop in which it initialises the information about each generator. This includes an initial guess of the generator output. In the case of OPF analysis, where the objective function typically involves economic and environmental considerations, it is necessary to include a cost factor (describing the cost of generating electricity) and an emission factor (describing the cost imposed on emissions from the generator) in terms of a carbon tax and CO_2 emission intensity factor.

The data instantiated by the *PowerGridMathematicalModelConstructor* agent is used in simulation tasks by an *PFandOPFAnalysis* agent.

3.3.4. *Simulation agent: Power flow and optimal power flow analysis*

The *PFandOPFAnalysis* agent acts as a wrapper for the Python package `PYPOWER` [106]. Fig. 9 shows an activity diagram. The agent supports both PF and OPF analysis. The output of PF analysis includes the voltage of each bus, along with their respective active and reactive powers, and information about branch (grid) losses. The output of OPF analysis also includes the output of each generator, along with the objective function value, typically representing the total operation cost. The corresponding CO_2 emissions are subsequently calculated using the generator output and its carbon emission intensity factor. These outputs are written back to the knowledge graph.

4. Results and discussion

Using the proposed knowledge graph method, a case study was performed to explore the outcome (generation mix, regional load shifting, *etc.*) of replacing fossil-fired generators with SMRs to move towards a

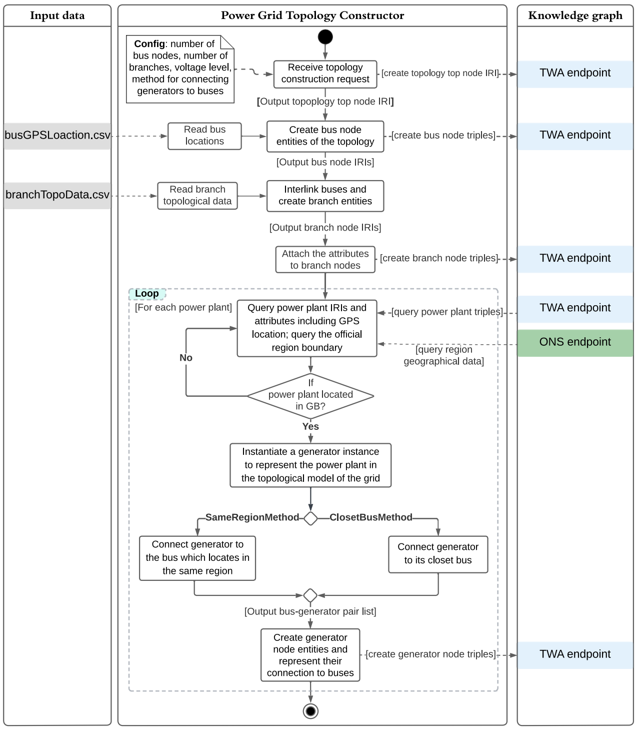

Fig. 7. Activities conducted by the **PowerGridTopologyConstructor** agent. "TWA endpoint" refers to the triple store maintaining the TWA knowledge while "ONS endpoint" denotes the ONS Linked dataset [100].

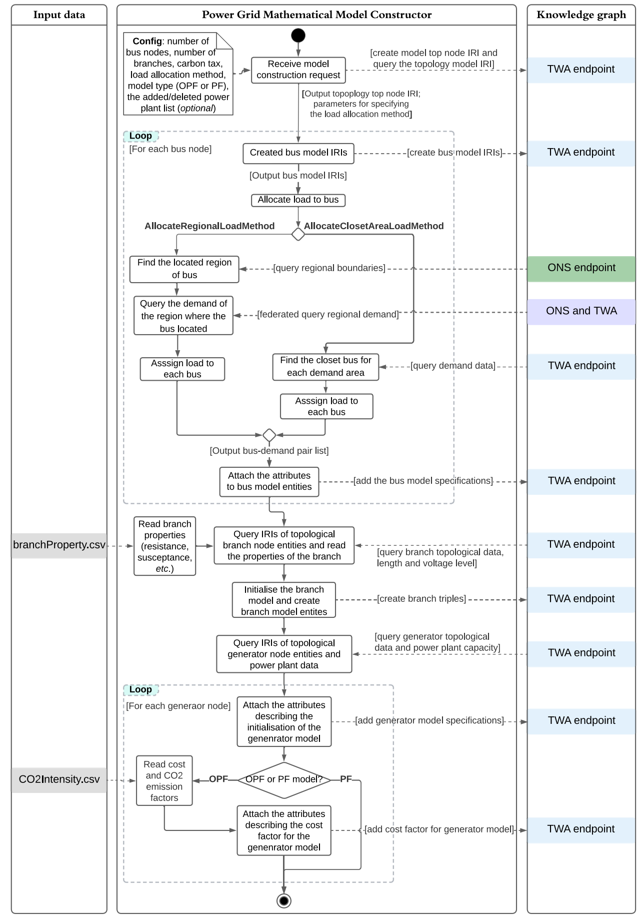

Fig. 8. Activities conducted by the **PowerGridMathematicalModelConstructor** agent. The shaded box "ONS and TWA" refers to both TWA and ONS endpoints that are used simultaneously in the federated SPARQL query.

zero-carbon emission target in the UK. A carbon tax (emission penalty) was applied in this analysis as the economic driving force to motivate the replacement. The study considers three scenarios representing varying levels of wind and solar availability, W_MS_M (medium), W_HS_H (high), and W_LS_L (low). The medium, high and low levels are based on weekly average, weekly maximum, and weekly minimum values (2022) for wind and solar power generation in the UK. See Fig. 10.

The study considers the placement of SMRs with specifications based on a Rolls-Royce prototype, with a design capacity of 470 MW and a reported Levelised Cost of Electricity (LCOE) ranging from 40 to 60 £/MWh [108]. The simulations in this study use an LCOE based on the upper bound of 60 £/MWh with a "balanced strategy" for SMR placement. The balanced strategy equally prioritises minimising risks and transmission distance (as a proxy for transmission losses) [76]. Each site permits a maximum of 4 SMRs. The 29-bus model [105] was used to conduct the analyses in the case study. This constrains the analyses to solutions that are feasible with the current grid.

4.1. Site selection agent

The SMR site selection was performed by a *SMRSiteSelector* agent. Fig. 11 shows an activity diagram. Potential sites are determined based on the sites of existing and decommissioned power plants of the type specified in the agent *Config*. In this study, we specifically consider fossil-fired and traditional nuclear power plant sites as candidates for deploying SMRs. The choice of whether to place, and how many SMRs to place on each site considers two objectives: safety and distance from centres of demand (as a proxy for transmission losses). The data to evaluate the objectives are obtained through geospatial queries of the knowledge graph. There is a trade-off between the objectives because while placing SMRs at a distance from populated areas increases safety, it will also increase transmission distance (and therefore transmission losses) as most of the populated areas overlap with the high-demand areas. The agent uses a genetic optimisation algorithm to find the

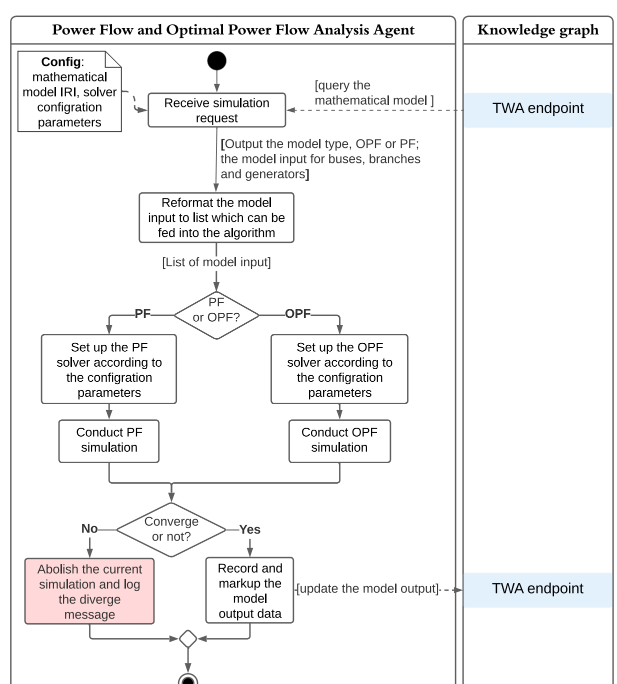

Fig. 9. Activities executed by the **PFandOPFAnalysis** agent.

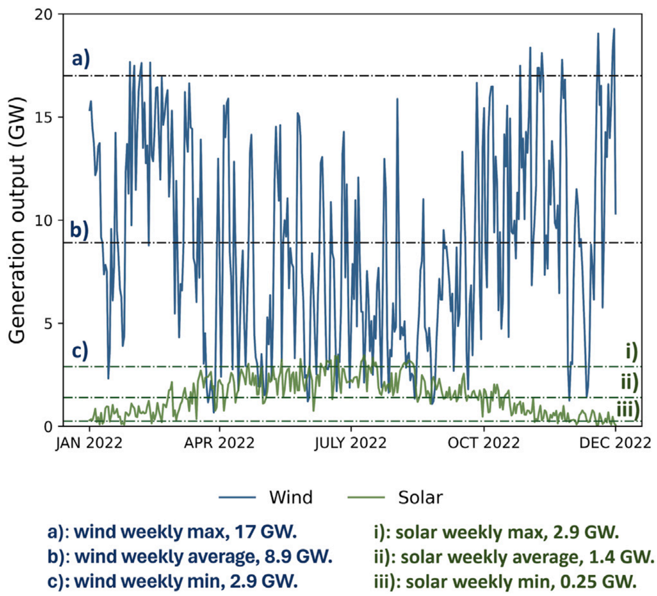

Fig. 10. Daily production of wind and solar energy in 2022 of GB [107].

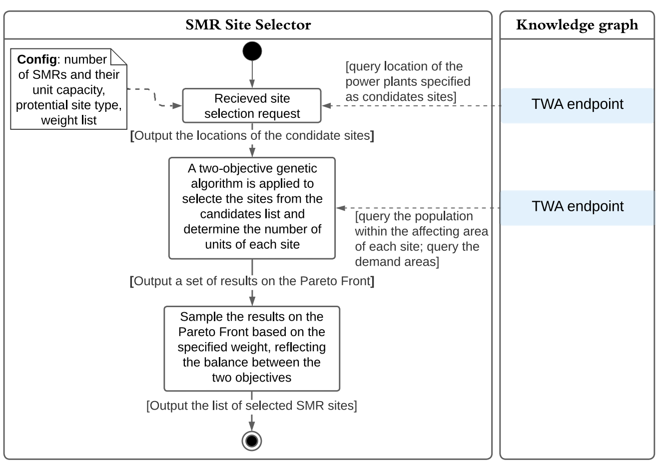

Fig. 11. Activities executed by the *SMRSiteSelector* agent.

corresponding Pareto Front, which is subsequently sampled to assess solutions with different relative weighting of the objectives. Each sampled result comprises a set of chosen sites and the number of SMRs on each site. Full details of the site selection algorithm are given by Xie et al. [76].

Fig. 12 shows the major data flows between the knowledge graph and the interactions of the agents employed in the case study. The derived information framework [85] was used to record the provenance of the information added to the knowledge graph by the agents. The execution of each agent is accompanied by the instantiation of a “derivation” and associated markup. Taking the *SMRSiteSelector* agent as an example, the outputs (information about SMR sites) are marked as *belongsTo* the derivation, which itself *isDerivedFrom* a list of inputs. The execution of the *PowerGridModelConstructor* is accompanied by the instantiation of a new derivation that *isDerivedFrom* the information about the selected sites and topological data about the grid and calculates information that *belongsTo* the *PowerGridModelConstructor* derivation. The execution of the *OPFAnalysisAgent* is accompanied by the instantiation of a new derivation that *isDerivedFrom* the information that *belongsTo* the *PowerGridModelConstructor* agent, and calculates data including generator outputs, branch losses, total operational cost,

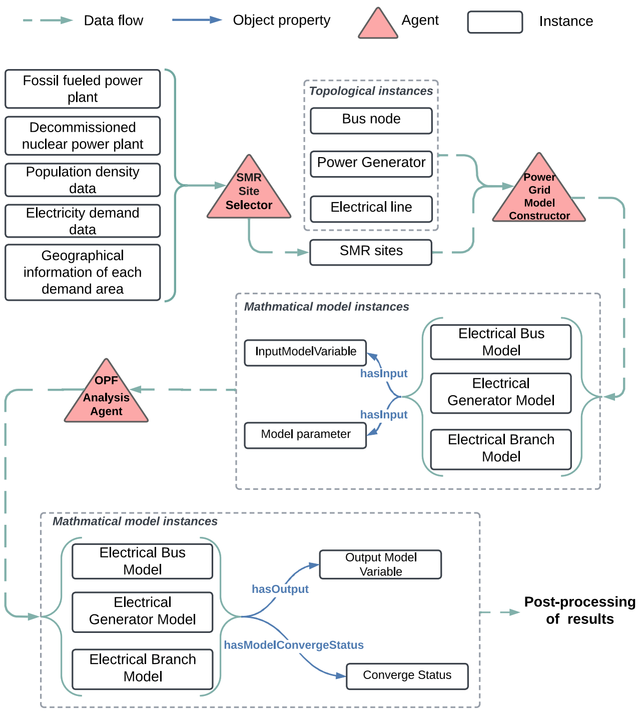

Fig. 12. The inputs, outputs, and interactions of the agents involved in the SMR replacement case study.

and emission cost due to carbon tax that *belongsTo* the *OPFAnalysisAgent* derivation.

4.2. Medium renewable availability scenario

Fig. 13 summarises the main outcomes of the $W_M S_M$ scenario as the carbon tax escalates from 0 to more than 100 £/tCO$_2$. “Base case” refers to the case without SMR adoption, with all other conditions remaining consistent with the scenario.

No SMRs are adopted at low levels of carbon tax (top row) due to the lack of economic viability, and the outputs from the base case and SMR adoption case are equivalent. Scotland and northern England predominantly source their electricity from clean energy, encompassing wind and conventional nuclear power. Scotland is a major power producer, contributing nearly 5 GW, and supplies power to England through the transmission grid (not shown). In the central regions of England, specifically Yorkshire & Humber and East Midlands, there is a substantial dependence on coal-fired generation. Despite the availability of capacity for natural gas generation, the use of coal remains economical at this level of carbon tax. While the West Midlands is characterised by a high proportion of solar generation, the total capacity is low. Among the regions generating more than 4 GW, only Scotland qualifies as “clean”. In contrast, the South East, East Midlands, and East England, despite a combined share of nuclear, wind and solar energy, are significant emitters due to a reliance on fossil fuel.

At a carbon tax of 50 £/tCO$_2$ (middle row), both the base case and SMR adoption case show the phasing out of coal-based power generation. In the base case, the use of coal is entirely replaced by natural gas, with natural gas now the dominant energy source across the majority of regions. The cleanest regions, Scotland and the North East, show minimal change because the economics of clean energy is unaffected by the carbon tax. The most noticeable change is observed in the East Midlands, where the output decreases from 4.5 GW to around 3 GW with the shift from coal to natural gas. In the SMR adoption case, the use of coal is displaced by the SMRs, with 19 SMRs providing 8.9 GW of power across Wales (8 units), South West (3 units),

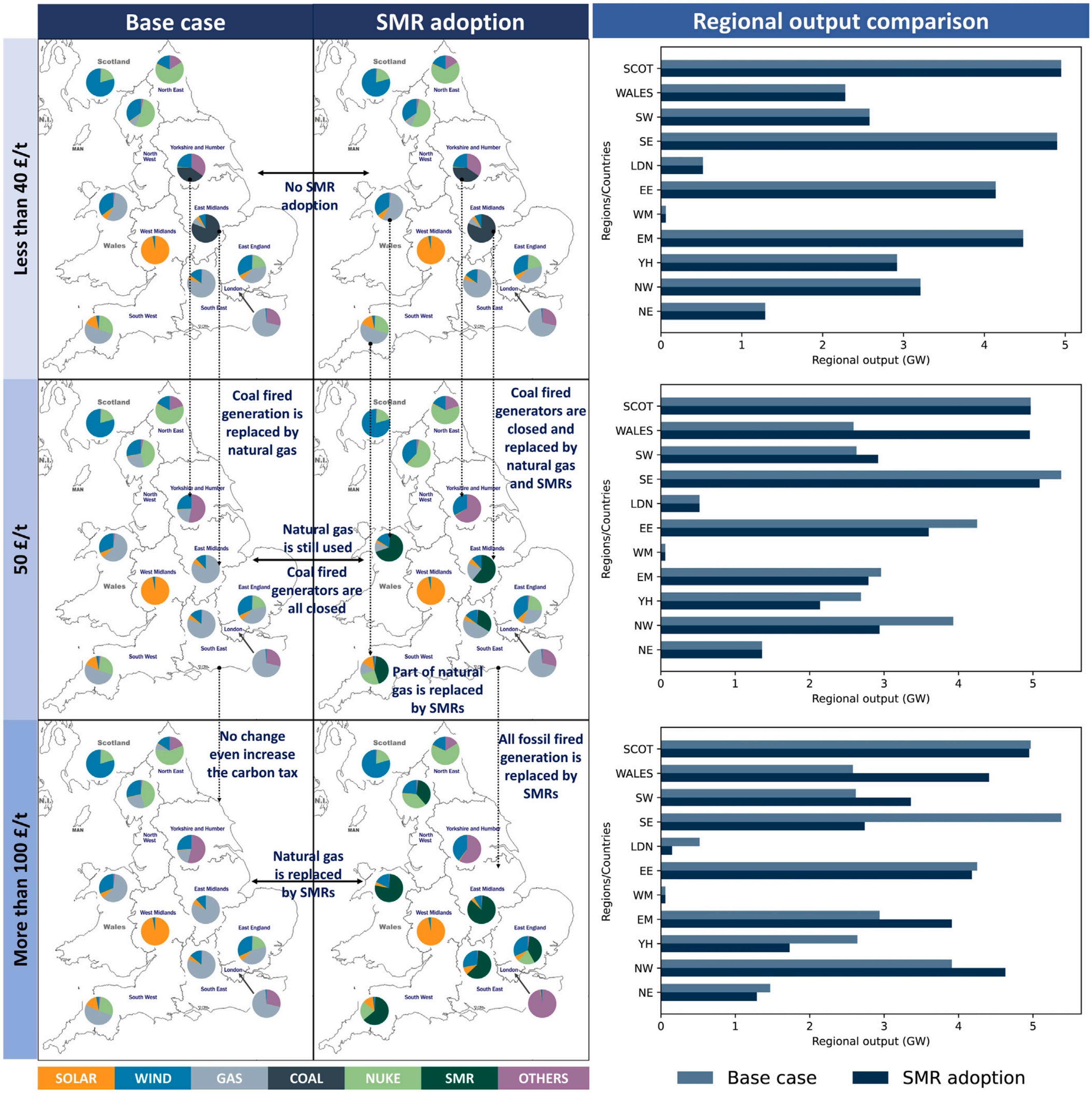

Fig. 13. W_MS_M scenario. Regional energy mix (left) and total power output (right). Scotland (*SCOT*), Wales (*WALES*), South West (*SW*), South East (*SE*), London (*LDN*), East England (*EE*), West Midlands (*WM*), East Midlands (*EM*), Yorkshire & Humber (*YH*), North West (*NW*) and North East (*NE*).

East Midlands (4 units), and South East (4 units). Scotland and the North East again show minimal change, with Scotland remaining as the largest power producer. Relative to the base case, the SMRs reduce the dependence on natural gas in southern regions, although natural gas remains cost-competitive so is not totally displaced. The SMRs double the power output from Wales relative to the base case, suggesting the potential for notable variations in bus voltage levels, branch losses and power flow direction.

At a carbon tax exceeding 100 £/tCO_2 (bottom row), the base case remains the same as at 50 £/tCO_2 because it has already attained optimal performance with no cleaner (*i.e.*, cheaper) alternatives available. In the SMR adoption case, the stringent emission penalties favour the use of SMRs over natural gas. An additional 14 SMR units have been integrated to replace the remaining natural gas generation, bringing the total to 33 units supplying 15.5 GW. This fulfils over half of demand, with the remainder provided by wind, solar and conventional nuclear generators operating at their maximum capacity under the prevailing W_MS_M availability. The North West (4 units) and East England (8 units) emerge as the new host locations, with both seeing an increase in their regional output. Aside from Wales, the South East shows a major change with output dropping to nearly half that of the corresponding base case due to the shift away from natural gas. Interestingly, the balanced placement strategy results in a significant proportion of the SMR adoption occurring in southern regions that traditionally rely on fossil fuels. This implies that choosing on-site replacement at fossil-fired sites may be a prudent strategy consistent with balancing risk and transmission losses.

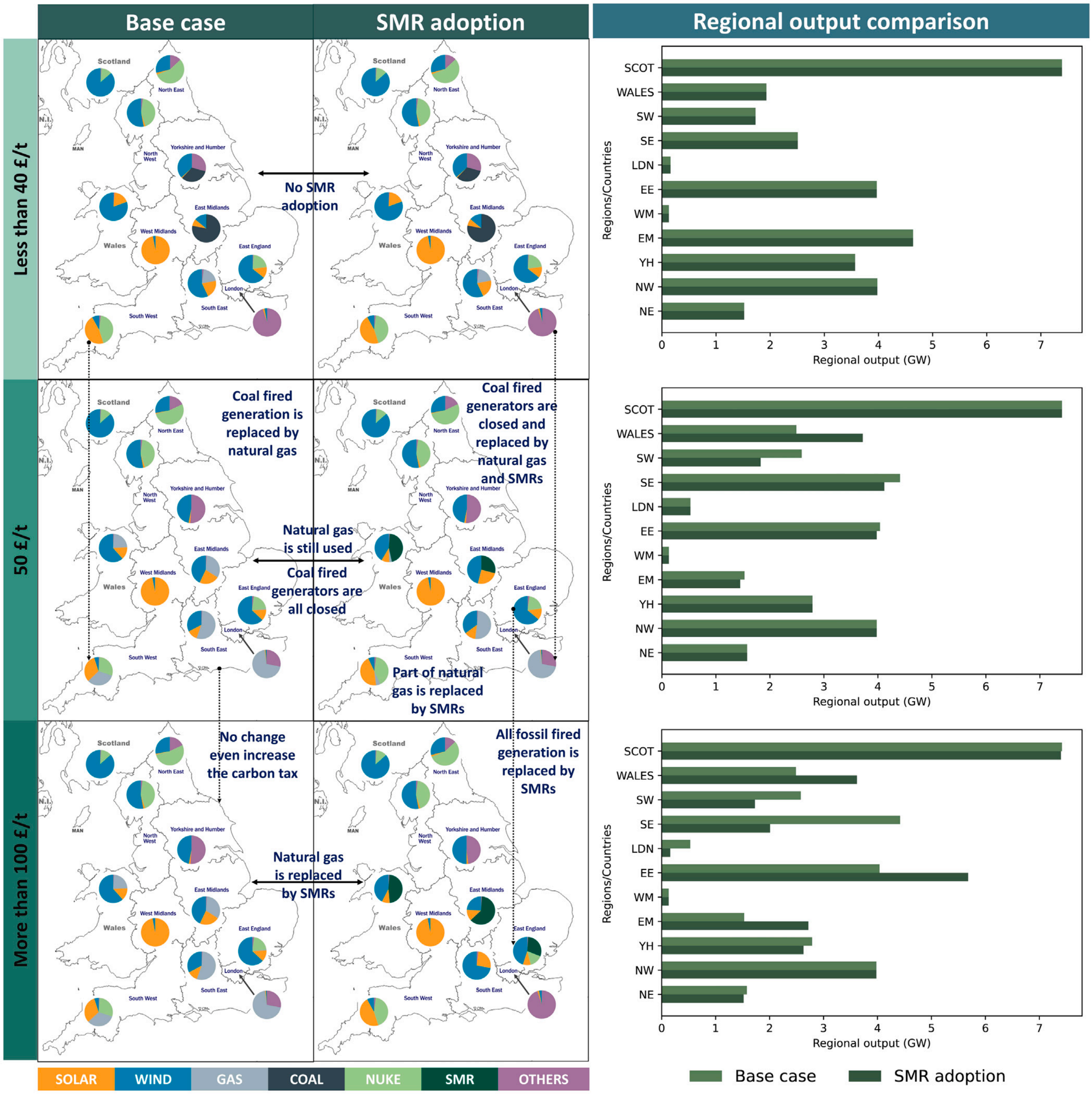

Fig. 14. W_HS_H scenario. Regional energy mix (left) and total power output (right).

4.3. High renewable availability scenario

Fig. 14 shows the main outcomes of the W_HS_H scenario. This reflects a hypothetical scenario to investigate the adoption of SMRs as an auxiliary technology in support of a policy that prioritises renewable energy, resulting in a significant increase in capacity.

No SMRs are adopted at low levels of carbon tax (top row) as per the W_MS_M scenario. The dependence on natural gas and coal (less visible on Fig. 14) is alleviated with the increased availability of wind and solar power. The wind power is such that output from Scotland now exceeds 7 GW, significantly surpassing other regions and intensifying dependence on Scotland. Solar capacity, concentrated in southern regions, is less than a fifth of total wind capacity and is insufficient to counterbalance this dependence. This results in greater losses because of increased long-distance power transmission (not shown). At a carbon tax of 50 £/tCO_2 (middle row), the use of coal is entirely replaced by natural gas in both the base case and SMR adoption case. In the SMR adoption case, 5 SMRs providing 2.4 GW of power are deployed, but the dominant status of Scotland persists, reflected in a relatively insignificant change in the output of the other regions. At a carbon tax exceeding 100 £/tCO_2 (bottom row), all fossil-fired power generation has been replaced by SMRs, with a total of 12 SMRs contributing 5.6 GW in Wales, the East Midlands and East England. The East Midlands is now the second-largest energy provider after Scotland.

The results of this scenario reflect that a predominant reliance on wind power has the tendency to concentrate power generation in specific locales, displacing power generation in proximity to areas of demand. This could pose a substantial challenge for high-demand areas,

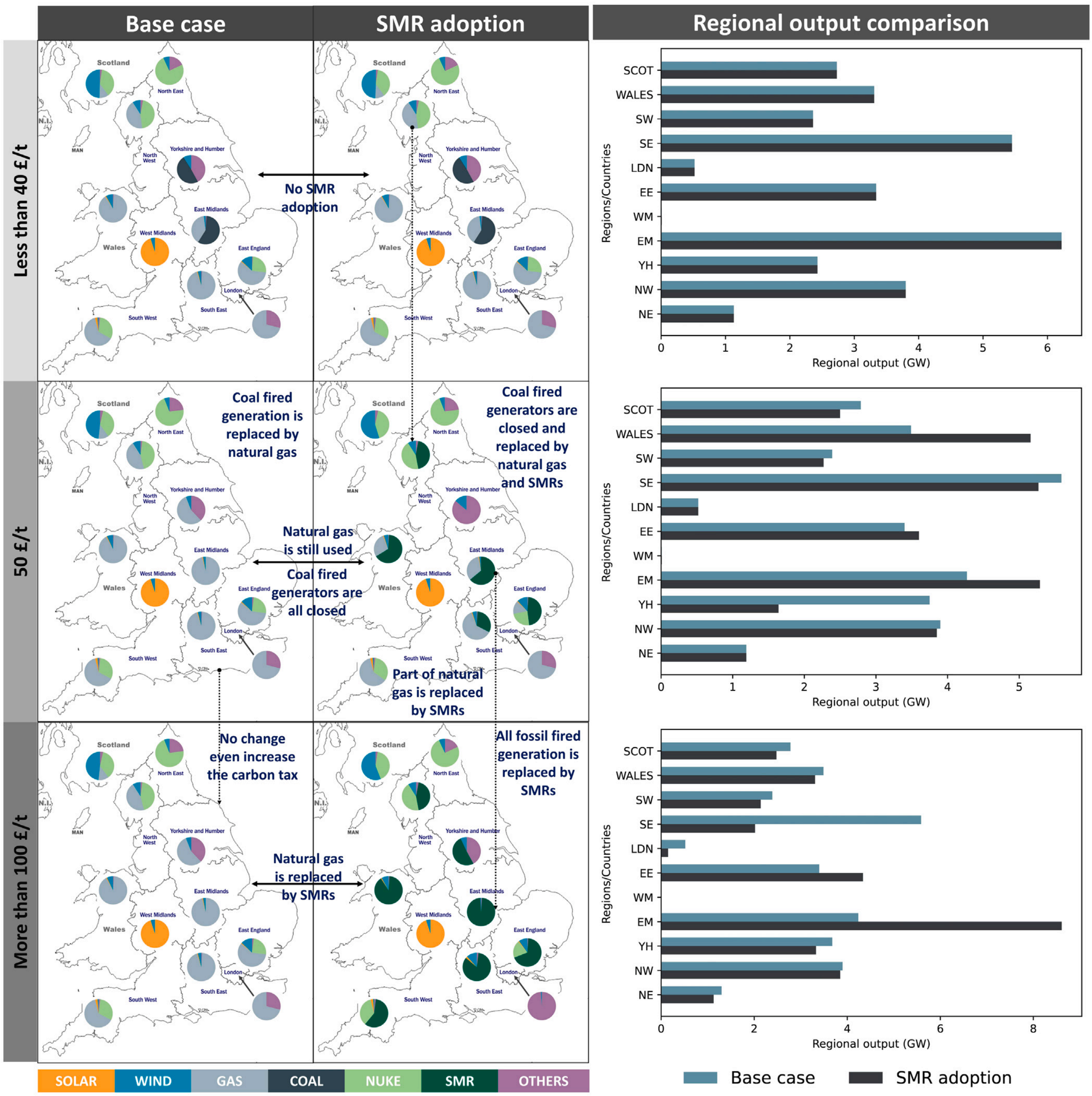

Fig. 15. W_LS_L scenario. Regional energy mix (left) and total power output (right).

including industrial zones in the middle of England around Liverpool, Manchester, Leeds, as well as London and regions like the South West that traditionally rely on local coal and natural gas plants, which now find themselves reliant on long-distance transmission of power. This would be particularly the case if the UK proceeds with its planned expansion of onshore wind capacity on Scotland [11]. In comparison, balanced siting strategy for SMRs can alleviate this, unlike solar and wind, which heavily depend on climatic and geographical conditions.

4.4. Low renewable availability scenario

Fig. 15 shows the main outcomes of the W_LS_L scenario. This reflects a hypothetical scenario in which SMRs are chosen as the primary energy source and the reliance on wind and solar energy is reduced.

Fossil fuels are extensively used at low levels of carbon tax (top row), with the East Midlands and South East as the largest power generators, commensurate with their substantial fossil fuel capacities. In contrast to the other scenarios, the reduction in the availability of wind power is such that Scotland is no longer the largest power generator. The adoption of SMRs displaces first coal and then natural gas as the carbon tax increases. At a carbon tax exceeding 100 £/tCO_2 (bottom row), all fossil-fired power generation has been replaced by SMRs, with a total of 49 SMRs that provide 23 GW of power. The most pronounced variation in regional output between the base case and SMR adoption case is in the South East and East Midlands. Only 3 SMRs with a capacity totalling approximately 1.4 GW are adopted in the South East, leading to a significant reduction in power output compared to the substantial natural gas capacity power generation in the base case. In contrast, 18 SMRs with a capacity exceeding 8 GW are placed in the East Midlands due to its location, not too far from areas of high demand and yet a reasonable distance from densely populated areas. Under this scenario, the East Midlands is the largest regional power generator, contributing to mitigating transmission losses by alleviating the burden of long-distance power transmission.

In summary, SMRs offer a flexible siting advantage when compared to wind and solar power. This facilitates adjustments aligned with the geospatial distribution of population and demand, providing a more manageable approach to addressing power supply for newly developed populated areas experiencing increases in demand. Relying on SMRs as the primary clean energy source offers a route to attaining a zero-emission target, while concurrently ensuring a stable and reliable power supply.

5. Conclusions

This paper presents a dynamic knowledge graph for power system analysis and decarbonisation, addressing data integration and interoperability challenges. Utilising ontologies for data modelling and computational agents for automation, we introduce the OntoEnergySystem ontology, and extend the existing OntoEIP and OntoPowSys to include a wider range of power system concepts. These ontologies enable the representation and linkage of information, offering a reusable framework for describing diverse power systems across different geospatial locations and structures.

A set of computational agents was developed to interact with the knowledge graph, ensuring dynamic behaviour as information propagates for self-consistency. These agents handle input/output tasks like populating the graph, querying data, and propagating changes. Other agents process data, invoking computational models for simulations and optimisations. A derived information framework [85] was used to mark up the inputs and outputs of the agents, allowing traceability of the provenance of dependent information.

A case study of the UK power system exemplified the application of ontologies and computational agents. Power plants were represented in the knowledge graph, linked to geographic data and land authority codes. This facilitated connections between power plant descriptions and hierarchically structured administrative areas in the UK. Electricity demand was ontologically represented as an observed feature associated with these areas, linking it to power plants. Population density data at a 1-km resolution were instantiated. Geospatial queries, leveraging administrative area information, allowed retrieval of details such as population in proximity to power plants and areas with high electricity consumption. Two topological models (10-bus and 29-bus) of the transmission grid were instantiated in the knowledge graph, forming the basis for simulation and optimisation tasks performed by computational agents.

The case study demonstrates the ability of the dynamic knowledge graph to analyse scenarios for optimised Small Modular Reactor (SMR) placement, aiming for a low-emission UK power system. Results reveal the energy mix in each UK region under various SMR deployment policies, highlighting the interplay with diverse geographic distribution and availability of wind and solar energy. This study broadens the use of dynamic knowledge graphs in power systems. Future work may extend domain ontologies to encompass concepts for describing various grid types, including distribution and smart grids. The approach could be applied to assess decarbonisation solutions in diverse geographical regions. The conceptual framework and information propagation approach introduced here have the potential to be integrated into a parallel world framework [21], enhancing support for scenario analysis and the practical application of dynamic knowledge graphs.

CRediT authorship contribution statement

Wanni Xie: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Feroz Farazi:** Writing – review & editing, Validation, Supervision, Software, Methodology, Data curation. **John Atherton:** Methodology. **Jiaru Bai:** Writing – review & editing, Software, Methodology. **Sebastian Mosbach:** Writing – review & editing, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Conceptualization. **Jethro Akroyd:** Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Markus Kraft:** Writing – review & editing, Supervision, Resources, Project administration, Methodology, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The codes developed for this work are available under an open-source license at https://github.com/cambridge-cares/TheWorldAvatar.

Declaration of Generative AI and AI-assisted technologies in the writing process

During the preparation of this work the authors used ChatGPT 3.5 in order to enhance the readability and language of the manuscript. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the publication.

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Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.egyai.2024.100359.

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