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A reference architecture for the American Multi-Modal Energy System enterprise

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ABSTRACT

The American Multimodal Energy System (AMES) is a system-of-systems comprised of four separate but interdependent infrastructure enterprises: the electric grid, the natural gas enterprise, the oil enterprise, and the coal enterprise. Their interdependence creates the need to better understand the underlying architecture in order to move towards a more sustainable, resilient and accessible energy system. Collectively, these requirements necessitate a sustainable energy transition that constitute a change in the AMES instantiated architecture; although it leaves its reference architecture largely unchanged. Consequently, from a model-based systems engineering perspective, identifying the underlying enterprise model's reference architecture becomes a high priority. This paper defines a reference architecture for the AMES and its four component energy enterprises in a single SysML model. The architecture includes (allocated) block definition and activity diagrams for each enterprise. The reference architecture was developed from the S&P Global Platts (GIS) Map Data Pro data set and the EIA Annual Energy Outlook dataset. This reference architecture serves as the foundation from which to accurately and consistently create mathematical and informatic digital twins of the AMES.

1. Introduction

The American Multimodal Energy System (AMES) is a ***system-of-systems*** comprised of four separate but interdependent infrastructure enterprises. The electric grid, natural gas enterprise, oil enterprise, and coal enterprise comprise the essential infrastructure that meet the energy demands of the 21st century in America. While each of these individual enterprises constitute a value chain in their own right, they also enable and support the value chains in the other energy enterprises. This interdependence instigates the need of Industrial Information Integration Engineering (IIIE) to better understand the underlying architecture in order to move towards a more sustainable, resilient and accessible integrated energy industry. Each of these three general requirements are discussed in turn.

1.1. The sustainable energy transition

From a sustainability perspective, the decarbonization of the AMES to meet a global target of not more than a 2 °C rise by 2050 is paramount [1–10]. Graphically, the Sankey diagram developed by the Lawrence Livermore National Laboratory shown in Fig. 1, depicts the AMES flow of energy from primary fuels to four energy consuming sectors [11]. It reveals that the three carbon-intensive fuels of natural gas, petroleum, and coal account for 80% of the AMES supply side. In the meantime, 37% of American energy supply and more importantly 100% of renewable energy supply flows through electric generation facilities where they are then routed to the residential, commercial, industrial and transportation sectors. On the demand side, 67% of all energy consumed is lost as rejected energy. The transportation sector, in particular, rejects 80% of its energy and is consequently the lead producer of greenhouse gas (GHG) emissions [12]. To significantly reduce the GHG emissions produced from fossil fuels, three ***architectural changes*** are simultaneously required of the integrated energy systems [2]. First, carbon-neutral renewable energy sources such as solar, wind, nuclear, geothermal and nuclear generation must be increasingly integrated into the grid and ultimately displace fossil-fuel fired generation plants; especially as they are retired at the end of their useful life [10,13–17]. Second, energy consumption technologies, like transportation and heating, that rely heavily on fossil-fuel combustion must switch fuels to electricity where they have opportunity to be powered by an

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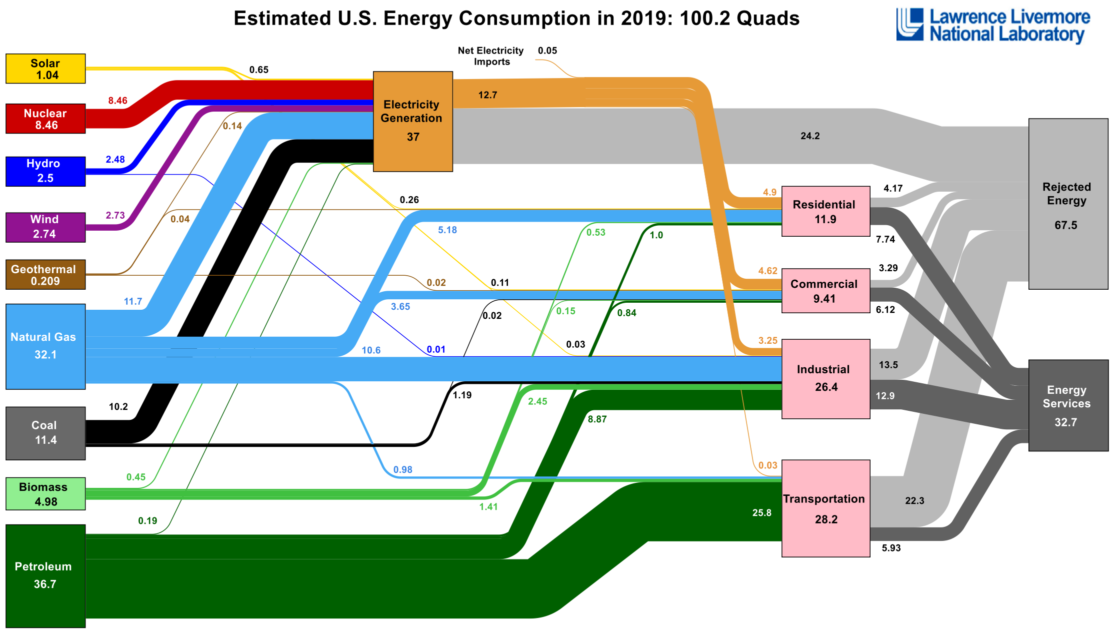

Fig. 1. A Sankey Diagram of U.S. Energy Consumption in 2019. The Lawrence Livermore National Laboratory has produced this visualization based primary data sources from the DOE and EIA [11].

increasingly decarbonized electric power. Lastly, energy-intensive technologies throughout the AMES must be systematically replaced with their more energy-efficient counterparts [18–23].

Together, these three architectural changes minimize the demand on the coal, oil, and natural gas enterprises. In the meantime, such a systemic shift towards the use of electricity requires a commensurate expansion of the electric grid. Such a ***sustainable energy transition*** is arguably the largest single engineering enterprise transformation in human history. Given the environmental consequences, the energy transition must be undertaken in a manner that not just meets the evolving requirements of its stakeholders, but also remains operational.

1.2. Engineered modeling solutions

Fortunately, from perspectives of Model-Based Systems Engineering (MBSE), Enterprise Modeling (EM), and Industrial Information Integration Engineering (IIIE) [24–27], the management of these architectural changes has methodological precedents. Notably, EM has been used in a manufacturing and supply chain context to direct changes in enterprise architecture in response to systemic challenges. Additionally, IIIE is an engineering discipline that overlaps and pulls from many other disciplines including energy, modeling architectures and the integration of information between enterprises [28]. By utilizing a standard ontology to model enterprises, their resources and processes can be accurately described, compared, and integrated [26,29,30]. With accurately designed enterprise models, the structures, processes, and value chains of said enterprises can be analyzed and optimized. These models can then be used to drive changes in the integration of enterprises and facilitate the optimal re-engineering of systems [26,31,32]. By directing the information integration of enterprises with MBSE and EM, value chains can be tied together in a standardized manner [26,33,34]. As the four energy infrastructures are supply chains in their own right, it follows that the management of architectural change in the EM literature applies directly to the architectural changes posed by the sustainable energy transition.

1.3. Resilience and reliability

From a resilience and reliability perspective, each of the AMES component enterprises must not just deliver their respective type of energy independently [1,35–39] but must also support the other AMES infrastructures [40]. For example, and as shown in Fig. 1, if a natural gas pipeline fails in the natural gas system it could take a natural gas power plant offline in the electric grid. Such a lack of electric generation capacity could then result in the temporary shut down of a natural gas processing plant; further reducing natural gas and electricity capacity. The New England electric power grid, in particular, remains susceptible to natural gas shortages during long cold spells when the fuel is used heavily for both space heating as well as electric generation [41]. Alternatively, the oil and natural gas systems rely on electricity to process their respective fuels and compress them during storage and transportation. Even the coal system requires electricity in safe and efficient mining.

As the AMES architecture moves through a sustainable energy transition, it must do so in a manner that is reliable and resilient to natural, economic and malicious disruptions. Using an integrated enterprise model of the AMES to guide the sustainable energy transition, will allow for system-wide vulnerabilities to be systematically identified and mitigated in a manner that is more comprehensive than if each enterprise were studied independently. For example, global climate change and severe weather events may place coastal energy facilities particularly at risk [42]. Additionally, economic shocks can affect the import and export energy resources and disrupt their relative balance in the AMES [43]. Lastly, malicious cyber-attacks can propagate failures not just within a given AMES infrastructure but across them as well as information and resources are integrated across all four energy infrastructures.

Finally, from an energy access perspective, the AMES must continue to cost-effectively and equitably provide readily available energy to the broader public [44]. Relative to many other nations, this requirement has been largely addressed in the United States. Nevertheless, certain issues remain. For example, in northern New England, people rely on carbon-intensive oil and propane for heating since heat pumps have limited performance in especially cold climates. Finally, solar and wind potential is often plentiful away from urban load centers and so may not be effectively utilized without additional electric transmission capacity [45–52]. Many of these energy access concerns are particularly poignant in Alaska and other arctic regions.

The three general requirements of energy sustainability, resilience, and access impose constraints on the evolution of the AMES integrated

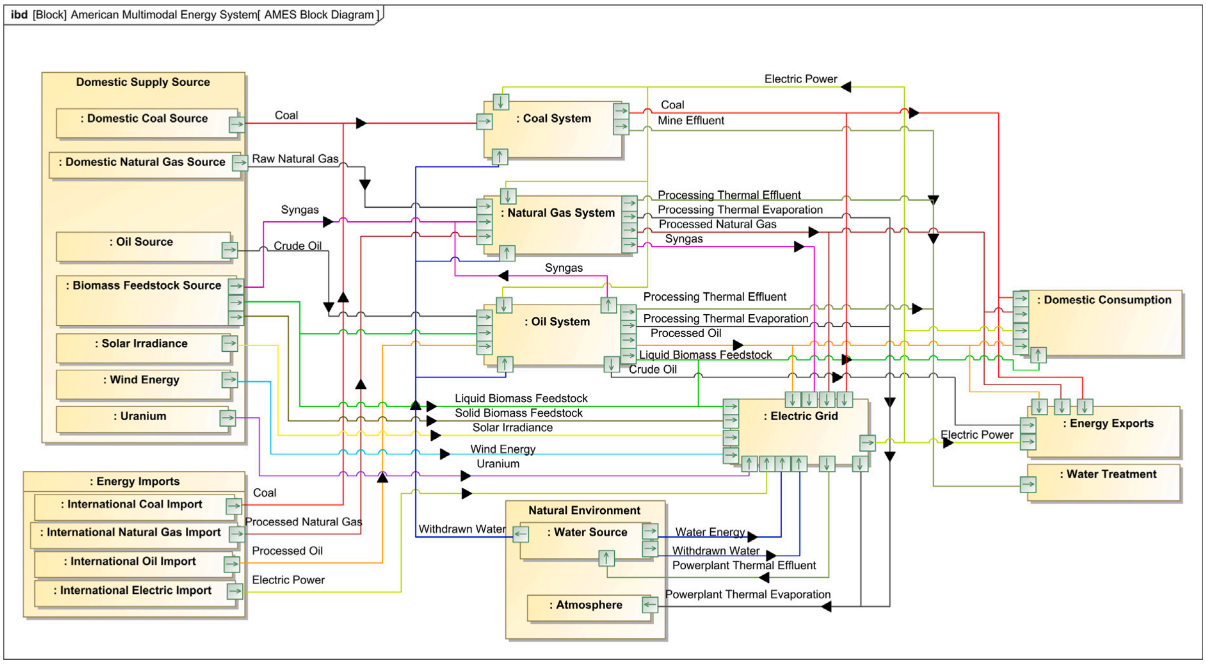

Fig. 2. The top level internal block diagram of the AMES. The domestic supply sources, the energy imports, natural environment, domestic consumption, energy exports, and water treatment are external to the AMES four subsystems of coal, natural gas, oil, and electric grid.

enterprise architecture. And yet, the AMES architecture remains relatively poorly understood from a holistic perspective [53–56]. The Sankey Diagram in Fig. 1, to our knowledge, presents the only graphical depiction of the AMES in its entirety. While this data visualization effectively conveys information concerning relative energy flows, from a model-based systems engineering [24] perspective, its highly simplified nature was not intended for architectural analysis and design. In addition to the Sankey model, the EIA has developed the National Energy Modeling System (NEMS) software to produce the yearly annual energy outlook [12]. Nevertheless, this software-based tool remains less than transparent and the EIA website itself states: "[The] NEMS is only used by a few organizations outside of the EIA. Most people who have requested NEMS in the past have found out that it was too difficult or rigid to use [57]".

1.4. Original contribution

In order to deploy a MBSE-methodology to the sustainable energy transition, this paper uses a ***data-driven approach*** to define a reference architecture as the foundation to creating a digital twin, in a single invariant SysML enterprise model describing the four main enterprises that comprise the unified AMES. When developing a digital twin of the AMES, the informatic operands passed across multiple energy systems must reflect the integration of information, matter, and energy between the energy enterprises from a standardized ontological foundation. By defining the reference architecture, this paper provides the foundation from which to consistently build a digital twin as an instantiated architecture for future mathematical modeling and analysis of the AMES. The top level block diagram in Fig. 2 presents the four subsystems of the AMES and the flow of operands between them and those entities defined as outside of the system boundary. Each of the four subsystems: the electric grid, the natural gas system, the oil system, and the coal system are in turn defined using class and activity diagrams with (allocation) swim-lanes. Integrating each of the sub-reference architecture class and activity diagrams as described in the AMES block diagram defines the entirety of the AMES reference architecture. As a result, the presented model defines all the pathways for integrating the information and energy passed between each respected energy industry.

This work assumes a working knowledge of the SysML (the Systems Modeling Language), as the ontological basis of this work, which is otherwise gained from several excellent texts [24,25,58]. For clarity, this paper uses system architecture and enterprise interchangeably recognizing enterprises are a type of system operated as either public, private, or a hybrid enterprises within the energy industry.

1.5. Scope

This paper restricts its scope to the AMES' four sub-systems. As this work uses a data-driven approach to accurately develop the AMES reference architecture, it restricts itself to the conventional energy technologies represented in the data. Most notably, the Platts Map Data Pro data set only includes transmission system resources and excludes those in the distribution system [59]. As the sustainable energy transition continues, it is possible, if not likely, that new clean energy technologies (e.g. hydrogen, carbon capture and sequestration) will emerge. As technologies become more prevalent and generate data, their information models can be integrated into the models presented in this paper allowing for a reusable model that can evolve as needed [60–62].

1.6. Paper outline

Section 2 starts with a description of the background literature and the datasets used to develop the enterprise model's reference architecture. The paper then presents the electric power grid's architecture in Section 3.1. The natural gas architecture is then presented in Section 3.2. The oil enterprise and coal enterprise architectures are then defined in Section 3.3 and Section 3.4 respectively. A discussion of dependencies between each of the integrated enterprises is presented in Section 4. The paper then presents future work of the AMES reference architecture. This includes simulation development for integrated planning and operations management. Finally, the paper is brought to a conclusion in Section 5.

2. Background

2.1. Standardized information integration ontology

While IIIE interacts with systems engineering and computer science in terms of engineering methods it also interacts with energy engineering at the application level [63–65]. This paper seeks to utilize systems engineering in the energy engineering space to integrate the four major energy enterprises into a standardized AMES model. Amongst many of the IIIE works there has been a focus on the standardization of inter-enterprise compatibility, communication, and synchronization of the information passed between enterprises [66]. In engineering the integration of industrial buildings and applications within a heterogeneous environment, many sources agree that there needs to be a single ontology from which these models are built to standardize the information that is passed between entities [67–69]. With recent ontology's being developed for such information integration including OWL and PLIB, there needs to be an ontology-driven methodology for developing normalized logical schema [70]. Through ontological harmonization of enterprise product models and reverse engineering techniques, semantically consistent inter-enterprise models can be developed to consistently capture the integration of multiple systems into a normalized database [71,72].

Using MBSE roots in SysML as a standardized ontology, this paper seeks to harmonize the product models of each energy enterprise into a singular integrated architecture from which to design future studies and models from. To create a standardized architecture for modeling the AMES requires a high level of system transparency and integrated compatibility between the systems with designed rationality and tractability of said integrations for consistent reuse [63,73]. An additional hurdle to the development of such an architecture is the strategic issue of interoperability of enterprises and the ability of said architecture to handle and enterprises evolution. The interoperability of an enterprise is inevitably enabled by the continuously evolving systems integrating with legacy systems [74,75]. One such solution to these IIIE challenges is an ontology-driven architecture, created by harmonizing the enterprise production models of each energy system from the basis of MBSE to allow for further evolution of technology and the AMES.

2.2. Modeling architectures

The three architectural changes described above constitute a change in the AMES *instantiated architecture* but leaves the AMES *reference architecture* largely unchanged. In order to deploy a MBSE-methodology to the sustainable energy transition, identifying the underlying reference architecture of the AMES becomes a high priority in meeting the paramount requirement of energy sustainability.

Definition 1 (- *Instantiated Architecture [25,76]*)**.** A case specific architecture, which represents a real-world scenario, or an example test case. At this level, the physical architecture consists of a set of instantiated resources, and the functional architecture consists of a set of instantiated system processes. The mapping defines which resources perform what processes.

Definition 2 (- *Reference Architecture [76]*)**.** *"The reference architecture captures the essence of existing architectures, and the vision of future needs and evolution to provide guidance to assist in developing new instantiated system architectures. …Such reference architecture facilitates a shared understanding across multiple products, organizations, or disciplines about the current architecture and the vision on the future direction. A reference architecture is based on concepts proven in practice. Most often preceding architectures are mined for these proven concepts. For architecture renovation and innovation validation and proof can be based on reference implementations and prototyping. In conclusion, the reference architecture generalizes instantiated system architectures to define an architecture that is generally applicable in a discipline. The reference architecture does however not generalize beyond its discipline."*

The primary benefit of a reference architecture is that it clearly identifies the system boundary, the resources of the enterprise, the activities of the enterprise processes, and the interfaces and interactions between them. This identification is of critical importance when the chosen system is particularly complex and heterogeneous; as in the case of the AMES. In the electric power grid (alone), there is a rich history of reference architecture development in the so-called "Common Information Model" [77,78] that has culminated in IEC Standards 61970, 61968, and 62325 [79–81]. Furthermore, it is important to recognize that a reference architecture, by design, can admit a wide variety of mathematical models of system behavior. For example, once the relevant classes of an electric power system have been identified in a reference architecture, depending on the need, one can still develop an AC or DC power flow analysis model, an AC or DC optimal power flow model, or a small signal or transient stability model. Naturally, the choice of mathematical modeling elements that are being superimposed on the reference architecture greatly affects the computational intensity of the mathematical model as a whole. Additionally, the chosen mathematical model may be implemented as a computational (simulation) model that is either centralized (on one processor) or distributed (on many). Furthermore, depending on the causal dependencies in the reference architecture, a distributed computational model may invoke fully parallel processing, or sequential co-simulation techniques [82,83]. This work leaves these mathematical modeling and computational implementation as choices outside the scope of this paper, but ultimately recognizes that the development of a reference architecture is a necessary first step.

2.3. Existing energy system literature

Normally, each of the four systems of the AMES are studied independently and each have their own extensive literature [84–88]. Increasingly, however, sustainability, resilience, and accessibility drivers have brought about greater attention to how these individual infrastructures depend on each other [39,89–96]. One dependence that has received considerable attention is the dependence of the electric grid on the natural gas system [41,97–103]. These works are motivated by the increasing role of natural gas-fired electricity generation relative to coal-fired facilities [104], and the importance of natural gas power plants in providing "flexible" operating reserves against variable renewable energy resources [105]. Similarly, some works have addressed the dependence of the electric grid on the oil [86,106] and coal systems [87,93,107]. Moving beyond the specific scope of the AMES, a related but extensive literature has developed on the co-dependence of the electric grid and water resources in the form of the Energy Water Nexus (EWN) [16,108–126]. Together, these works provide an insight into the resource and process complexity of the AMES. Furthermore, they also demonstrate the potential benefits of analyzing and optimizing the AMES as a single system-of-systems rather than each system independently [127]. Other works have sought to model multi-energy systems [96,128–141] making use of energy hubs to facilitate and track the flows of energy often focusing on the interactions of electricity, natural gas, distributed heating, and renewable sources. These approaches lack a SysML approach to explicitly define each component with their allocated processes and associations within the defined architecture. Additionally, specifically under the IIIE methodologies, research has analyzed life cycle assessments (LCA) and efficiencies of energy systems including the coal enterprise, oil and gas integration, environmental impacts, efficiency measures for the USA, and energy demand models [142–147].

It is worth mentioning that much of these works focus on a single interaction between two energy systems and consequently, to our knowledge, this is the first work to address the architecture of the AMES as a whole modeling electric, natural gas, oil, and coal enterprises in a single invariant SysML model. Furthermore, because the focus is usually on a single interaction, there has been little effort [109,148,149] to deploy a model-based systems engineering methodology where a system boundary is rigorously defined and then later elaborated in terms of physical interfaces and functional interactions. Ultimately, a complete architectural description is necessary to ensure that 1. energy and mass conservation laws are respected, 2. all environmental aspects are identified in environmental impact assessments [150], and 3. the greatest potential for synergistic outcomes are found. Finally, the use of model-based systems engineering, enterprise modeling, and industrial information integration engineering conventions (such as SysML) maximizes the potential for cross-disciplinary communication, coordination, and information to be integrated between enterprises.

2.4. Data-driven approach

This paper takes a ***data-driven approach*** and uses the S&P Global Platts (GIS) Map Data Pro data set [59] and the EIA Annual Energy Outlook dataset [12] to deduce the AMES reference architecture. The S&P Global Platts (GIS) Map Data Pro data set [59] is a proprietary data set available through the S&P Global Platts website. It is labeled with metadata that correspond to classes and attributes in the AMES formal resources. The classes and their associated behaviors are shown here, but their attributes have been suppressed for brevity. The interested reader is referred to original references for attribute metadata. Next, each GIS layer of the Platts dataset includes descriptions of facility types and their associated products. This data can be used to deduce the associated process(es) of these facilities. Finally, the process technologies for all of the AMES constituent energy facilities are well known. Therefore, this work relies on engineering textbook knowledge of these facilities to supplement the Platts and EIA datasets with low-level knowledge of input–output interfaces.

While the choice of a ***data-driven approach*** leads straightforwardly to a well-validated reference architecture model as the first step towards a digital twin, it is not without its limitations. First, the scope of this work is limited to only the energy systems themselves and not the end-use sectors outside of the AMES. Second, because Platts and EIA datasets only include bulk, wholesale, and transmission level assets, distribution-level and retail-level assets are outside the scope of the work. Finally, any assets outside of the conventional electric grid, natural gas system, oil system, and coal system are naturally out of scope as well. This includes non-conventional energy technologies and carriers (e.g. bio-energy, hydrogen, ammonia, etc.) which have yet to make a sizable impact on American energy infrastructure.

3. Modeling

This paper uses the Systems Modeling Language (SysML) [24,25,58,151–154] to define the AMES reference architecture. More specifically, the metadata of the input datasets are conserved, reorganized and drawn within SysML block definition and activity diagrams. This data-driven approach produces a SysML reference architecture that includes: 1. the different facilities that comprise the AMES resources and 2. their processes that comprise the AMES functionality and allocated architecture. Fig. 2 shows the system boundary of the AMES around its four constituent energy systems of electricity, oil, natural gas and coal. The high level flows of matter and energy between these four energy systems and across the system boundary are also defined. The matter and energy flows in Fig. 2 also restrict the set of operands in the AMES. While the Platts dataset does specify a much larger number of energy products, this analysis, for tractability, has classified all flows of matter and energy into the following set of operands: coal, raw natural gas, processed natural gas, crude oil, processed oil, syngas, liquid biomass feedstock, solid biomass feedstock, solar irradiance, wind energy, uranium, water energy (for cooling), electric power, withdrawn water, mine effluent, processing effluent, and thermal effluent. Therefore, Fig. 2 shows the input flow of these quantities of matter/energy operands from the domestic supply sources, the energy imports, and the natural environment across the system boundary and the output flow of these quantities to domestic consumption, energy exports, water treatment facilities, and the natural environment. In all cases, these input/output flows are specified in mass flow rates (e.g. Kg/time) or power (W) or both where the associated matter has an intrinsic energy content (e.g. heating value of natural gas).

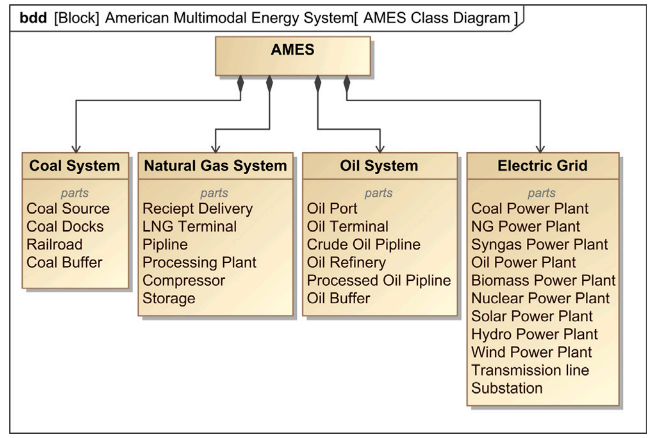

Fig. 3. AMES block definition diagram showing its four component systems.

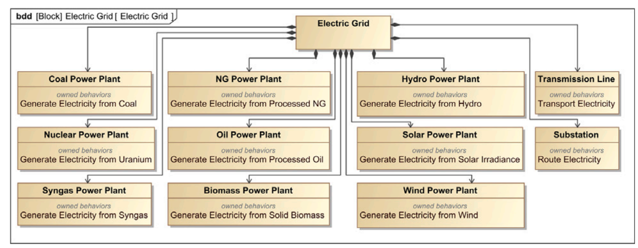

Fig. 4. Electric grid block definition diagram showing its component physical resources.

From a form perspective, Fig. 3 presents a class diagram of the AMES and its four constituent energy systems as classes. For graphical simplicity, each of these energy system classes adopt attributes to represent their component infrastructure facilities and resources. Furthermore, association links are removed for graphical clarity and may be otherwise deduced from the associated activity diagram. The following subsections elaborate the form and function of these systems.

3.1. Electric power enterprise

The electric power enterprise is comprised of resources for the generation, transmission, and routing of electric power. Power plants comprise a majority of the different types of resources within the electric grid. Each power plant type is designated by the primary fuel category used to generate electric power. There are nine different types of power plants present: coal, natural gas, syngas, oil, biomass, nuclear, solar, hydro, and wind. These power plants are connected to the electric grid by transmission lines (to the distribution system). The last component of the electric grid that realizes the end of the electric grid value chain is substations where the electric power leaves the transmission system. Fig. 4 presents the formal decomposition of the AMES electric grid architecture.

Each of the individual resources within the electric power system have their respective processes. Fig. 5 presents the electric grid activity

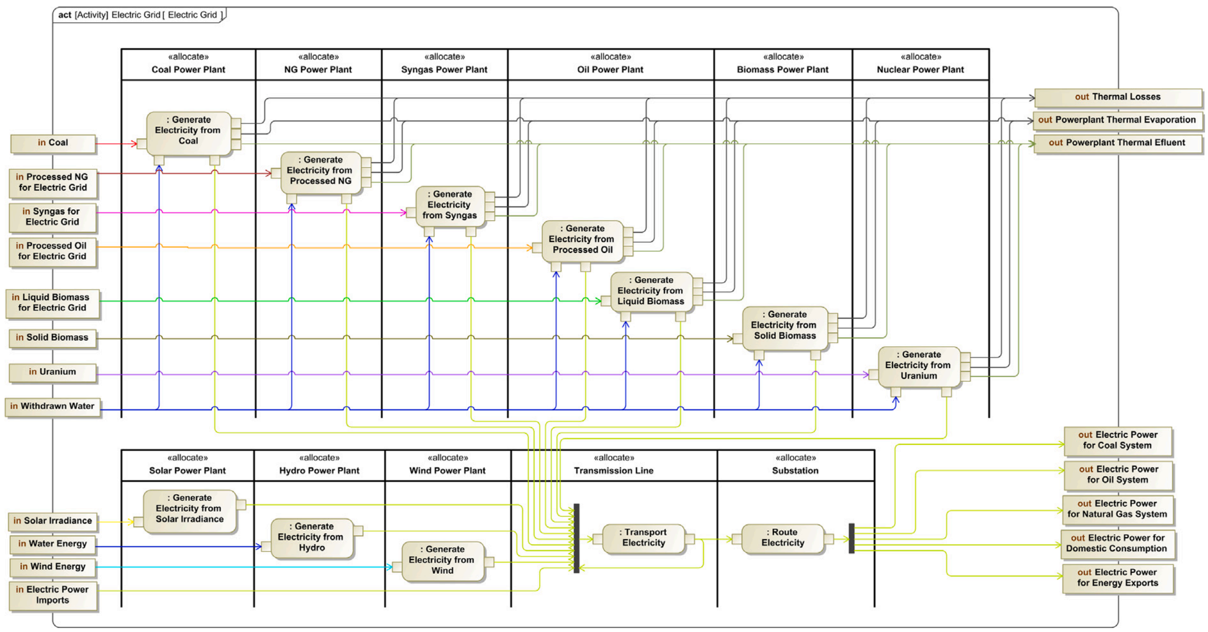

Fig. 5. Electric grid activity diagram with allocated swim-lanes.

diagram that shows these processes allocated onto their respective form in swim-lanes and follows the flows of matter and energy between the processes. Each power plant has their respective generate electric power process from their designated fuel source. The thermal generation processes Generate Electricity from Coal, Generate Electricity from Processed NG, Generate Electricity from Syngas, Generate Electricity from Processed Oil, Generate Electricity from Liquid Biomass, Generate Electricity from Solid Biomass, and Generate Electricity from Uranium each take their respective fuel source and withdrawn water as inputs and result in electric power, thermal losses, power plant thermal effluent, and power plant thermal evaporation. Aside from electric power, all of the remaining outputs immediately leave the system boundary. In contrast, the electric power is then transported by the transmission lines. The electric grid value chain is completed at the substation which routes the electric power to the other AMES energy enterprises or to the electric distribution system outside the scope of this reference architecture.

3.2. Natural gas enterprise

The natural gas enterprise is comprised of resources for the import, export, processing and delivery of natural gas. The receipt delivery and Liquefied Natural Gas (LNG) terminals are responsible for importing and exporting natural gas into and out of the natural gas system. These resources take both international and domestic imports into the United States' natural gas pipeline infrastructure. Pipelines and compressors are present for facilitating the transportation of natural gas. Additionally, processing plants are present for processing raw natural gas. Finally, storage facilities store syngas as well as raw and processed natural gas. Fig. 6 presents the formal decomposition of the AMES natural gas system architecture.

Each of the individual resources within the natural gas system have their respective processes. Fig. 7 presents the natural gas activity diagram. It shows natural gas processes allocated onto their respective form in swim-lanes and follows their flow of matter and energy. The Receipt Delivery facility can import and store syngas, raw natural gas, and processed natural gas as well as export the processed natural gas out of the system boundary. The LNG Terminal can import, store and export natural gas. Once inside the natural gas system, pipelines transport each of the operands, syngas, raw natural gas and processed natural

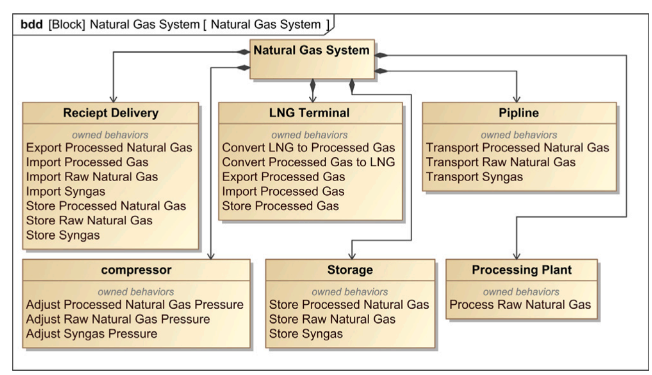

Fig. 6. Natural Gas system block definition diagram showing its component physical resources.

gas, through the United States. This includes pipelines that transport directly to natural gas electric power plants in the electric grid. With the inputs of raw natural gas, electric power and withdrawn water, processing plants process raw natural gas to produce processed natural gas and processing effluent. Compressors stimulate the transportation of the different types of natural gas by adjusting the associated pressure. Finally, storage facilities store syngas as well as raw and processed natural gas.

3.3. Oil enterprise

The oil enterprise is comprised of resources for the import, export, and delivery of oil. The oil port and oil terminal are responsible for importing and exporting oil into and out of the oil system. These resources take both international and domestic imports into the United States' oil pipeline infrastructure. Crude and processed oil pipelines are present for facilitating the transportation of oil and liquid biomass. Oil refineries allow for the processing of crude oil into processed oil, and oil buffers allow for storage within the oil system infrastructure. Fig. 8 presents the formal decomposition of the AMES oil system architecture.

Each of the individual resources within the oil system have their respective processes. Fig. 10 presents the oil activity diagram. It shows

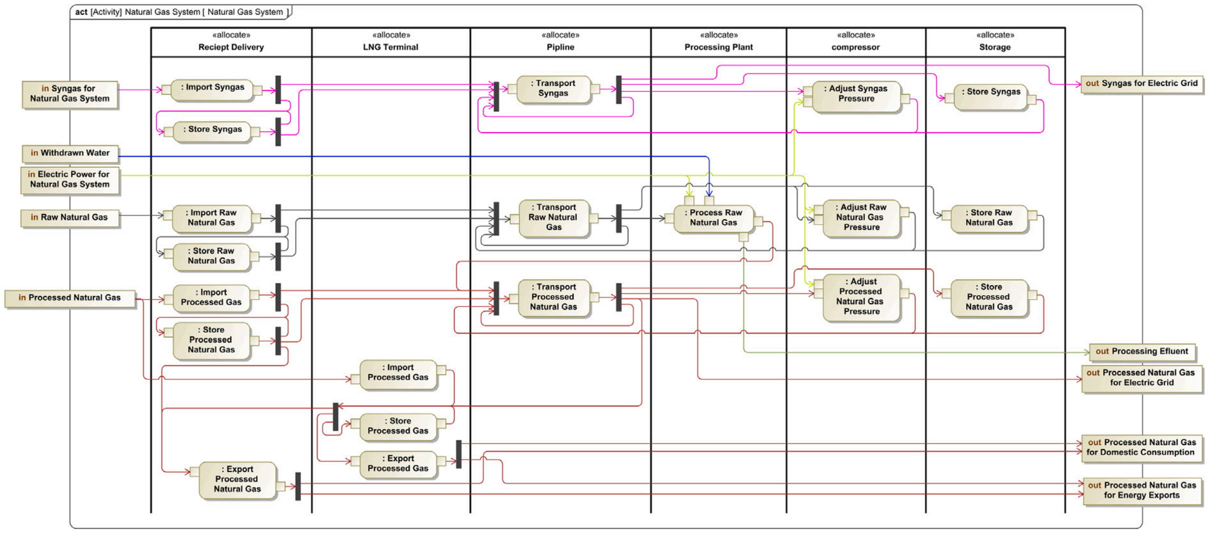

Fig. 7. Natural gas system activity diagram with allocated swim-lanes.

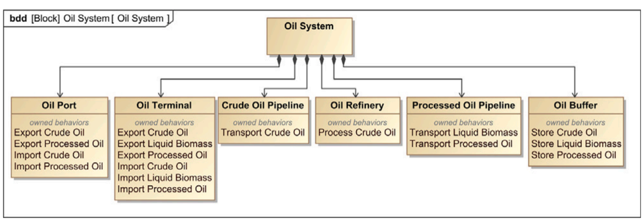

Fig. 8. Oil system block definition diagram showing its component physical resources.

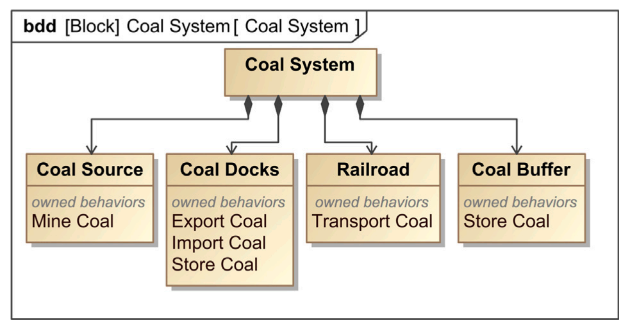

Fig. 9. Coal system block definition diagram showing its component physical resources.

the oil system's processes allocated onto their respective form in swim-lanes and follows their flows of matter and energy. The Oil Terminal facility can import and export crude oil, processed oil and liquid biomass to and from outside the system boundary. The Oil Port can also import and export crude and processed oil. Once inside the oil system, the crude oil pipeline can transport crude oil from an oil port or terminal to an oil refinery where the crude oil is processed into processed oil. This process requires the input of crude oil, electricity and withdrawn water to produce processed oil, syngas [60] and processing effluent. The processed oil can then be transported by the processed oil pipelines. These processed oil pipelines transport processed oil and liquid biomass within the oil system and directly to oil and liquid biomass electric power plants in the electric grid. Additionally, all three operands, crude oil, processed oil, and syngas can be stored within the oil system by oil buffers.

3.4. Coal enterprise

The coal enterprise is comprised of resources for the import, export, and delivery of coal. The coal sources are responsible for mining domestic sources of coal and introducing coal into the United States coal system. Coal docks are also responsible for the import and export of coal. Railroads are responsible for transporting coal across the United States and to coal electric power plants in the electric grid. Finally, coal buffers allow for the storage of coal within the system boundary. Fig. 9 presents the formal decomposition of the AMES coal system architecture.

Each of the individual resources within the coal system have their respective processes. Fig. 11 presents the coal activity diagram. It shows these processes allocated onto their respective form in swim-lanes and follows their flow of matter and energy. With the input of electric power and withdrawn water, the coal source can mine coal to produce coal and mine effluent. Alternatively, the coal docks can import coal into the coal system which can then be transported by the railroads. The coal can then be stored within a coal buffer or exported out of the coal system boundary by a coal dock.

4. Discussion

The activity diagrams in Figs. 5, 7, 10, 11 each show the individual energy enterprises that when integrated together form the AMES shown in Fig. 2. When following the flows of matter and energy through the AMES, it becomes apparent that every subsystem is connected to the other. The coal enterprise produces and imports coal that is delivered to the electric grid for electric power generation. The oil enterprise is able to produce and deliver syngas to the natural gas enterprise as well as deliver processed oil and liquid biomass to the electric grid for electric power generation. The natural gas enterprise is able to deliver syngas and processed natural gas to the electric grid for electric power generation. Finally, the electric grid is able to deliver electric power to the coal enterprise for mining, the oil enterprise for processing crude oil, and to the natural gas enterprise for processing raw natural gas and gas compression. Each of these connections allow the electric grid to produce electric power from the other energy enterprises' fuel sources and subsequently deliver power to the United States. Additionally, the electric power allows for the production and processing of operands in the coal, oil, and natural gas enterprises so that they may provide fuel sources back to the electric grid and the rest of the United States' fuel demands.

Understanding the nature of such interdependencies within the AMES reference architecture facilitates changes to the AMES as it is

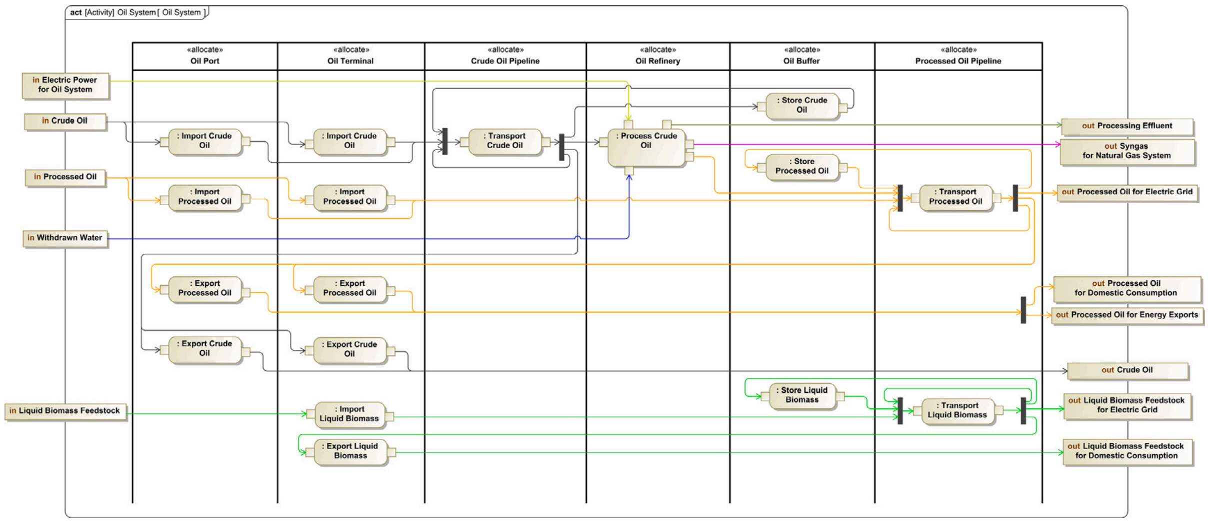

Fig. 10. Oil system activity diagram with allocated swim-lanes.

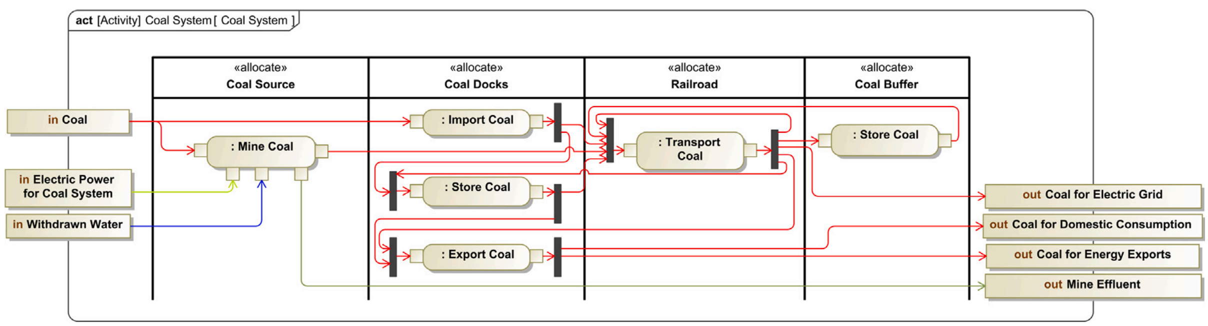

Fig. 11. Coal system activity diagram with allocated swim-lanes.

currently instantiated [155–157]. This knowledge becomes particularly important in avoiding cross-sectoral cascading failures [36,90,158]. For example, if a natural gas pipeline fails, there is not only a loss of natural gas being delivered for heating, but for electric power generation as well. Unavailable electric power plants not only diminishes the grid's ability to meet residential, commercial, and industrial demand, but also the load demanded by the other energy systems.

These interdependencies in the AMES reference architecture often exaggerate "infrastructure lock-in" effects that impede the forward-motion of the sustainable energy transition [159–163]. As coal power plants are decommissioned, natural gas power plants are often installed in their place with commensurate reductions in greenhouse gas emissions. These benefits, however, are not realized until sufficient natural gas pipeline capacity is secured; either on existing or potentially new pipelines. Similarly, electric power transmission capacity often impedes the full utilization of remote solar and wind generation resources. Alternatively, the presence of excess processing and transmission capacity for coal, oil, and natural gas makes it very easy and economical to rely on these sources in the electric power sector. For example, the electric power grid is likely to retain its reliance on the natural gas enterprise for a long time because so much of the country relies on natural gas for heating. In short, an effective "deep" decarbonization strategy requires the coordination of all four energy sectors and not just one alone.

4.1. Integrated planning and operations and model development

By planning future infrastructure developments and shifts with an integrated view of the whole AMES, developments with the greatest beneficial impacts can be planned and installed. The information integrated between all energy enterprises allows for a holistic planning effort that incentivizes simultaneous developments in multiple energy systems such that they compliment, rather than impede, each other. For example, if a coal mine is decommissioned in the coal enterprise, then a coal power plant in the electric grid could be replaced with a less carbon-intensive power plant. The EWN literature has already demonstrated similar benefits [117–120,164,165]. For example, the straightforward installation of water storage capacity has been shown to alleviate power balance constraints in the electric power grid where the installation of battery energy storage is at a premium. Similarly, the natural gas–electricity literature has shown pairing natural gas electric power plants with variable energy resources (VER) such as wind turbines provides a smaller carbon footprint with renewable wind energy and natural gas replacing coal [99,166,167]. Additionally, the fast ramping capacity of natural gas power plants provides reliability in maintaining a stable grid in the presence of VERs. In all of these cases, one or more layers of planning and operations management decision-making are superimposed on the underlying interdependent infrastructure enterprise's instantiated mathematical model.

4.2. Dynamic simulation model development

The development of the AMES reference architecture facilitates the subsequent development of instantiated mathematical models and simulations of system behavior. As a relevant precedent, the energy-water nexus reference architecture [109,148] led to the development of holistic mathematical models [108,110,112,115,168] which were later implemented as numerical simulations. To this end, the reference architecture provides the starting point for a ***transparent*** objected-oriented software design grounded in "digital twin" principles. Much like the National Energy Modeling System (NEMS) [169], the AMES reference architecture can be used to model and simulate the effect of potential policies and future infrastructure developments. By using the reference architecture's standardized ontology to define components and their interactions, one can instantiate an existing or simulated architecture. For example, using the Platts Map Data Pro [59] to guide the installation of resources and their subsequent associations, a SysML-compliant model of the AMES can be created. By then varying the ratios of instantiated technologies belonging to the instantiated model variant, different scenarios can be analyzed to further advance the AMES development. Furthermore, additional IIIE methodologies could them be applied such as LCAs, automated production management simulations, or energy demand models [143,145–147].

Just as the AMES reference architecture allows for the simulation and analysis of differing policies across the entirety of the AMES, it also allows for integrated operations management and power flow analysis. As seen in past energy-water nexus works, the mathematical models were later used to conduct sensitivity analyses and identify input/output trade-offs [110,114,116,120,149]. Such an approach of translating a reference architecture into a dynamic simulation/optimization model has been further generalized using hetero-functional graph theory [170]. As demonstrated in previous work [171], the use of continuous, timed, and arc-constant colored Petri nets facilitate the transition of a reference architecture into a (generic) hetero-functional minimum cost flow optimization problem. By introducing a device model for each capability independently, the modeler can control the relevant time scale, and thereby eliminate fast dynamics with steady state approximations. This allows for each device model to be integrated into the model with the same choice of relevant temporal resolution. Applying these device models can be viewed as a generalization of a similar procedure that has been demonstrated for electric power system modeling and simulation [172]. As each individual capability receives their own device model, the energy flows of differing types throughout the system can all be optimized together towards a well defined objective.

4.3. Structural analysis model development

Additionally, recent theoretical works [37,170,173] have shown that SysML-based reference architectures of interdependent infrastructure systems can be translated, without loss, into mathematical structural models called hetero-functional graphs (HFG). These HFGs can then be used to study the AMES structural resilience under varying scenarios [37,173]. By allocating function onto instantiated individual resources, capabilities are formed which can be chained together to complete a value chain and define deliverable services. Through tracking the number of deliverable services present in the instantiated model, the structural resilience can be analyzed [173]. By changing the ratios of these instantiated technologies from the reference architecture, the number of deliverable services will also vary; thereby changing the associated structural resilience. Alternatively, the instantiated model could be placed under attack, which would dictate the gradual removal of capabilities, and decrease the structural resilience as the instantiated model degrades. Using the AMES reference architecture to guide the instantiation of various scenarios, future AMES technology compositions can be analyzed to guide the energy transition.

4.4. Pathways to a sustainable energy transition

Returning to the original motivation of the paper, the AMES reference architecture serves as a critical step in a Model-Based Systems Engineering methodology to the sustainable energy transition. In that regard, the AMES reference architecture remains invariant while the instantiated architecture undergoes three architectural changes. The well-received United States Deep Decarbonization Pathways report [7] identifies these three changes as: 1. the increased penetration of renewable energy technologies into the electric power system 2. the increased penetration of energy-efficient (consumption) technologies of all types, and 3. a systematic electrification of energy consuming technologies. Furthermore, it identified four viable scenarios that mix the relative importance of these three architectural changes. Because all of these architectural changes are reflected already in the S&P Global Platts (GIS) Map Data Pro data set, the AMES reference architecture can be instantiated straightforwardly to create digital twins of these four viable scenarios. In that regard, the implicit assumption of stationarity in the dataset does not impede modeling and analysis of the AMES instantiated architecture despite the profound changes required by the sustainable energy transition.

5. Conclusion

The American Multi-modal Energy System reference architecture is an invariant reference architecture that describes the electric grid, the oil enterprise, the natural gas enterprise, and the coal enterprise as well as their inter-dependencies. As American energy demands in the 21st evolve to meet new requirements for energy sustainability, resilience, and access, the AMES instantiated architecture will also evolve, but the AMES reference architecture ontology will remain largely unchanged. Instead, the ratios of instantiated elements will change resulting in more carbon-intense resources being instantiated less and carbon-lite or carbon-free resources being instantiated more. This AMES reference architecture provides the consistent basis from which to run simulations on new policies and the associated changes of instantiated architecture. Furthermore, the AMES reference architecture facilitates the formulation of new optimal planning and operations management decisions. As previously demonstrated in the NG-Electricity nexus literature and the energy-water nexus literature, these decisions can identify synergistic strategies that simultaneously enhance infrastructure cost, reliability and sustainability. Such synergistic strategies are often able to overcome typical "infrastructure lock-in" scenarios and the ensuing "trilemma" debates on energy sustainability, resilience, and access. In short, holistic AMES enterprise models present new possibilities for energy infrastructure integration and coordination that may have been otherwise overlooked when addressing each energy enterprise independently. Through future work exploring the static and dynamic simulations of the AMES, this reference architecture provides the first ontologically grounded step towards guiding the energy transition.

CRediT authorship contribution statement

Dakota J. Thompson: Methodology, software, Validation, Writing – original draft, Writing – review & editing, Visualization. **Amro M. Farid:** Conceptualization, Methodology, Validation, Writing – review & editing, Supervision, Project Administration.

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 authors do not have permission to share data.

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