A MULTISCALE MODELING AND OPTIMIZATION FRAMEWORK FOR THE DESIGN OF ENERGY SYSTEMS WITH EMBEDDED LIFE CYCLE CONSIDERATIONS

A Thesis

by

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ABSTRACT

The role of dynamic energy storage in future energy systems driven by a mix of intermittent renewable power generation and dense energy carriers (DECs) cannot be understated. Reliable energy storage could pay dividends in terms on grid resilience and energy security as well. Nevertheless, in the context of promoting a systematic energy transition towards net-carbon neutrality by 2050, the long-term environmental impact of energy storage from the perspective of materials utilization and supporting sustainable power generation mandates a thorough evaluation. To this end, the article presents a modeling and optimization framework developed in the *energiapy* package to analyze the at-scale life-cycle impact of different technology pathways. The mixed integer programming (MIP) framework is applied towards the design of future integrated energy systems consisting of both renewable power generation through solar or wind power, DECs production, and battery energy storage. The trade-offs between the levelized cost of energy and the environmental impacts, the potential to exploit synergies between value chains, and the comparison of different cost and technology scenarios are elucidated upon.

DEDICATION

To my mother Liying and my father Shaofeng.

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NOMENCLATURE

MIP	Mixed Integer Programming
MILP	Mixed Integer Linear Programming
MINLP	Mixed Integer Nonlinear Programming
mpLP	Multiparametric Linear Programming
DECs	Dense Energy Carriers
ESS	Energy Storage System
EIA	Energy Information Administration
EES	Electrical Energy Storage
PSH	Pumped Storage Hydropower
BES	Battery Energy Storage
VRB	Vanadium Redox (Flow) Battery
DOD	Depth of Discharge
SOC	State of Charge
ZEBRA	Zero Emission Battery Research
CAN	Composite Asymmetric Nonwoven
EV	Electric Vehicle
ORNL	Oak Ridge National Laboratory
O&M	Operation and Management
GHG	Greenhouse Gas
CCUS	Carbon Capture, Utilization and Sequestration
GWP	Global Warming Potential
NREL	National Renewable Energy Laboratory

NSRDB	National Solar Radiation Database
DNI	Direct Normal Irradiation
ERCOT	Electric Reliability Council of Texas
CAPEX	Capital Expenditure
CAES	Compressed Air Energy storage
MILP	Mixed Integer Linear Programming
OPEX	Operating Expenditure
WF	Wind Farm
NMC	Nickel Manganese Cobalt
LFP	Lithium Iron phosphate

TABLE OF CONTENTS

Page

ABSTRACT ii

DEDICATION iii

ACKNOWLEDGMENTS iv

CONTRIBUTORS AND FUNDING SOURCES v

NOMENCLATURE vi

TABLE OF CONTENTS viii

LIST OF FIGURES x

LIST OF TABLES xii

1. INTRODUCTION AND LITERATURE REVIEW 1

2. BACKGROUND 4

   2.1 Renewable power generation 4
   2.2 Energy storage 4
      2.2.1 Electrochemical battery storage 5
      2.2.2 Non-electrochemical energy storage 8
   2.3 Material transition 11

3. MODELING AND OPTIMIZATION FRAMEWORK 15

   3.1 General energy system data acquisition and collection 15
   3.2 Overview of embedded components 19
   3.3 Model formulation 21

4. COMPUTATIONAL EXAMPLES 30

   4.1 Scenario analysis 32
      4.1.1 Meeting different demand loads 33
      4.1.2 Changing technology pathways 38

5. CONCLUSION 42

6. FURTHER STUDY 43

REFERENCES 46

APPENDIX A. 52

A.1 Wind farm economic model 52
A.2 CCUS model 56

APPENDIX B. KEY CONSTRAINT OF THE FRAMEWORK 58

B.1 Key constraint and framework implementation in material and electricity distribution model 58
B.2 Nomenclature of sets 63
B.3 Nomenclature of parameters 63
B.4 Nomenclature of variables 64

LIST OF FIGURES

FIGURE Page

1.1 Integrated energy system pathways. 3

2.1 Material flows for electric vehicle (EV) manufacturing. 13

3.1 Superstructure for wind farm using Resource-Task Network (RTN) 16

3.2 Conversion factor for solar photovoltaics (PV) array in Houston. 16

3.3 Conversion factor for natural gas in Houston. 17

3.4 Varying demand factor for power obtained from ERCOT for the houston region. 18

3.5 A schematic representation of electrochemical battery storage model 28

4.1 Capacity contribution of WF1 process. This further illustrated that mobility transition with hydrogen as a mobility fuel is indeed a feasible pathway when tackling the intermittent issue of wind energy production. DAC: direct air capture, LiI_c and LiI_d: lithium ion battery charge and discharge process, respectively, AKE: alkaline water electrolysis, $H2_{Lc}$ and $H2_{Ld}$: liquid hydrogen charge and discharge process 31

4.2 The GWP value of the network. 31

4.3 Capacity utilization of WF1. The utilization value fluctuates between full utilized to 70 33

4.4 Superstructure for wind energy-EV/Hydrogen-HV system model using Resource-Task Network (RTN). 34

4.5 Schedule for hydrogen storage for demand=1000 MW scenario. Note that the model chooses to rely on storage of power in the chemical form (H_2) for large scale storage instead of batteries. Note that hydrogen storage is relatively long-term and experiences lower storage loses. 36

4.6 Schedule for battery energy storage for demand=100 MW scenario. For the moderate demand scenario, the model chooses both battery energy storage as well as production and storage of hydrogen to meet a varying demand. Hence, a mix of both options can tackle both seasonal and diurnal variability. However, given the low capacity realized, it can be inferred that batteries merely supplement hydrogen storage. 37

4.7 Schedule for hydrogen storage for demand=100 MW scenario. Hydrogen storage is setup alongside battery energy storage. 37

4.8 Superstructure for PV/WF system model using Resource-Task Network (RTN). 38

4.9 Schedule for battery energy storage for using solely PVs, material of PV3: Cadmium telluride (CdTe). 39

4.10 Schedule for battery energy storage for using solely PVs and excluding Li-ion battery. 39

4.11 Capacity contribution for using solely PVs and excluding Li-ion battery. The Cadmium Telluride solar PV is shown to be the most cost conscious option. While more expensive than wind farms, the associated emissions are lower. 40

4.12 Capacity utilization for WF A-C and PV A-C combination for the 10MW case mirrors the demand profile, as the demand is met directly and entirely through power generation and no storage is necessary. 40

4.13 GWP of the four scenarios. 41

4.14 Cost of the four scenarios. 41

6.1 An important piece of future energy systems–Electric Vehicles. 45

B.1 Sets declaration. 58

B.2 Parameter set up. 59

B.3 Variables declaration. 60

B.4 Framework implementation of constraint B.1 60

B.5 Framework implementation of constraint B.2 61

B.6 Framework implementation of constraint B.3 61

B.7 Framework implementation of constraint B.4 62

B.8 Framework implementation of constraint B.5 62

B.9 Framework implementation of constraint B.6 62

LIST OF TABLES

TABLE Page

2.1 Economic aspects of various electrical energy storage technology options 11

2.2 Environmental aspect of EES 14

4.1 Data of the main components in the scenarios 34

1. INTRODUCTION AND LITERATURE REVIEW

In 2021, renewable energy sources accounted for about 12.2% of total U.S. energy consumption and around 20.1% of electricity generation (EIA). The intermittent availability of solar and wind energy could exacerbate the need for dynamic energy storage to meet variable and asynchronous energy demand. While electro-chemical battery storage is apt for such applications, the high global warming and toxicity potential of the constituent materials has challenged the notion that the large-scale dispatch of renewable technologies, in itself, is enough to drive the energy transition. To this end, it becomes important to analyze these systems in the context of circular economic considerations.

Moreover, the challenges in terms of integration impede the stable operation of the grid by posing many operational and control challenges. Firstly, renewable intermittency is subject to both diurnal and seasonal variations. Secondly, there exits a mismatch between resource availability and energy demand, which poses a critical challenge in maintaining energy efficiency, deployment, and market penetrability. In the context of decentralized power generation at residential and commercial points of energy consumption, surplus energy can also be reversed to both lend stability to the grid by supplementing power generation, while also providing economic incentive.

Currently, economies with a large share of renewables, Texas for example, continue to be supplemented by conventional power generation, which are dispatchable and provide a high degree of control over the power output. Nevertheless, coal and natural gas power generation have a high carbon intensity. Sustainable and robust energy storage system (ESS) will play a vital and requisite role in mitigating the fluctuation by storing superfluous generated energy during peak wind hours to be used during periods of high demand. However, investment costs and accompanying pollution need to be carefully evaluated (1; 2).

Nevertheless, for heavy industries like iron and steel, cement and chemicals, renewable energy account for less than 1% of the combined energy demand (3). Currently, a renewable energy mix of electricity, solar, wind, and nuclear is still the chief source being used to supply the loads according to Marco (4).

The variability and uncertainty of power output are the two rudimentary obstacles of the bulk integration of renewable energy sources with the existing grid. The trend of growing demand for energy storage will definitely last for a long periods as the penetration of renewable energy into the electric grid increases year by year because of the aforementioned strengths and marked reduction in cost. There is a big opportunity to realize a sustainable energy transition through the integration of ESS with renewable power. ESS with high power ratings and a long operation will play a formidable role in making variable renewable energy (VRE) attractive.

Energy storage mechanisms also face many challenges such as storage capacity, response time, efficiency,cost, durability, material constraint, recycle potential, water and land requirements, toxicity potential, and life cycle green house gas emission to name a few. Moreover, the subsequent complexity of determination of supply network and trade offs. In the presented work, a framework is developed to analyze the at scale impact of various power generation and energy storage technologies that meet the requisite dynamicity for application in modern grids. The remainder of this paper is constructed as follows. Chapter 2 presents a overview of EES technology pathway where readers could acquire general insights and expand their understanding of the trends of EES. Chapter 3 describes the model formulation and solution strategy which is aimed to provide utility operators in decision-making and future planning for the best optimisation solution. Chapter 5 provides a summary on overall findings from the review. Lastly, Chapter 6 intensifies the conclusions and potential future works.

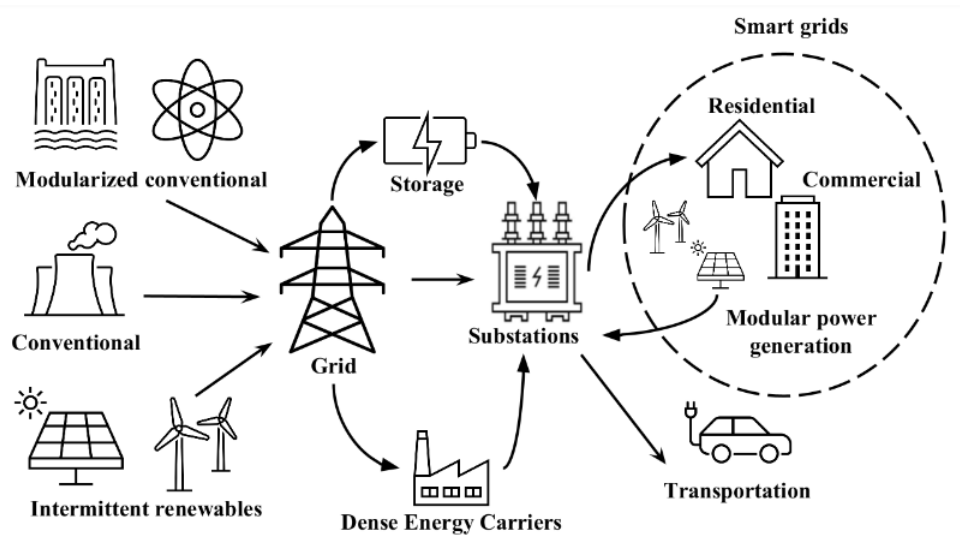

Figure 1.1: Integrated energy system pathways.

2. BACKGROUND

Mature and promising electrical energy storage (EES) and power generation technologies from the author's point of view which are particularly largely used in wind farm are briefly reviewed in regards to their main technical characteristics, life cycle impact, and costs of implementation.

For power generation, we mainly focus on the renewable generation of power through wind farms (WFs) or solar photovoltaics (PVs) of different makes. Further, battery energy storage is appropriate for the dynamic dispatch requried to tackle intermittency. To this end, we consider various forms of battery storage. The WFs, PVs, and batteries all vary significantly in terms of their material utilization and costs.

2.1 Renewable power generation

Arrays of wind mills have already seen utility scale application driven largely by improvements in efficiency and the reduction in costs in recent years which has made renewable energy generation techno-economically competitive. Moreover, these trends are expected to continue unabated in the coming decades, especially given that some of the considered processes are yet to attain the techno-economic maturity required for large scale deployment. Also, wind is intermittent and, hence, needs to be used in tandem with energy storage to regulate the system and realize a resilient system. Additionally, although battery storage does have the advantage of not being restricted by the geological conditions, making it indispensable to reduce the need for grid scale storage in locations where PSH is not feasible, the post-use of battery materials is yet to be adequately addressed. Nonetheless, researchers are making effort towards modular PSH as well which is more deployable and conscious.

2.2 Energy storage

Presently PSH is most widely used at the utility scale amongst all the technology pathways. Nonetheless, PSH is not applicable for all locations and in spite of promoting the modularization of the technology, it is predictable that will be a booming in electro-chemical battery storage in the next twenty or thirty years. The renewable power generated in the system is sourced directly to a grid. Lithium ion battery, lead-acid battery, and nickle cadmium battery all are the mature technologies in wind turbine and competing battery technologies such as sodium-sulfur, sodium-metal halide, zinc-brine, vanadium redox batteries are also likely to reach technical maturity.

2.2.1 Electrochemical battery storage

The battery electricity storage systems are mainly used as ancillary services or for supporting the large-scale wind integration in the existing power system, by providing grid stabilization, frequency regulation and wind energy smoothing. Battery is one of the common used electrical energy storage system and includes several different types. Battery energy storage (BES) can be separated as both conventional (lead-acid, NaS, Ni-Cd, Li-ion) and flow batteries (VRB, Zn-Br) focusing on their technical characteristics and life cycle cost.

Lead-acid battery. The most widely used rechargeable battery currently for application in small wind power system is the lead–acid battery. Lead oxide (PbO_2) and lead (Pb) serve as the cathode and anode, respectively, with sulfuric acid serving as the electrolyte. Compared to other rechargeable batteries, lead–acid batteries have relatively low energy density (25-35 Wh/Kg) (5). Despite this, their ability to supply high surge currents means that the cells have a relatively large power-to-weight ratio. Their limited life cycles (6), short discharge time (1 min to 8 h) and low energy density make them not good choices for energy time-shift purposes. Lead-acid battery life is highly dependent on depth of discharge (DOD) where typically the battery is cycled between 50% and 80%. Lead-acid batteries should not be typically operated at low state of charge (SOC), otherwise it suffers from significant degradation in design lifetime. The SOC is generally prevented from going below 20% when an extended battery life is desired.

NaS battery. NaS batteries use molten sodium and molten sulfur as the two electrodes, and employs beta alumina as the solid electrolyte. The reactions normally require a temperature of 574-624 K to ensure the electrodes are in liquid states, which leads to a high reactivity (7). The operating temperature is too high which can limit its application on energy storage particularly regarding to the safety issue. NaS batteries are one of the most proven electrochemical storage technologies in MW scale. NaS batteries have shown capabilities in power quality applications and power time shift, with relatively high overall efficiency (75–85%), 4500 life cycles, expected lifetime of 15 years, and discharge time up to 7 h (8; 9). The power rating is scalable, promising more utility-scale demonstrations in the future (10).

$NaNiCl_2$ battery. Sodium–nickel–chloride batteries, known as ZEBRA (Zero Emission Battery Research), are high-temperature batteries (270–350 °C), in which nickel chloride is employed as the cathode instead of sulfur (11). $NaNiCl_2$ batteries have shown relatively high overall efficiency (86–88%), 2500-3000 life cycles, expected lifetime of 15 years, and discharge time up to 5 h (6). They have been commercially available since about 1995 and have been successfully employed in several mobile applications. In general, more research is needed to address the energy density and environmental issues of Na-ion batteries for their large-scale adoption in the grid-scale services (12; 13).

Li-ion battery. One of the most common electrochemical energy storage system in large scale wind turbine is Li-ion battery. It uses lithium metal oxide as cathode material and graphitic carbon as anode. The electrolyte is normally a non-aqueous organic liquid containing dissolved lithium salts, such as $LiClO_4$ (8). High energy density (200 Wh/kg), long lifetime (10,000 cycles), and relatively high efficiency (0.85–0.95) have offered sufficient motivation for the development of these batteries (14).The Li-ion battery energy storage system can smooth the fluctuation of wind power quickly and effectively. It can provide certain power support for the power grid when it fails. It can stabilize the voltage and frequency of the system and effectively ameliorates the performance of the wind power system. There are two sources in present lithium extraction, which are rock-based (spodumene, lepidolite, etc.) and brine-based. The levelized time-lag between project establishment and full release of production capacity is 3 years for rock-based lithium and 7 years for brine-based. As a result, suppliers struggled to keep up with fast-growing demand due to this ineluctable constraint (15; 16). Chen et al developed a self-driven lithium extraction method which was enabled by a composite asymmetric non-woven (CAN) and it's expected to reduce the energy consumption of lithium extraction from both rock and seawater/brine and thus saving energy costs (17).

Vanadium Redox (Flow) Battery. The VRB is one of the most mature flow battery systems (14). The VRB stores energy by using vanadium redox couples (V^{2+}/V^{3+} and V^{4+}/V^{5+}) in two electrolyte tanks. VRBs exploit the vanadium in these four oxidation states which makes the flow battery have only one active element in both anolyte and catholyte. During the charge/discharge cycles, H+ ions are exchanged through the ion selective membrane (18; 19). It has high life cycles (up to 13000) (6) and high efficiency (20) which means that it's a good candidate of electrochemical energy storage. However, the energy density is only 10-35 Wh/kg (6) and by the nature of flow battery system, the volume of VRB is much larger than other batteries. As a result, they are often stored in containers or even buildings which is not easy to move. At the same time, they also need a relatively mild temperature (5-40 °C) which can be applied to few scenes. These shortcomings affect the application in EVs, but they meet the needs of energy storage stations especially large-scale one, in which need safe and stable energy storage equipment. VRB would be the first choice from this aspect.

Zn-Br Battery. Zn-Br flow batteries belong to the hybrid flow batteries category. In a Zn-Br battery, two aqueous electrolyte solutions contain the reactive components, which are based on zinc and bromine elements, stored in two external tanks (19). It have inherent advantage in cost because the price of electrolyte determines the overall cost of batteries to a large extent (accounts for 30% of the total cost). The electrolyte consists of zinc, a common metal is readily available and inexpensive and bromine which is even more common and can be extracted from sewage. This innate trait determines the cost advantage of it. Although the issue of low efficiency (0.6-0.7) due to self-discharge phenomenon needs to be addressed (6), the capital cost is really low, similar to common lead-acid batteries. It can be seen that the price advantage is very obvious which lays a good foundation for the large-scale application of Zn-Br battery.

Ni-Cd battery. Other than lead-acid batteries, the other commonly used batteries in wind power generation systems are Ni-Cd batteries (also known as alkaline batteries). A Ni-Cd battery uses nickel hydroxide and metallic cadmium as the two electrodes and an aqueous alkali solution as the electrolyte. It normally has relatively high robust reliability and low maintenance requirements. They offer relatively high energy density (55-75 Wh/kg), low maintenance need, and life cycles between 2000 and 2500. The life cycle is highly depended on DoD so that it can reach 50,000 cycles in 10% DoD (8). The weaknesses of Ni-Cd batteries are: cadmium and nickel are toxic heavy metals, resulting in environmental hazards (21; 22); the battery suffers from the memory effect – the maximum capacity can be dramatically decreased if the battery is repeatedly recharged after being only partially discharged (23).

2.2.2 Non-electrochemical energy storage

Hydrogen, belonging to the category of power to gas energy storage, basically is a form of supplementary interweaved alternative for energy storage that can be employed to address the intermittency issues. There are chiefly two key technology pathways which are the blue and green pathways in the background of future energy systems which attempt to eliminate the technologically mature but carbon intensive grey pathways (24). Basically, blue pathway refers to hydrogen produced from natural gas through steam methane reforming and supported by carbon capture and storage viz. the CO_2 emitted during the manufacturing process is captured and stored permanently underground (25). Green pathway signifies that hydrogen is produced by electrolysis of water. Contemporarily, approximately three-quarters of global hydrogen production (70 Mt H_2/yr) comes from SMR, with a marginal contribution (0.5 Mt H_2/yr) which is integrated with carbon sequestration. Electrolysis of water, on the other hand, accounts for merely 0.1% of total H_2 production owing to prohibitive costs mainly because of expensive catalyst like platinum and a large energy requirement (24). Hydrogen as an energy source can be stored in the form of pressurized gas, liquefied gas in cryogenic tanks or in chemical compounds like ammonia and methanol as dense energy carriers (DECs) (6) while the first two modes are susceptible to storage losses as energy is also required for compression and liquefaction. While low energy metal hydride storage has been explored, the need for rare earth metals and the associated cost have confined their commercialization. For large scale storage, geological structure could play an essential role due to the reduction of the storage cost and storage losses significantly. However, this belies the requirement for investment in gas pipelines or other transportation methods. Large volume storage options such as underground caverns and depleted oil wells (DOWs) might whereas not always be locally procurable, which necessitates research into modular storage option (Rahul Kakodkar et al., 2022).

Energy density of hydrogen is as high as Li-ion batteries, which indicates the need for significantly smaller storage reservoirs compared to PHS and CAES. The stored hydrogen can be converted back to the electricity by fuel cells (compatible for mobile applications), gas-fired turbines, or gas-fired engines. Nowadays the comparatively low overall efficiency and enormous amount of capital costs are two chief obstacles in commercial application of hydrogen-based storage in grid-scale applications (6). Tractebel Overdick, a Belgian marine engineering company, has unveiled a solution for large-scale hydrogen storage at the sea, using offshore wind farm to produce and compress hydrogen and seabed salt cavern to store hydrogen. When there is a need on land, hydrogen produced by offshore platforms is piped directly to land; when the current demand is low, hydrogen is temporarily stored in salt caverns and then distributed when the demand is high, playing a role of peak regulation.

Pumped Storage Hydropower. PSH, belonging to the scope of mechanical energy storage systems, as the earliest large-capacity energy storage technology, has been widely used since the middle of the 20th century and has gradually become the most widely used one in the world. In times of excess energy, water is pumped from the lower to the upper reservoir, and is then released through a turbine to generate electricity during times of peak demand (Blakers 2015). There are various configurations of this technology, including open loop (one or more of the reservoirs are connected to a natural body of water) and closed loop (reservoirs are separate from natural waterways) (26). PSH offers quick synchronization, short response time, and the versatility to serve as both a load and a generator. PSH is very efficient in ensuring renewable energy supply is smoothed out over periods of peak energy demand. Wind energy require availability of certain climatic conditions to ensure uninterrupted supply, which is not always present (27). PSH can store the electricity generated by these resources and supply it when there is peak load energy demand, thus providing balancing services (28). The capital cost of PSH is quite high, however, the ratio between total investment and total processed electricity is far lower than other energy storage schemes (29). Comparing to BES, its life time is far longer although capital cost is high. Current new direction of PSH is modular PSH. Oak Ridge National Laboratory (ORNL) concluded a 4-year research, testing, and analysis project investigating a new lab-developed PSH technology, and results indicate promising cost and commercialization potential. It is a modular, scalable energy storage technology designed for a long life (>30 years), high round-trip efficiency (ratio of energy put in compared to energy retrieved from storage), and low cost.

Thermal energy storage. Electricity can be used to produce thermal energy, which can be stored until it is needed. One example is electricity can be reserved in thermal storage medium like molten salt during times of low demand and later water is heated to produce steam of high temperature and pressure by utilizing thermal storage medium to drive the turbo-generator to generate electricity. Another example is that electricity can be used to produce chilled water or ice during times of low demand and later used for cooling during periods of peak electricity consumption (30).

Economic data consists of capital cost, fixed operation and management (O&M) cost, variable O&M cost, life cycle and lifetime is shown in Table 2.1.

EES	Capital Cost ($/kWh)	Fixed O&M Cost ($/kW-yr)	Variable O&M Cost ($/kWh)	Life Cycle	Lifetime (yr)
Lead-acid Battery	350 (31)	11 (31)	0.0003 (31)	2500 (32)	10 (6)
NaS Battery	750 (31)	11 (31)	0.0019 (6)	4500 (31)	12 (6)
$NaNiCl_2$ Battery	875 (33)	5.9 (6)	0.0006 (6)	4500 (34)	15 (6)
Li-ion Battery	500 (35)	9 (35)	0.0003 (35)	2500 (33)	10 (6)
VRB	965 (31)	11.5 (31)	0.00035 (31)	5000 (31)	10 (6)
Zn-Br	265 (34)	4.6 (6)	0.0006 (6)	7500 (6)	7 (6)
PSH	104 (26)	24.5 (31)	0 (34)	20000 (36)	50 (36)
Hydrogen (fuel cell)	50 (36)	28.51 (26)	0.001 (26)	20000 (36)	20 (36)

Table 2.1: Economic aspects of various electrical energy storage technology options

2.3 Material transition

Greenhouse gas (GHG) emissions associated with the implementation of technology through the utilization of mined, recovered, refined, processed and molded materials can be significant. Emission consists of the functional use of technology (direct) and the implementation and manufacture of technology (indirect). Indirect emissions also refer to annualized emissions over the life time of the material production and are unavoidable as the recovery and processing of materials unavoidably releases carbon and other refuse. An example is that while renewable power generation technologies are emission-free at the point of service, the requirement for materials including metal and polymer could still result in high indirect emissions during the whole life cycle, as shown in Figure 2.1. Indirect emission and carbon sequestration through material production are both front ended, whereas direct emission and carbon capture and utilization happen throughout the temporal horizon.

The energy transition has challenged the demand for metals such as lithium (Li), nickel (Ni), cobalt (Co) which have a high human toxicity potential. For example, solid oxide fuel cells require materials which have supply constraints. A 250 kW cell needs 150 kg Nickle Oxide, 67 kg Yttrium-stabilized Zirconium (8% mole Y), and 0.62 kg Lanthanum-Strontium-Manganite (LSM). However, the global proven reserves of yttrium oxide stands at a mere 450,000 tons. Metal needed to transition entire TX fleet to EVs is also significant. Just the present widely applied Li-ion batteries need: 0.176 million metric tons (MMT) Lithium, 0.770 MMT Nickle, 0.44 MMT Manganese and 0.308 MMT Cobalt, which contribute 1.25%, 0.81%, 0.03%, 4.33% of global proven reserves, respectively. Water consumption associated with the implementation of technology through the utilization of recovered, refined, and processed materials should not be ignored, since it takes ~1892.7 tons of water per ton of lithium. Besides there is a potential to increase water toxicity.

The demand for non-metallic materials cannot be overlooked either. Polymeric materials are produced through mature technologies which have largely reached their full efficiency potentials, allowing better use of both energy and hydrocarbon feedstock. For example EVs now use a significantly higher amount of polymers (43). Per vehicle contain 150 kg polymer composites which are polypropylene (32%), polyurethane (17%) and PVC (16%). Polymer chains can also act as sinks for carbon, and their use has the potential to adhere to circular economic considerations through recycling and repurposing.

It is essential to note that it's not necessary to be carbon neutral at every stage yet the target is net carbon neutrality. This can be achieved by balancing emissions of carbon dioxide with its removal (often through carbon offsetting) or by eliminating emissions from society. It is understood that net-carbon neutrality over the lifetime of technology use can neither be quantitatively assessed nor realized without accounting for the flows of carbon comprehensively from well to wheel. Notably, promising carbon capture utilization and sequestration (CCUS) technologies are yet to achieve techno-economic maturity suitable for large-scale deployment. Nevertheless, in the near term, the utilization of carbon-based materials with circular economic benefits, the production of synthetic fuels, co-production and retrofitting of existing hydrocarbon facilities could be instrumental in promoting de-carbonization. It is imperative to note that the technology transition will also elicit a transition of energy resource feedstocks and infrastructural materials. The synergies between the constituent value chains are especially apparent in the carbon chain with products with myriad applications and characteristics being derived from the same raw materials such as 1) power generation, 2) energy storage through either electrochemical process or non-electrochemical process, 3) fuels production, 4) metals for construction of power production and energy storage facilities and 5) the synthesis of polymer materials for grid infrastructure. There is also potential for the recycle of materials spanning different value chains. Three points with regard to material transition needed to be illustrated is 1) the production of high value and long-lasting materials in order to reduce carbon emission, 2) material requirements to realize decarbonization, 3) circular pathways for the recycle and upcycle of carbon.

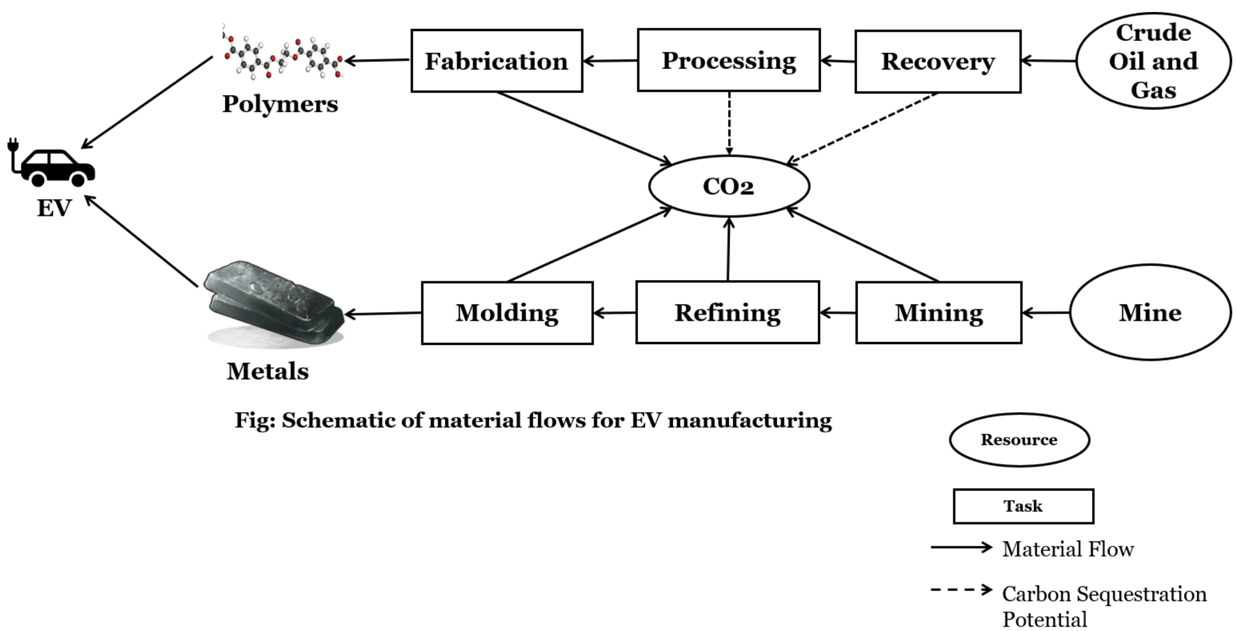

Figure 2.1: Material flows for electric vehicle (EV) manufacturing.

EES	Lifecycle GHG Emission (kgCO_2-eq/kWh)	Critical material of supply chain	Recycling potential	Environmental impact
Lead-acid battery	3.1 for VRLA type (37)	Antimony (29)	High recycle rates (99% in US) and high material value (38)	Lead and cadmium: Heavy metal contamination and toxicity
Na-S battery	2.8 (37)	Graphite (29)	Low material value (29)	Graphite dust, water pollution from acids
$NaNiCl_2$ battery		Nickel (29)	High material value	Nickle: water depletion
Li-ion battery	2.5 (37)	For NMC and LFP: graphite, fluorine, phosphate rock, lithium; For NMC: Cobalt (29)	Low material value except for cobalt in NMC, can reuse EV batteries for EES in wind farm (29)	Graphite dust, water intense in mining, water pollution from acids and large volume of waste rock
VRB	3.4 (37)	Vanadium (29)	Low material value, battery can be reused with new electrolyte (29)	Lower environmental impact compared to Li-ion battery, environmentally friendly (20)
Zn-Br battery	0.03 in manufacturing (39)	Zinc (29)	Both electrode and diaphragm materials are plastics (recyclable)	Abiotic resource depletion (40)
Ni-Cd battery	3.1 (37)	Nickel (29)	High recycling rates (95%) and value	Ni and Cd: toxicity of the heavy metals (6), technically low efficiency causes more disposal handling issue
PSH	18.5 (41)	Construction materials, water	Water	Destroy trees and animals and reduce water quality
Hydrogen	0 using water, 3 using natural gas (42)	Water or natural gas	Low	Producing CO_2 in natural gas pathway

Table 2.2: Environmental aspect of EES

3. MODELING AND OPTIMIZATION FRAMEWORK

In the following section, we discuss the solution methodology to resolve the simultaneous optimization of the material and energy transition using the features in the framework. In the example, we seek to evaluate the total emissions (direct + material sourcing) for different technology pathways and material (metals and polymer) required for construction.The schematic of this energy system model is shown in Figure 3.1. We take three cases of wind farm for distinct material compositions and allow multiple energy storage options, viz. Li-ion, NaCad, NaS batteries. Further, wind and solar are allowed to meet the power demand directly without storage. The model does not allow the purchase of electricity directly from the grid.

The framework was developed using the *energiapy* (44) python module. Notably, *energiapy* utilizes a hierarchical modeling paradigm, wherein resources are converted by process, which are in turn set up through the utilization of materials. The set of available processes are introduced at locations, and bespoke scenarios are generated and then formulated as MILP instances. All the required data sets are provided at appropriate resolutions and scopes, e.g. capital and operational expenditure are provided at the process level, intermittent renewable availability, daily demand, and resource prices are provided at the location level. Furthermore, constraints are available for: 1) balance of resource flows, 2) balance of material flows, 3) scheduling of resource purchase, discharge, production, inventory, 4) tracking of emission, and 6) costing. The objective considers the cost of establishing and operating processes and resource purchase.

3.1 General energy system data acquisition and collection

Computation techniques necessitate accurate data when testing, data-driven optimization is no exception. National Renewable Energy Laboratory (NREL) hosts databases such as the National Solar Radiation Database (NSRDB) which provides data for solar irradiance and wind speeds at five minute intervals. The solar Direct Normal Irradiation (DNI) and wind speeds at average one hour intervals in Harris County are gathered from the National Solar Radiation Database (NSRDB).

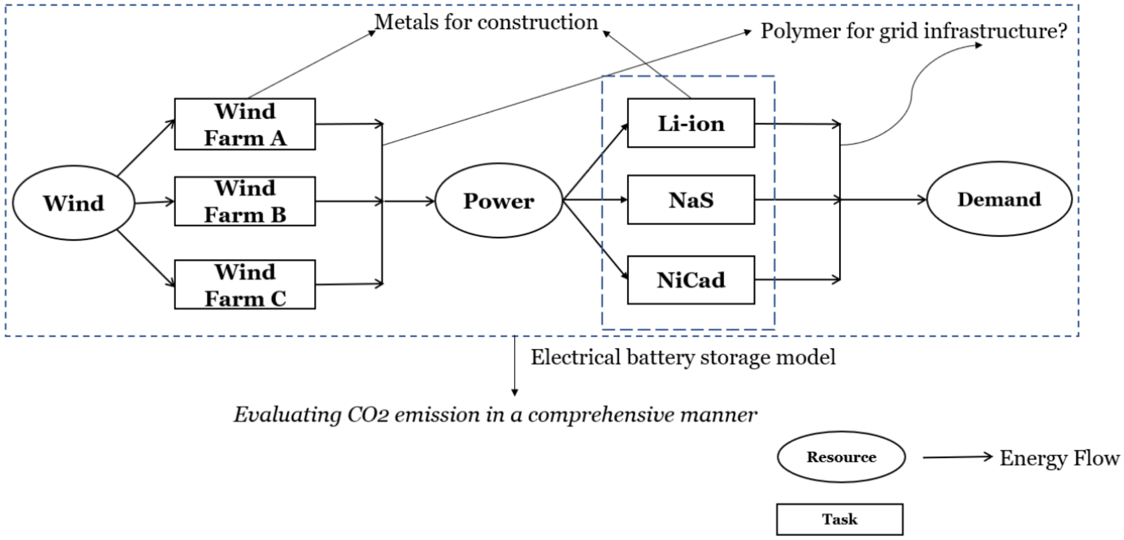

Figure 3.1: Superstructure for wind farm using Resource-Task Network (RTN) .

As such, a total of 8760 (24*365) data points should be presented per year, and the example conversion factor for solar photovoltaics (PV) array in Houston is shown in Figure 3.2.

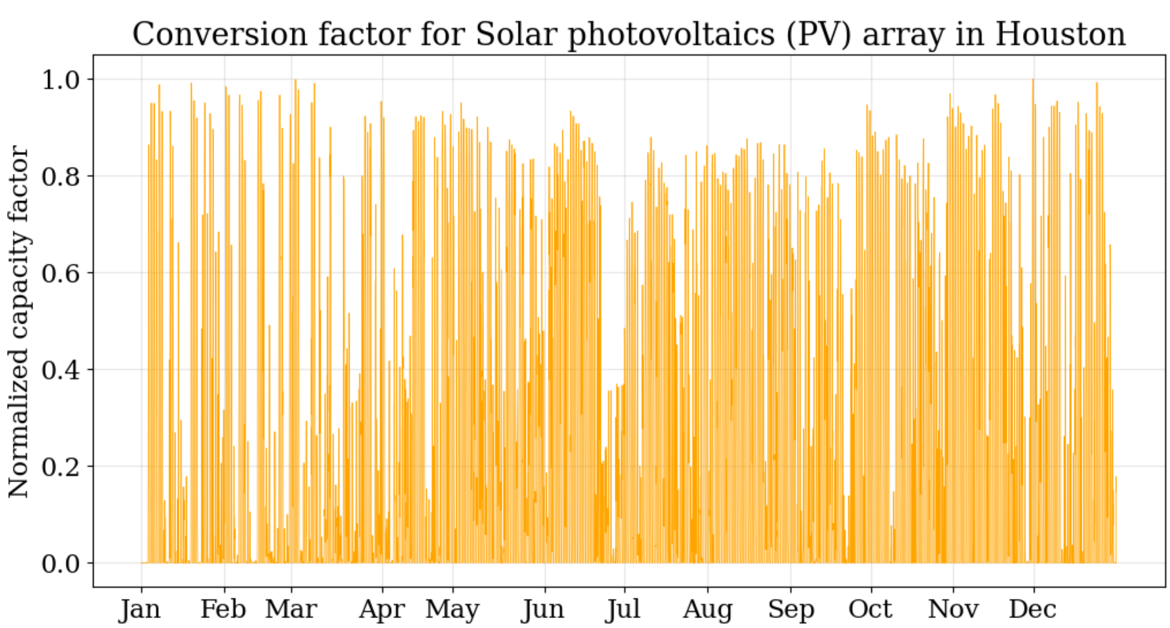

Figure 3.2: Conversion factor for solar photovoltaics (PV) array in Houston.

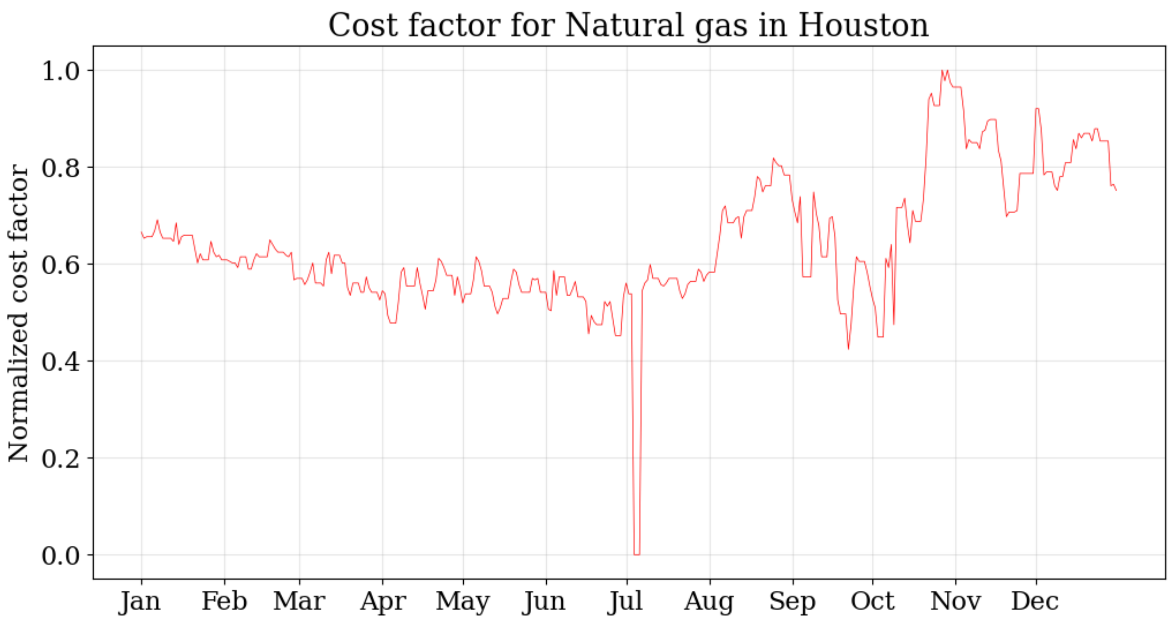

Figure 3.3: Conversion factor for natural gas in Houston.

Further, the electricity demand data can be collected from the Electric Reliability Council of Texas (ERCOT). The natural gas price data from Henry Hub can be collected from US Energy Information Administration. The cost data includes Capital Expenditure (CAPEX), fixed operations and maintenance (O&M) cost and variable operations and maintenance (O&M) cost for myriad energy storage processes. The availability of solar energy could be estimated using solar direct normal irradiance (DNI). Similarly, wind energy availability can be calculated using wind speed data.

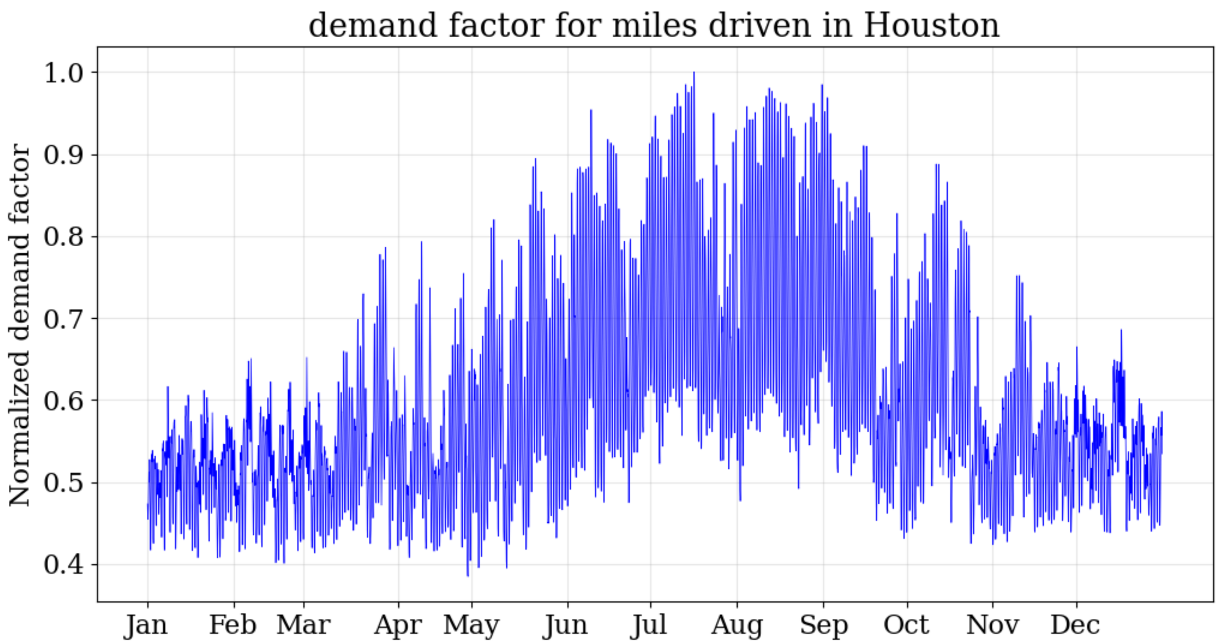

Figure 3.4: Varying demand factor for power obtained from ERCOT for the houston region.

3.2 Overview of embedded components

Transition scenarios contain diversified energy feedstock, multiple technology options for the production of energy vectors and power generation. As such, the problem allows the energy and material. The framework is modeled using embedded energiapy components, namely *Resource, Material, Process, Location, and Scenario*. The temporal scales of the problem are itself declared apriori, as shown below. Note that here, the scales are indexed a 0, 1, 2. Scale 0, has one discretization and represent a year. Similarly scales 1 and 2 represent days and hours respectively. Overall the problem has $1 \times 365 \times 24 = 8760$ temporal indices.

```
scales = Temporal_scale(discretization_list=[1, 365, 24])
```

The resources that flow through the system can be declared as *energiapy.Resource* objects. As shown below, they can include various characteristics such as whether they meet a particular demand or can be stored, the basis, associated GWP values, etc. Note that there is no distinction drawn in terms of the resource representing energy, mass, or even information flows.

```
Charge = Resource(name='Charge', sell=False,
    store_max=100, basis='MW', label='Battery energy')
```

The *energiapy.Material* object can be used to declare materials needed for establishing processes (*energiapy.Process* objects). Materials in turn could consume resources for their production, and have associated toxicity, GWPs, etc. An example declaration is shown below:

```
Ni = Material(name='Ni', gwp=7.64, resource_cons = {H2O: 80},
    toxicity=67, basis= 'kg', label='Nickel'))
```

Process objects include, power generation, hydrogen production, energy storage. These can essentially convert resources, and utilize materials for their establishment. The *Process* object contains key information, such as conversion, capital and operational expenditure, maximum production rates, production modes, etc. Processes can be declared as shown:

```
WF1 = Process(name='WF1', conversion={Wind: -5, Power: 1},
```

```
    capex=1377, fopex=2117, vopex=300,
    prod_max=100, gwp=42700, land=1800000,
    material_cons = {Steel: 292, Fe:44, CuP: 4,
    Al: 4, Epoxy: 16, Polyester: 16,
    Vinyl_easter: 12, Glass_fibre: 12},
    label='Wind mill array')
```

The goal is to simultaneously address the energy, resource, and material transition meanwhile minimize the environmental impact. The *energiapy.Location* object is essentially declared as a set of processes. The required resources and materials are drawn from the *energiapy.Process* object itself. The location also requires the provision of the scales at which the factors for varying resource price, resource demand, and process capacity are resolved.

```
HO = Location(name='HO', processes= process_set,
    demand_factor= {Power: ercot},
    capacity_factor = {PV1: pandas.DataFrame(weather['dni']),
    WF1: pandas.DataFrame(weather['wind_speed'])},
    scales=scales, label='Houston', demand_scale_level=2,
    capacity_scale_level= 2, cost_scale_level= 1)
```

energiapy.Location objects are then appended to an *energiapy.Scenario* object to produce a certain deterministic manifestation of the modeled system. Note that the system can also be multi-location, in which case the network attribute is set to an *energiapy.Network* object. Scenarios essentially contain all the necessary information to generate mathematical models of the required type, viz. LP, MILP, MINLP, mpLP. Scenarios also require the scales of the problems to be stated. For example, in the scenario declared below, the demand and schedule levels are set at an hourly resolution (scale 2), whereas, the network level is set at an annual scale (scale 0):

```
scenario = Scenario(name= 'xmp', network= HO, scales= scales,
```

```
expenditure_scale_level= 2, scheduling_scale_level= 2,
network_scale_level= 0, demand_scale_level= 2,
label= 'case study')
```

Moreover, an entire energy system can be modeled through the constraints selected by the user. The system can then be optimized to the objective either minimizing cost, maximizing production or utilization, minimizing environmental impact or even the combination of them, which eventually becomes a multi-objective problem. In the presented example, the model was formulated as shown:

```
milp = formulate(scenario= scenario, demand = 100,
 constraints={Constraints.cost, Constraints.inventory,
 Constraints.production, Constraints.land,
 Constraints.resource_balance, Constraints.emission},
 objective= Objective.cost)
```

The model can then be solved using the appropriate solver for the problem class. In this case, we used the gurobi solver (45) to solve the MILP. The solve functionality provides an *energiapy.Results* object, which can then be used for analysis and visualization of the solution output. The solve functionality requires the provision of both the MILP instance, as well as the *energiapy.Scenario* object.

```
solve(scenario = scenario, instance= milp, solver= 'gurobi',
 name=f"Material_case_study")
```

To this end, the modeling and optimization framework developed within *energiapy* is highly generalizable and can be used to analyze bespoke scenarios for multiple locations, or even multi-location formulations. Moreover, the model formulation can be optimized towards multiple, even competing, objectives such as emission, cost, demand.

3.3 Model formulation

In this section, a *Scenario* instance is formulated from the scenario, concise sets and corresponding variables are declared, corresponding constraints are generated based on the nature of the model chosen, and eventually a MILP is formulated in the presented example. 17 resources, 29 materials and for annual operation, there will be a total of 271745 continuous, 32 binary variables wherein in the resource and material availability of each resource and material are restricted.

Below is the key onstraints of the model:

Nameplate inventory constraint:

$$Inv(l,r,y,d,h) \leq Cap^S(l,r,y) \tag{3.1}$$

Max storage facility constraint:

$$Cap^S(l,r,y) \leq Store^{max}(l,r) \tag{3.2}$$

Min storage facility constraint

$$Cap^S(l,r,y) \geq Store^{min}(l,r) \tag{3.3}$$

Nameplate production constraint

$$Prod(l,p,y,d,h) \leq Cap^P(l,r,y) \tag{3.4}$$

Production facility constraint

$$Cap^P(l,p,y) \leq Prod_{max}(l,p) \tag{3.5}$$

Min production facility constraint

$$Cap^P(l,p,y) \geq Prod_{min}(l,p) \tag{3.6}$$

Process land constraint

$$Land_p(l,p,y) = land^p_{dict} \times Cap^P(l,p,y) \tag{3.7}$$

Location land constraint

$$Land_l(l,y) = \sum(Land_p(l,p,y)), \forall p \in Process \tag{3.8}$$

Network land constraint

$$Land_n(y) = \sum(Land_l(l,y)), \forall l \in L \tag{3.9}$$

Location land restriction constraint

$$Land_l(l,y) \leq land_{restriction} \tag{3.10}$$

Demand constraint

$$discharge = cluster_{wt}(y,d,h) \times demand_{target} \tag{3.11}$$

Inventory balance constraint

$$cluster_{wt}(y,d,h) \times (consumption + produced - discharge + transported) = storage \tag{3.12}$$

Resource consumption constraint

$$C(l,r,y,d,h) \leq C^{max}(l,r) \tag{3.13}$$

Resource purchase constraint

$$B(l,r,y,d,h) = R(l,r) \times cost_{factor}(l,r,y,d,h) \times C(l,r,y,d,h) \tag{3.14}$$

Location production constraint

$$P^l(l,p,y) = \sum cluster_{wt}(scale) \times P(l,p,scale), \forall scale \in Scale \tag{3.15}$$

Location discharge constraint

$$\sum cluster_{wt}(scale) \times S(l,r,scale), \forall scale \in Scale \tag{3.16}$$

Location consumption constraint

$$C^l(l,r,y) = \sum cluster_{wt}(scale) \times C(l,r,scale), \forall scale \in Scale \tag{3.17}$$

Location purchase constraint

$$B^l(l,r,y) = \sum cluster_{wt}(scale) \times B(l,r,scale), \forall scale \in Scale \tag{3.18}$$

Network production constraint

$$P^n(p,y) = \sum P^l(l,p,y), \forall l \in L \tag{3.19}$$

Network discharge constraint

$$S^n(r,y) = \sum S^l(l,r,y), \forall l \in L \tag{3.20}$$

Network consumption constraint

$$C^n(r, y) = \sum C^l(l, r, y), \forall l \in L \tag{3.21}$$

Network purchase constraint

$$B^n(r, y) = \sum B^l(l, r, y), \forall l \in L \tag{3.22}$$

Global warming potential process constraint across wind farm

$$GWP_{WF}(l, WF, y) = GWP_{dict}(l, WF) \times Cap^P(l, WF, y) \tag{3.23}$$

Global warming potential resource constraint

$$GWP_r(l, r, y) = r_{GWPdict}(l, r) \times C^l(l, r, y) \tag{3.24}$$

Global warming potential material constraint

$$GWP_{material}(l, WF, y) = \sum (material_{GWPdict}(l, m) \times WF_{materialdict}(WF, m)) \times Cap^P(l, WF, y),$$

$\forall m \in material_{dict}$(3.25)

Global warming potential location constraint

$$GWP_l(l, y) = GWP_{WF} + GWP_r + GWP_{material} \tag{3.26}$$

In which,

$$GWP_{WF} = \sum GWP_{WF}(l, WF, y), \forall WF \in P \tag{3.27}$$

$$GWP_r = \sum GWP_p(l, r, y), \forall r \in R \tag{3.28}$$

$$GWP_m = \sum GWP_p(l, m, y), \forall m \in M \tag{3.29}$$

Global warming potential network constraint

$$GWP_n(y) = \sum GWP_l(l, y), \forall l \in L \tag{3.30}$$

Global warming potential network reduction constraint

$$GWP_{nr}(y) \leq GWP_n(y) \times (1 - GWP_{reduction-percentage}), \forall l \in L \tag{3.31}$$

The objective of the model is to minimize the total cost and maximize the demand incurred by the system. The cost objective minimizes the levelized total cost borne by the system. The total cost consists of the annualized capital expenditure, operational expenditure, and material purchase cost. (Y is set of years in the planning horizon)

$$min \sum cost_y^{total}, \forall y \in Y \tag{3.32}$$

$$cost_y^{total} = CAP_y^{total} + OPEX_y^{total} + p_y^{total} + transport_y^{total} + CAP_{penalty}, \forall y \in Y \tag{3.33}$$

The key constraint of electrochemical battery storage model and the sample software implementation is shown below. Here p, l, h, r represent storage technology process, location, hour and resource, respectively:

Hourly capacity constraint

$$minC_p \times y_{l,r} \leq C_{l,r} \leq maxC_p \times y_{l,r}, \forall l \in L, p \in Process, r \in R \tag{3.34}$$

Wind power generation constraint:

$$0 \leq P_h \leq GP_h \tag{3.35}$$

$$P_h^c + P_h = GP_h \tag{3.36}$$

$$P_h^d + P_h \leq L_h \tag{3.37}$$

$$P_h^c \leq P_r \times y_h \tag{3.38}$$

$$P_h^d \leq P_r \times (1 - y_h) \tag{3.39}$$

The sample software implementation of Constraint (4.38) and (4.39) is shown below.

$$C_{l,p,h} = C_{l,p,h-1} \times (1-\eta_p) + P_{l,p,h}^c \times ec_p - P_{l,p,h}^d / ed_p (k \geq 2), \forall l \in L, p \in Process, h \in H \tag{3.40}$$

where P_h is the wind power generation in hour h, P_h^c is the charging power in hour h, P_h^d is the discharging power in hour h, GP_h is the maximum wind power can be generated in hour h, L_h is the load in hour h, P_r is the nominal power rating of the storage facilities in the unit of kW, y_h is binary variables, η is the self discharge efficiency, $S_{l,p,h}$ is the stored capacity for process l at location l in hour h, $Electric_h$ is the electricity purchased from outside, ec_p and ed_p is charged and discharged efficiency of process p, respectively.

Stored constraint:

$$S_{l,p,h} = P_{l,p,h}^c - P_{l,p,h}^d + S_{l,p,h-1}, \forall l \in L, p \in Process, h \in H \tag{3.41}$$

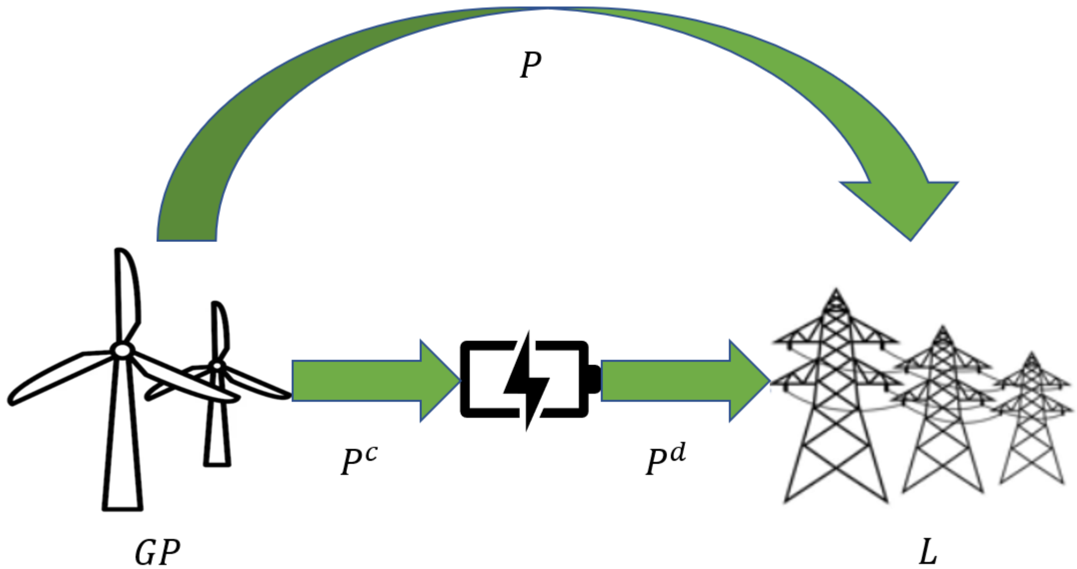

Figure 3.5: A schematic representation of electrochemical battery storage model

Demand constraint (efficiency factor=eff_p may vary):

$$P^d_{l,p,h} + P_{l,p,h} \times eff_p + Electric_h \geq Demand_h, \forall l \in L, p \in Process, h \in H \tag{3.42}$$

Objective function is to minimize cost:

$$min \sum CAP_{l,p} \times C_p + OPEX_{l,p} \times C_p + p_E \times Electricity_h \tag{3.43}$$

where p_E is price of electricity

Meanwhile it's important to address environmental burden (46):

$$EB = \sum_{k-1}^{k} G_k ef_k \tag{3.44}$$

where G_k are emissions from GHGs, ef_k is the GWP factor of GHGs relative to CO_2 GWP, and k is either CO_2, CH_4, or N_2O.

Optimal network design should be cognizant of emissions over the lifetime of process components and material sourcing. Taking CO_2 as an example for greenhouse gas, total carbon dioxide emission is as follows:

$$G_{CO_2} = G_{CO_2}^{direct} + G_{CO_2}^{annualized} \tag{3.45}$$

where G_{CO_2}, $G_{CO_2}^{direct}$, $G_{CO_2}^{annualized}$ represent the total carbon dioxide emission, direct carbon dioxide emission and annualized carbon dioxide emission.

4. COMPUTATIONAL EXAMPLES

The framework is applied towards the simultaneous design and schedule optimization of the material and energy transition to compare the impact of different technology pathways. Of key interest is the trade-off between the levelized cost of the system and the environmental impact.

A primary motivation for WF adoption is the reduction of emissions. To have an appreciable impact on climate change, reductions are required at scale which cannot be analyzed accurately without modeling renewable-grid interactions, which refer to WF-grid interactions in this case. Moreover, to accurately determine the net environmental impact, the flow of material needs to be modeled explicitly, so as to account for emission stemming from the production and procurement of material requisite for setting up wind farms and ancillary systems such as grid connections. Methodologically, estimates of the impacts of high WF penetration should explicitly model (1) the dependence of power demand on WF use, and (2) material composition and cost of wind turbine.

First, a base case is implemented without the consideration of GWP reduction. The subsequent scenarios seek to reduce the net GWP, and the cost of the system is analyzed. The generality of the framework allows it to be applied towards the analysis of myriad cost and GWP reduction scenarios. Three WFs and three PVs are tested in this model, by assigning different material composition and cost. Moreover, the option of meeting power demand through the production of hydrogen using alkaline water electrolysis (AWE), with hydrogen storage, is also investigated. The options for biomass and biogas power generation are also included in the model. As a whole, the model can be applied towards the problem of transitioning the mobility fleet towards sustainable alternatives, viz. methanol, hydrogen, electricity.

Data pertaining to the constituent processes of the system, the energy and material value chain, associated technology and resource purchase costs, GHG emissions are used to formulate a mixed integer programming (MIP) model. The framework utilizes the *energipy* python module. The results.output function shows that the objective cost is 8.2 hundred million to meet a demand of 1000 MW. The capacity contribution of WF1 process is shown in 4.1. The result of network GWP is shown in Figure 4.2 and they are very slightly different.

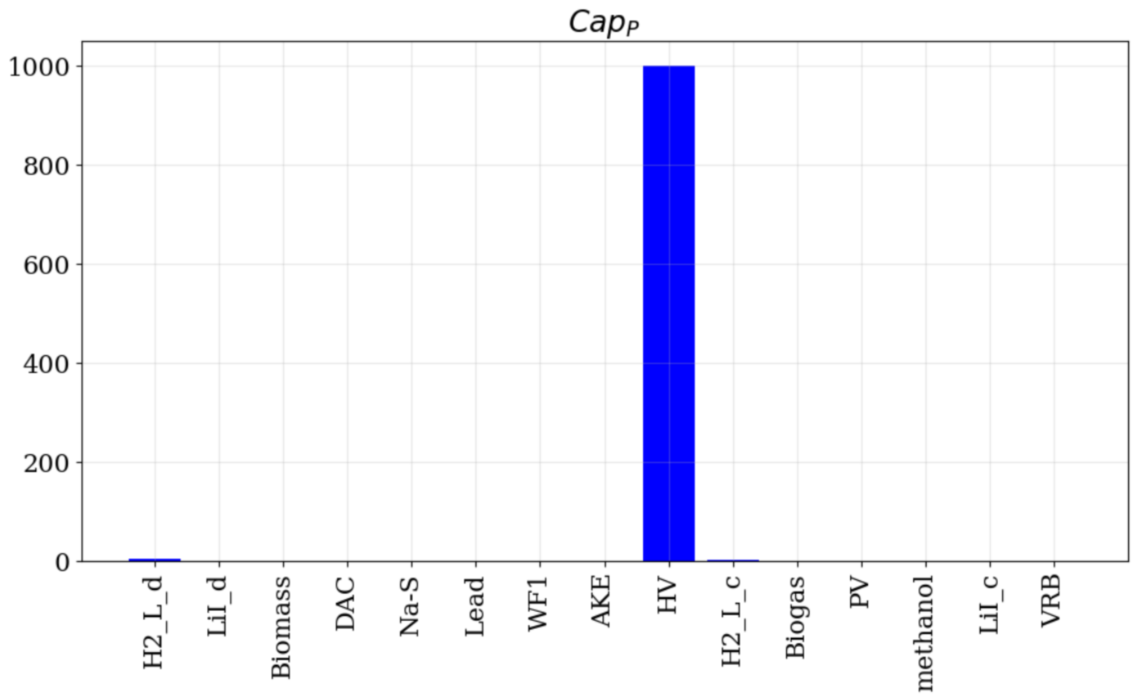

Figure 4.1: Capacity contribution of WF1 process. This further illustrated that mobility transition with hydrogen as a mobility fuel is indeed a feasible pathway when tackling the intermittent issue of wind energy production. DAC: direct air capture, LiI_c and LiI_d: lithium ion battery charge and discharge process, respectively, AKE: alkaline water electrolysis, $H2_{Lc}$ and $H2_{Ld}$: liquid hydrogen charge and discharge process

Figure 4.2: The GWP value of the network.

4.1 Scenario analysis

Scenario analysis is the process of estimating the expected value of a case after a given period of time, assuming that specific changes in the values of the case's key factors take place, such as resource and technology cost, material composition, and demand load.

Scenario analysis is also commonly used to estimate changes to a case's value in response to unfavorable events and may be used to examine a theoretical worst-case scenario. The sense behind it basically is if the configuration if an optimal design is determined for the worst-case scenario, feasibility is ensured for a range of scenarios.

Based on mathematical programming, scenario analysis provides a process to estimate variation in the value of a portfolio based on the occurrence of different situations, which are scenarios, following the principles of "what if" analysis. Sensitivity analysis is simply how different values of an independent variable affect a dependent variable under specific conditions, i.e. scenarios.

These assessments can be used for decision-making to evaluate trade-offs within a given investment as related to a variety of potential events. Relying on the results of the analysis, decision-makers can judge if the level of risk present is deserved to invest (47).

The idea behind scenario analysis in multi-scale energy system modeling is to characterize and compare the impacts of various energy transition scenarios. A multi-scale scenario is ranging of various time horizon and location dependant, and therefore the model need to take both spatial and temporal variability of available resources, conversion efficiencies, material and energy requirements, and policy choices into consideration (48).

Optimization-based scenario analysis specifically in this model considers the following as inputs: i. Time and location dependent wind availability ii. Power demand iii. Cost, emission, land and production constraint iv. Available storage infrastructure and return an optimal solution that comprises: i. Process and storage unit capacities ii. Land, cost and GWP at process, location and network iii. Time dependent production rates and operating modes for each process iv. Material and energy flow rates between processes v. Inventory management for storage of resources. Essentially, the framework can be used for scenario analysis through the consideration of myriad values for the material compositions of the system. Figure 4.3 shows the capacity utilized by WF1.

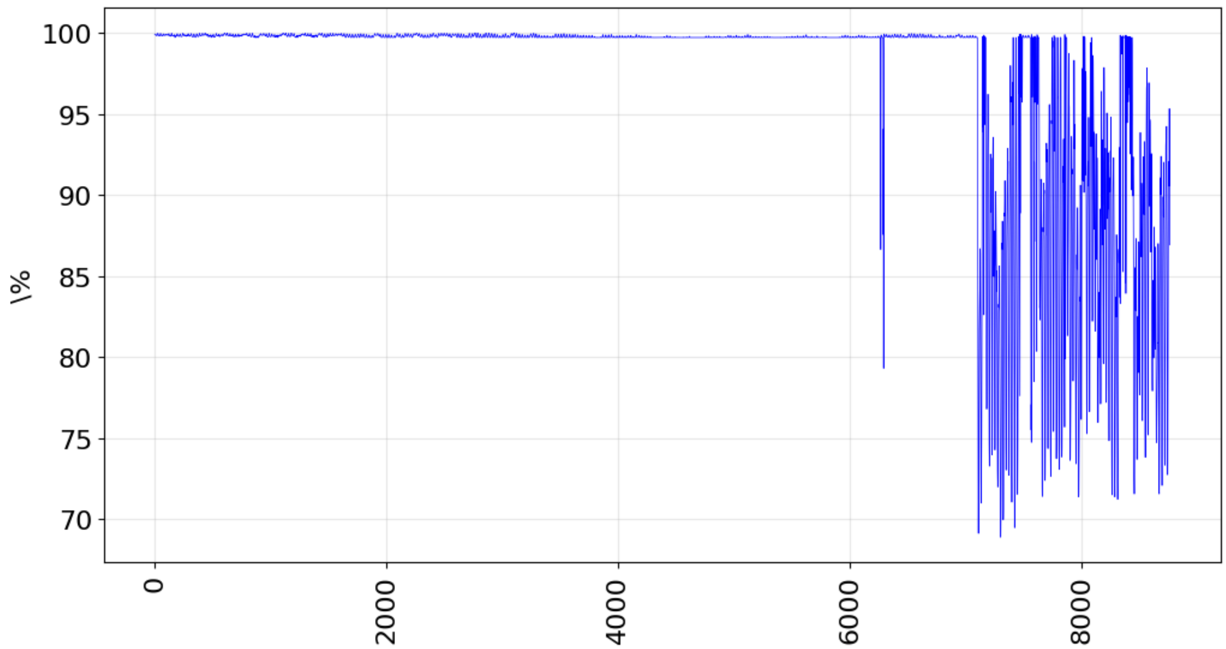

Figure 4.3: Capacity utilization of WF1. The utilization value fluctuates between full utilized to 70

4.1.1 Meeting different demand loads

In the beginning, the schematic of the Wind energy-EV/Hydrogen-HV system model is shown in Figure 4.4. Decision variables within the framework cover both strategic and operational aspects of the energy system, including which processes are implemented as well as daily production of hydrogen through each process. The implemented case study focuses on solely wind energy for the generation of power and alkaline water electrolysis (AWE) for the production of hydrogen; batteries for energy storage.

The data for the main component (power source and storage system) of the case study is shown in Table 4.1.

Component	material (WF is in tons)	Conversion efficiency
PV1	Monocrystalline	20%
PV2	Polycrystalline	16%
PV3	Cadmium telluride	33%
WF1	Steel:292, Fe:44, etc.	20%
WF2	Steel:316, Fe:20, etc.	33%
WF3	Steel:330, Fe:85, etc.	40%
LiR-ion	Rock-based lithium	85%
LiB-ion	Brine-based lithium	95%

Table 4.1: Data of the main components in the scenarios

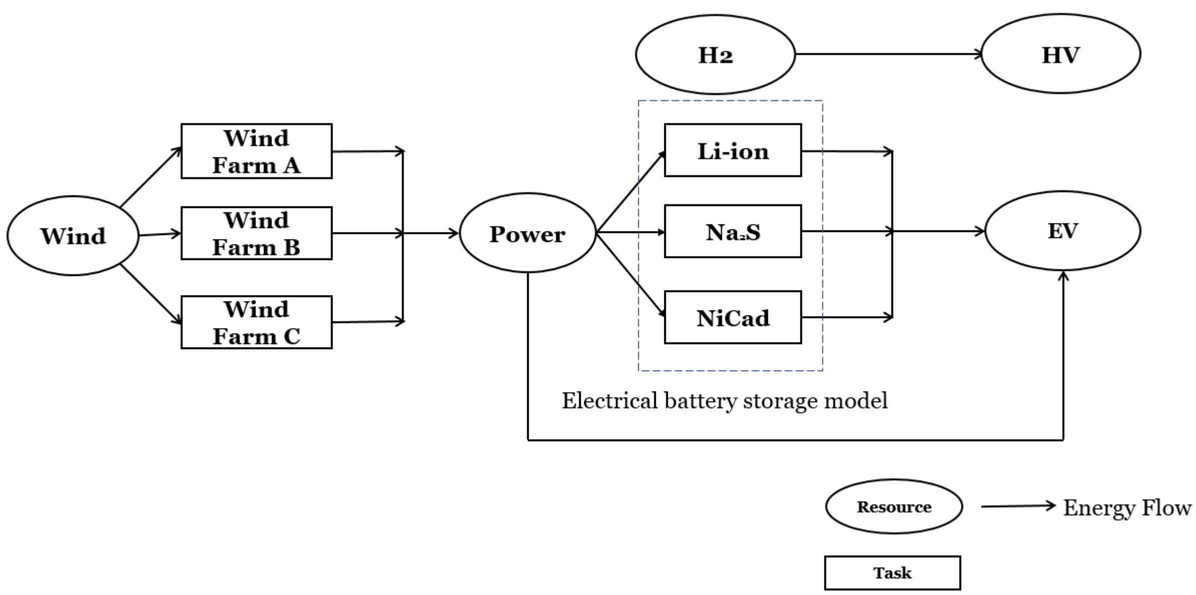

Figure 4.4: Superstructure for wind energy-EV/Hydrogen-HV system model using Resource-Task Network (RTN).

First, the model utilized windtoolkit to create the power source, namely wind turbine over the

8760 (365 days 24 hours) time intervals for one year to either be stored in the BES or meet the demand of EV or Hydrogen vehicle (HV). In other words, the stored electricity might be discharged to meet the demand in some time of the year. Figure 3.4 illustrate the demand factor of vehicles. A constant demand of 1000 MW per time interval is assumed in this model. The wind energy going directly to meeting demand is the same as the total wind energy amount from the power source with an unavoidable loss in energy conversion process. Apparently in this mode, the model does not store any energy in the BES as it prefers to meet the demand in a hydrogen production and direct combination pathway. This result exactly shows its characteristic to address the intermittency issue, and further a more reliable alternative to store is through DECs. The reason behind this result can be various interpretations. One reason could be the long planning time horizon, the other reason might be the hydrogen production costs less in this scenario. Extra possible reason includes the demand is high enough compared to the size or capacity of BES.

The first interpretation of the results makes the most sense since the time period planning is one year and normally, battery is not very good at storing energy for a long time period. Battery generally store energy for only one week at its maximum. This may cause a huge energy loss if choosing BES. Moreover, the contributor of cost in the whole system comprises the costs of the EES, which depends on the capacity of them. Hence, the cheapest choice is utilizing zero capacity which means none of the BES are used meanwhile the demand is met by wind energy directly as well as hydrogen production.

The high demand demonstrated that BES was in idle since there was not any excess wind energy can be stored. The energy supplied from the WF was to meet the high demand directly, and the system rather chose to schedule hydrogen for the demand.

Following this, the demand was decreased to 100 MW and 10 MW to verify the explanation. Figure 4.6 shows the schedule for battery energy storage for demand=100 MW and 10 MW , respectively. Figure 4.7 shows the schedule for hydrogen production for demand=100 MW and 10 MW, respectively. For demand=100 MW scenario, we can clearly see that because of the significant decreasing demand compared to 1000 MW case, the BES start to work but in a low storage manner. The system still chose to produce hydrogen and direct way to meet the demand. For demand=10 MW scenario, a possible speculation is that the system directly chose to meet the demand directly without storage and because of the demand is relative low, there is no need for hydrogen production as well. The 10MW scenario requires neither hydrogen or battery storage as the demand can be met entirely by oversizing the power generation system.

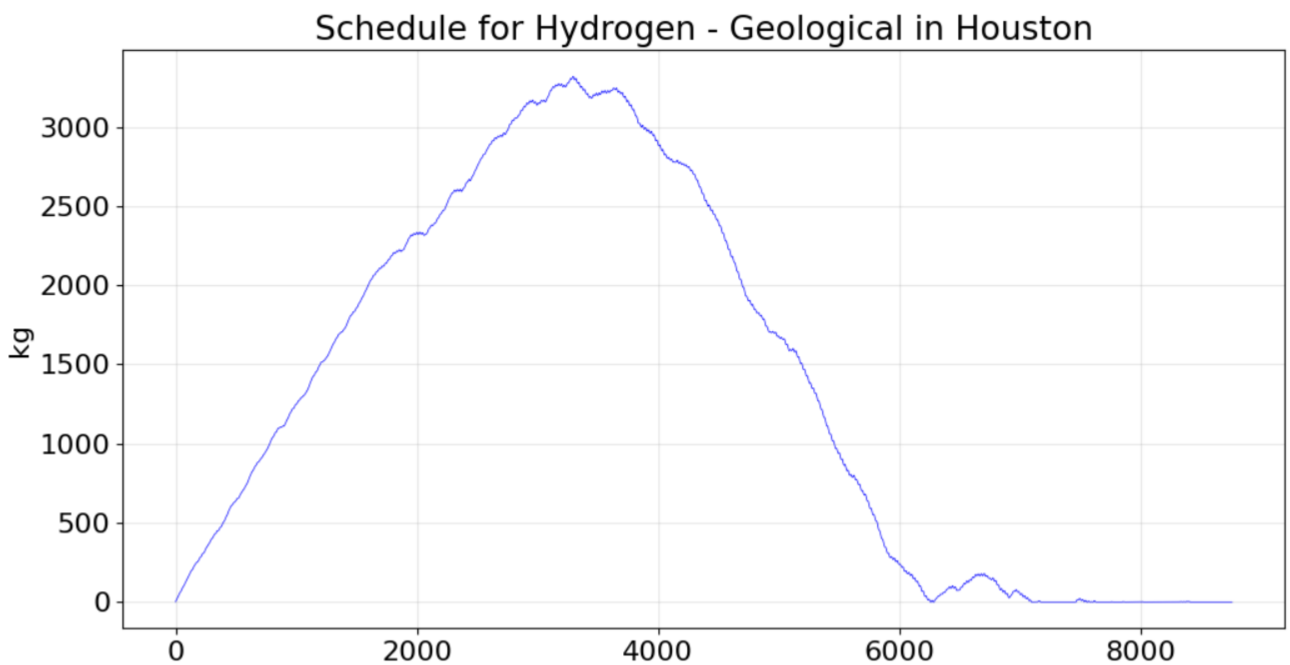

Figure 4.5: Schedule for hydrogen storage for demand=1000 MW scenario. Note that the model chooses to rely on storage of power in the chemical form (H_2) for large scale storage instead of batteries. Note that hydrogen storage is relatively long-term and experiences lower storage loses.

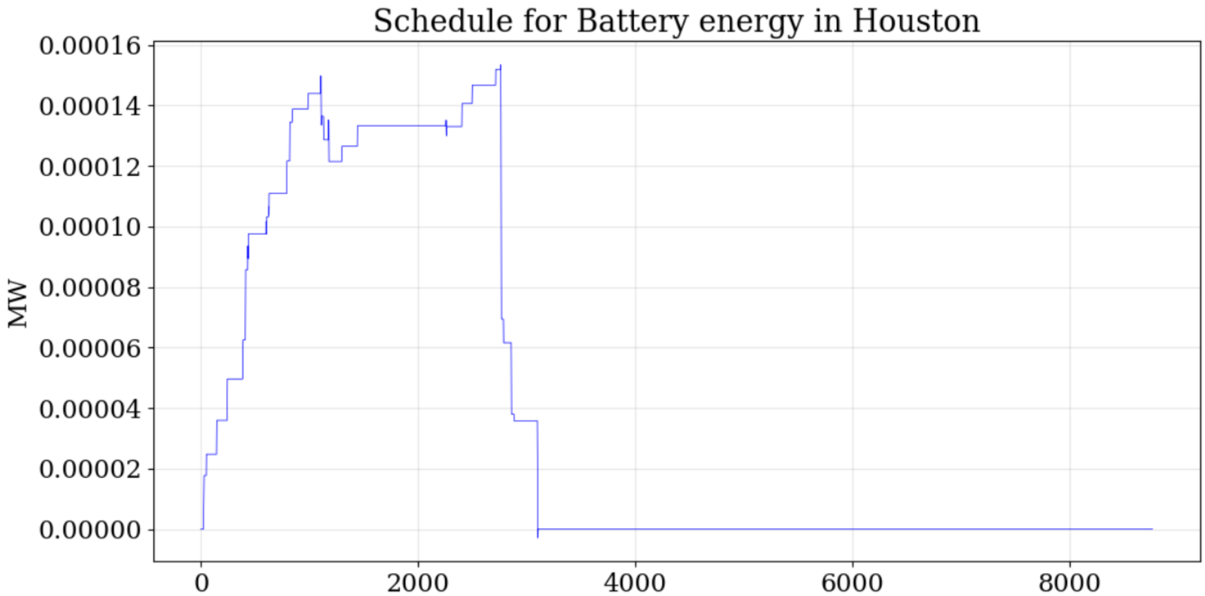

Figure 4.6: Schedule for battery energy storage for demand=100 MW scenario. For the moderate demand scenario, the model chooses both battery energy storage as well as production and storage of hydrogen to meet a varying demand. Hence, a mix of both options can tackle both seasonal and diurnal variability. However, given the low capacity realized, it can be inferred that batteries merely supplement hydrogen storage.

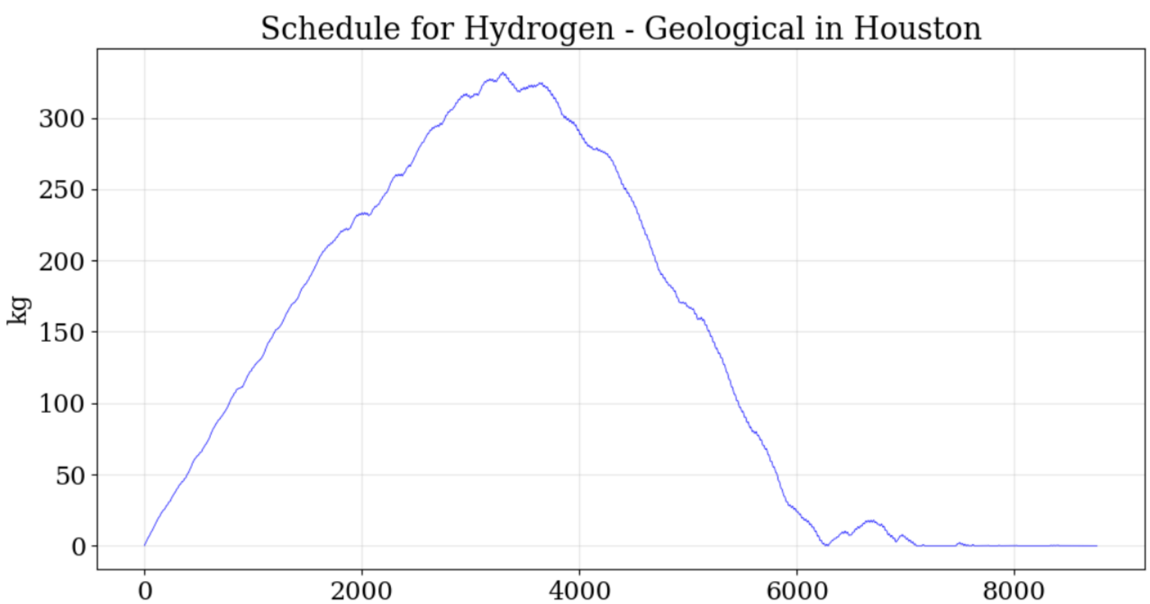

Figure 4.7: Schedule for hydrogen storage for demand=100 MW scenario. Hydrogen storage is setup alongside battery energy storage.

4.1.2 Changing technology pathways

Since the GWP is quite similar in solely 3 WFs case, the system was changed to demand=10 MW scenario and tested the different PV/WF combination, as shown in Figure 4.8. The schedule for battery energy for four scenarios, I. WF A-C and PV A-C, II. Solely PVs, III. Solely WFs, IV. Solely PVs and Li-ion battery is excluded. Figures 4.9 and 4.10 show scenario II and IV, respectively. The significant point of Figure 4.9 is that solar PV panel required more battery storage because the solar energy is only available during the day. The first three scenarios all chose LiB battery as the storage system, indicating its high performance. As thus, the fourth case was tested, however, the system does not choose any storage pathway. Also, this result is consistent with its higher conversion efficiency, lower GWP and price compared to LiR. The capacity utilization of the four scenarios are shown in Figure 4.12. The GWP and cost of the four cases are shown in Figures 4.13 and 4.14, respectively. As we can see, the cost will be increasing if decreasing the GWP.

Next, the system is able to track the emissions to the level of material use, hence, the same process WF1 with LiR-ion battery or LiB-ion battery was investigated. Results show that GWP is 420808 and 507153 $kgCO_2eq/MW$, respectively. Hence, even if the same storage technology Li-ion battery is used, the source of the materials can lead to significantly different GWP (20% higher in LiB-ion battery).

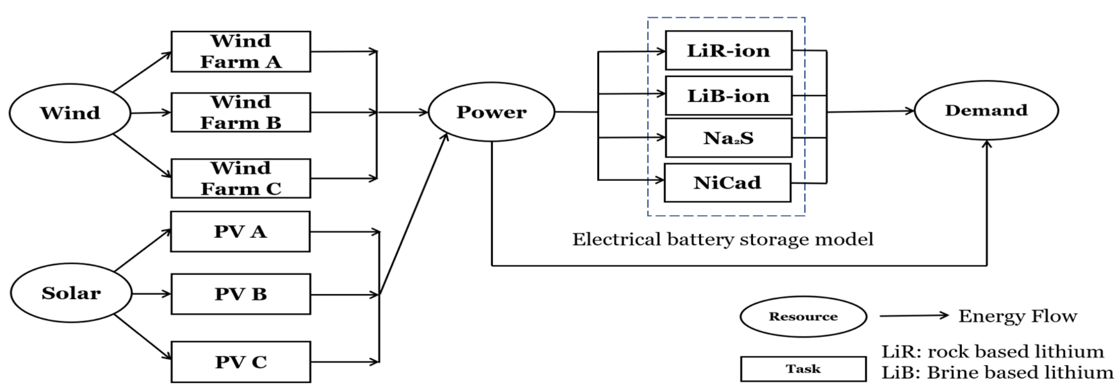

Figure 4.8: Superstructure for PV/WF system model using Resource-Task Network (RTN).

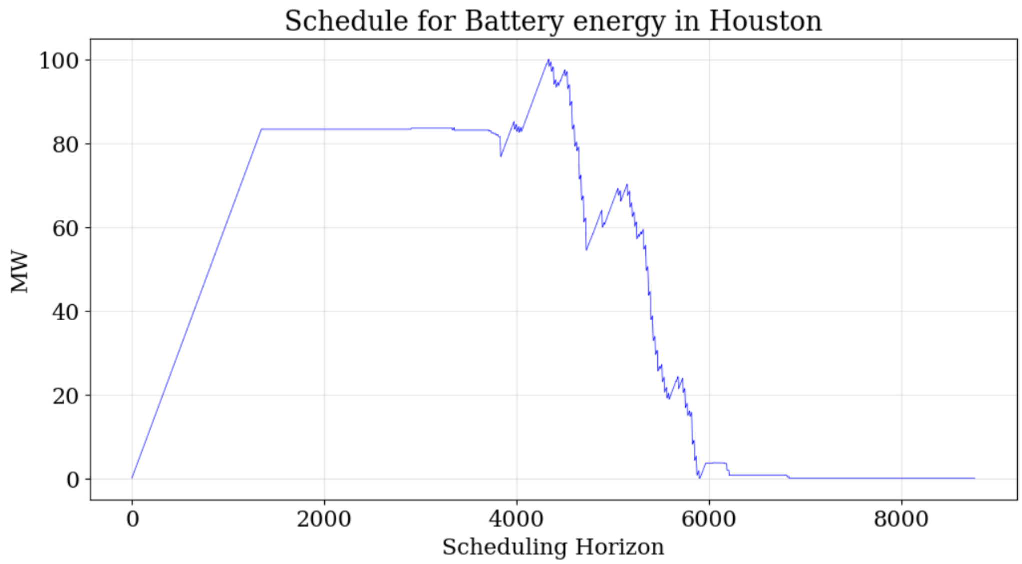

Figure 4.9: Schedule for battery energy storage for using solely PVs, material of PV3: Cadmium telluride (CdTe).

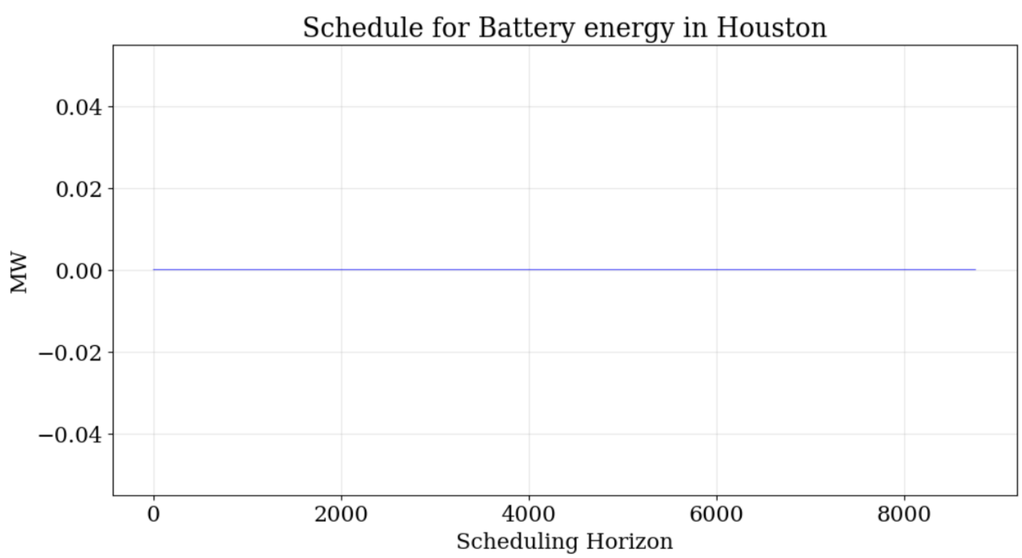

Figure 4.10: Schedule for battery energy storage for using solely PVs and excluding Li-ion battery.

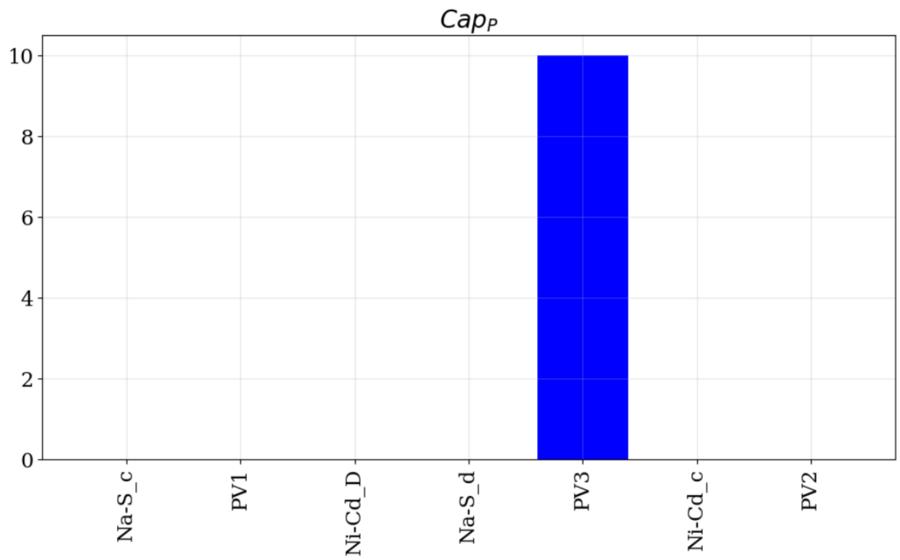

Figure 4.11: Capacity contribution for using solely PVs and excluding Li-ion battery. The Cadmium Telluride solar PV is shown to be the most cost conscious option. While more expensive than wind farms, the associated emissions are lower.

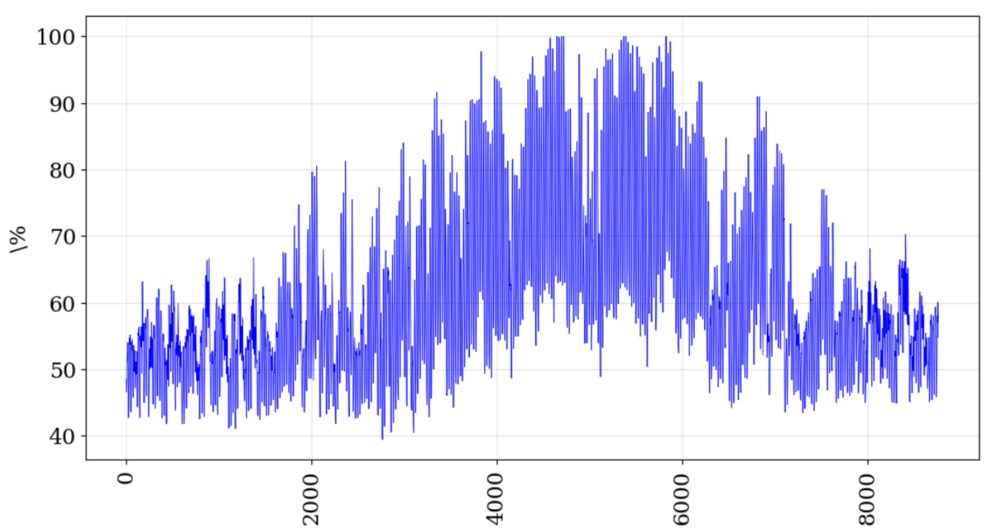

Figure 4.12: Capacity utilization for WF A-C and PV A-C combination for the 10MW case mirrors the demand profile, as the demand is met directly and entirely through power generation and no storage is necessary.

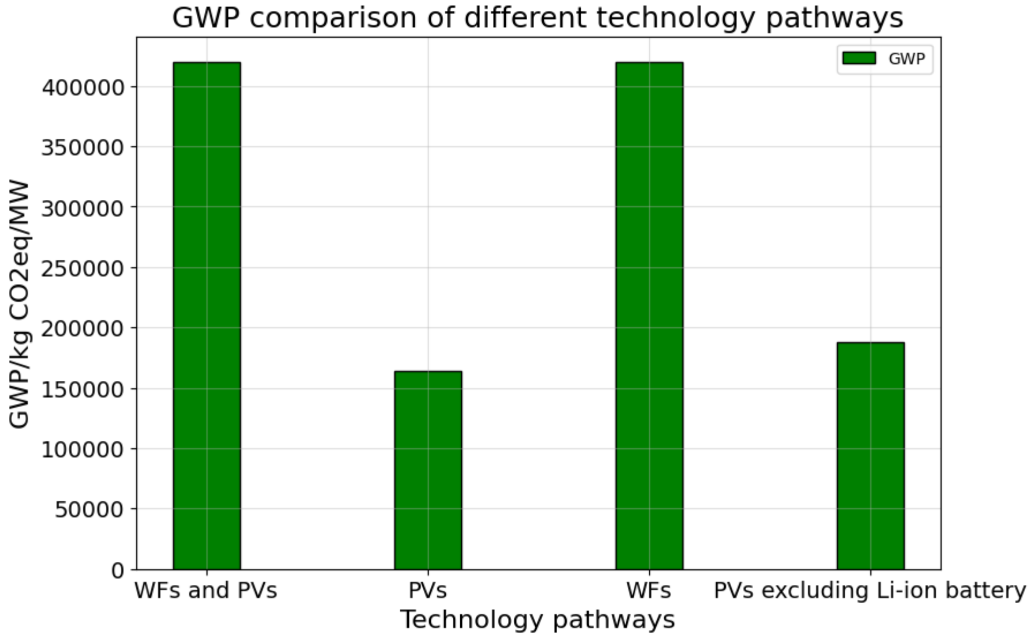

Figure 4.13: GWP of the four scenarios.

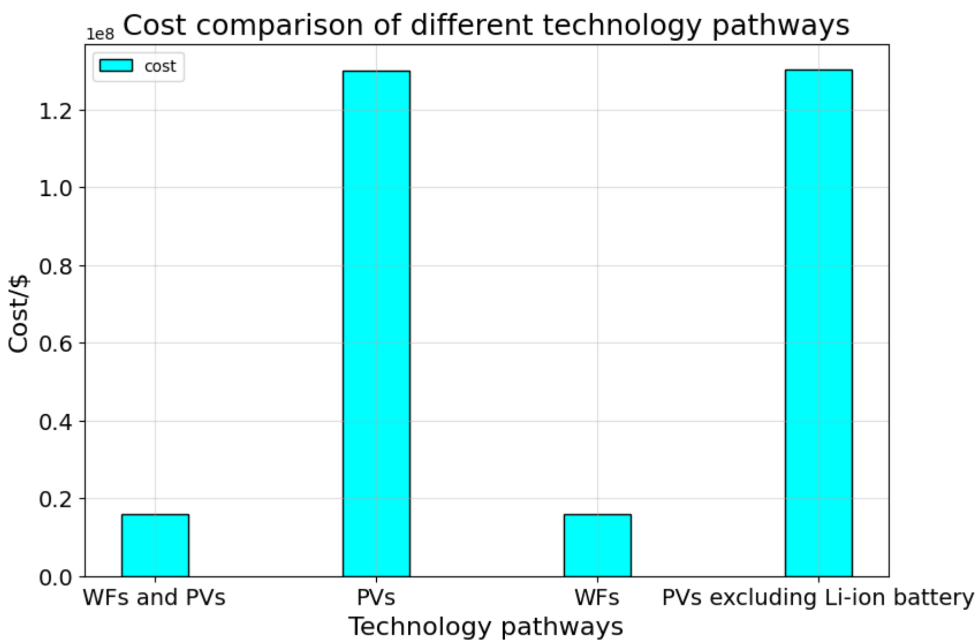

Figure 4.14: Cost of the four scenarios.

5. CONCLUSION

A comprehensive model library consisting of biomass, biogas, carbon dioxide based methanol, different types of battery storage and other renewable process has been appended to the prototype to allow users to develop integrated energy system formulations. The framework stores the large amount of data in the form of interrelated databases.Values such as lower and upper bound of production and storage capacities, material constraints, GWP and resource (water) consumption are embedded in the system. Users can pull data from the corresponding databases and embedded data to formulate constraints and objectives to build a full scale model. The formulation of such constraints and objectives is also demonstrated. The formulated model can be afterwards solved using the solvers like Gurobi. Since environmental impact and material shortage are pressing issue, this model sought to minimize GHG emissions as an environmental impact indicator as well as cost to not only provide the decision makers with techno-economic insights into transition pathways for decarbonsing energy systems but balance the trade-offs between cost and environmental impact.

As the first generation of wind turbine starts to reach their designed life time and thus be eliminated, it's necessary to optimize the layout implement of next generation wind farm and meanwhile evaluate the combination of whole renewable grid demand. For this purpose, a wind farm-based grid economic model was introduced and under developed, and following one of the vital component-energy storage model was suggested. It's unavoidable that there still emits GHG over the course, therefore a CCUS model was proposed. Moreover, it's natural to think of the material constraint to construct in wind farm, thus a distribution model was presented. It should be noted that the trade-offs between centralized and decentralized still need further study. As above mentioned, when wind turbine reach their designed life time, it will become so-called new industrial solid waste. If a reasonable approach is not established, solid waste may become the obstruction point of the whole supply chain. Another issue could be pointed out is there is a new technology route suggesting application of sodium-ion battery or recycling and echelon utilization of waste batteries which are environmentally benign but it takes time for them to be commercialized.

6. FURTHER STUDY

The paradigm will be improved to involve more environmental relating constraints, such as material toxicity and lifetime, time-variant costing data, and process parameters range picked by user. The carbon emissions of different modes of transportation to deliver materials from source area to processing plant to the renewable facility construction site will be accounted for the comprehensive evaluation of the carbon emission. In addition, the constraints of the model need more work, in this way they can represent the system precisely. The effects of carbon credits and cost to consumer has presented in the recent paper by Baratsas et. al (49). Similar work includes (50) proposed the concept of hydrogen credits the first time and a framework of trading hydrogen credits is designed to stimulate hydrogen economy. The green hydrogen credit system is closely coupled with the carbon credit market and it will provide a new pathway towards the carbon neutral future. When collecting data for each material object, energy storage and generation process, there is significant distinction in the data that make it confused to determine which sources of information to model. It's understandable that there are many factors or assumptions that have affected this variation in data such as publication year, size of facilities, and others. Thus, setting a range for life time, GHG emissions and water consumption would be a good method to handle this and the user can determine which specific data value they want to use.

Environmental burden is one of the important point which should not be overlooked even if material transition is realized. One aspect can be added to the environmental consideration is nitrogen dioxide, which is not strictly classified as a greenhouse gas. Nevertheless, they are important in the process of creation of tropospheric ozone which is a greenhouse gas. Hence, in the further work, it's essential to take account for mitigating the emission of NO_2 to the sustainable end. (51) proposed a techno-ecological synergy methodology of NO_2 abatement with reforestation meanwhile accounting for seasonal and growth dynamics of the forest ecosystem, which is a suitable model to refer. It should be highlighted that the prospective output of the study is not to determine certain or specific values of investment, revenue or GHG emissions to the system, rather what we are focusing on is more lying in alleviating the trade-offs between diverse technology pathways in electrical energy storage, identifying niche application areas for proposed technologies and at the end developing to a comprehensive framework for global decision making and planning.On top of that, there is uncertainty in input data such as lifetime and GWP, increasing the intractability of programming problem. Further, we could study hybrid network, eg. solar, wind and hydro in the framework. Another point is that we can integrate electric vehicles and renewable energy-based generation together which is a promising solution to the pressing issue of global warming. Another aspect of integrating means that old EV batteries can be reused to store excess locally generated renewable energy, which can act as a supplemental process to the model. (52) analyzed that the carbon footprint of a lithium-ion EV battery can be reduced by up to 17% if it is reused before being recycled. Batteries with reduced energy storage capacity can be repurposed to store wind and solar energy. The research is key to manufacturing lithium-ion batteries for electric vehicles that are designed for sustainability instead of performance. Hence, a comprehensive model of renewable-grid-connected EV-PV/WF charging systems deserves to be further explored. Besides, in early 2022 some of the provinces in China is experiencing power shortages and brownouts due to high temperatures and lack of precipitation meanwhile the dominant power generation route is PSH. A question may be raised naturally which is if we should develop EVs in the context of electricity shortage. As a matter of fact, part of the renewable electricity can go into storage and the rest can be charged to EV. In fact, we can treat the battery inside the cars as a mini energy storage equipment so we can imagine that when the number of EVs is large enough, with the characteristics of being able to charge or discharge, it could play a significant role of "cutting peak and filling valley" on the power grid. That's, EVs are fully charged at night and used normally during the day then the excess electricity can be returned to the grid during the day and the power company pays the day rate. In this way, people can make some profit as well because the electricity price is different during the day and at night. Fig. 6.1 shows the graphical interpretation of this network.The EVs are actually a piece of the future energy framework and in this case. However, during the repeated charging and discharging process the battery life would sustain a lot of damage, as a result the trade-off between making benefit from selling electricity and damaging battery life should be accounted for.

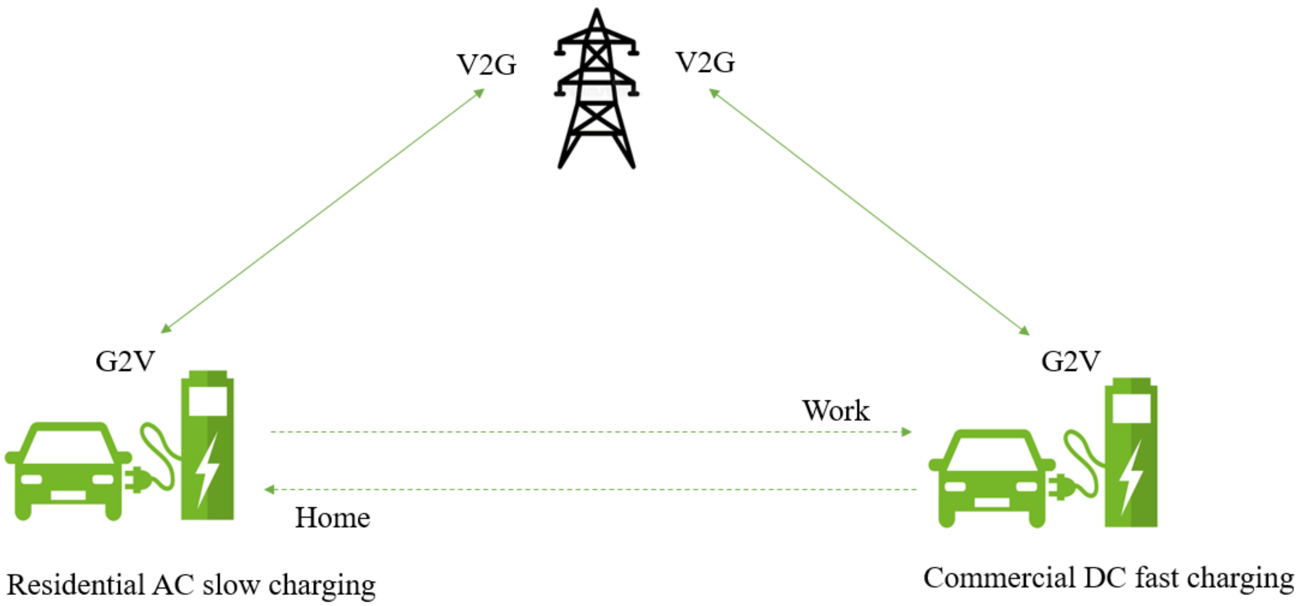

Figure 6.1: An important piece of future energy systems–Electric Vehicles.

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APPENDIX A

The framework is modeled as a mixed-integer linear program (MILP) which allows for integrated design, planning, and scheduling. In this chapter, the key constraints of the framework are elucidated. The Appendix A.1 describes a massive economic network in wind farm. The CCUS model are presented in Appendix A.2. The electrochemical battery storage model has already described in Section 4.3 which is determined for each hour of the planning period and the production distribution supply network model has already demonstrated in Section 4.3 as well.

A.1 Wind farm economic model

The cash flow for a given wind farm (WF) can be modelled as maximum (53):

$$CF(j) = WF_{rev}(j) + L(j) + RV(j) - CAP(j) - OPEX(j) - LP(j) - TOR_{tax}(j) - EP(j) \tag{A.1}$$

OPEX include expenses for regular inspection and maintenance, labor of technicians, insurance and land lease.

where L, RV, CAP, OPEX, LP, TOR_{tax}, EP represent the loan funds, residue value of fixed assets, the capital cost, operational costs , repayment of the loan and interest, tax on revenue of the WF for year j and electricity purchase. Note that selling price of electricity may vary.

n is the life time of wind turbine station, assume n=26, 1 year for construction, 25 years for operation. A good quality, modern wind turbine will generally last for 20 years, although this can be extended to 25 years or longer depending on environmental factors and the correct maintenance procedures being followed.Assume good maintenance.

The revenue of wind farm WF_{rev} is as follows:

$$WF_{rev} = \begin{cases} 0, & \text{if } j \text{ is between 0 and 1} \\ Q_j \times P \times (1 - D_j), & \text{if } j \text{ is between 2 and 26} \end{cases} \tag{A.2}$$

where Q_j refers to power generation in year j, in kWh; P refers to the bus-bar price in \$/kwh; and D_j indicates rate of natural degradation.

L and CAP are expressed by:

$$L_j = \begin{cases} d \times CAP, & \text{if } j \text{ is 0} \\ 0, & \text{if } j\text{>0} \end{cases} \tag{A.3}$$

The efficiency of wind turbine modules decreases due to natural degradation with prolonged usage. The degradation rate is assumed at 3% in the first operational year, and 0.7% for the following operational years (24).

$$CAP_j = \begin{cases} CAP, & \text{if } j \text{ is 0} \\ 0, & \text{if } j\text{>0} \end{cases} \tag{A.4}$$

where d denotes the debt ratio in the capital structure; and CAP denotes capital expenditures.

$$CAP = A \times P \times C \tag{A.5}$$

where A is the area of wind farm in m^2, C refers to total cost in \$/W which consists of two parts, cost of wind turbine module (C_m) and balance of system (BOS) (C_{BOS}) which refers to everything needed aside from WT modules to make the WF functional, which includes inverters, fixed support, combiner boxes, cables for grid infrastructure, and other items

$$C = C_m + C_{BOS} \tag{A.6}$$

C_m can be evaluated by:

$$C_m = C_0 m \times (\frac{N_j}{N_0})^{-\alpha_1} \tag{A.7}$$

where C_0 refers to the module cost in 2021; N_j denotes cumulative wind power installed capacity in the year j (2022-2060); N_0 indicates the initial wind power installed capacity in 2021; and α is the learning index for solar modules. C_{BOS} is expressed in a similar way:

$$C_{BOS} = C_{0B} \times (\frac{N_j}{N_0})^{-\alpha_2} \tag{A.8}$$

where C_{0B} refers to the BOS cost of WF in 2021; and α_2 is the learning index of WF BOS RV(j) and LP(j) are expressed by:

$$RV(j) = \begin{cases} 0, & \text{if } j < 26 \\ CAP \times 0.05, & \text{if } j = 26 \end{cases} \tag{A.9}$$

$$LP(j) = \begin{cases} \frac{(L_1+r_0)\times r\times(1+r)^{15}}{(1+r)^{14}-1}, & \text{if } j \text{ is between 2 and 16} \\ 0, & \text{if } j = \text{else years} \end{cases} \tag{A.10}$$

where r is the interest rate of loan during loan-payment period from first to 15th years; and r_0 refers to the interest of the construction period, including financing cost and borrowing interest. The value of r_0 is selected here as 1% of the total capital expenditures:

$$r_0 = 1\% \times CAP \tag{A.11}$$

OPEX(j) is expressed as:

$$OPEX(j) = \begin{cases} A \times P \times OMY, & \text{if } j \text{ is between 2 and 26} \\ 0, & \text{if j is between 0 and 1} \end{cases} \tag{A.12}$$

where OMY refers to annual operation and maintenance unit cost in year j, in $/(W*year):

$$OMY = 1\% \times C \tag{A.13}$$

$TOR_{tax}(j)$ has three components, namely value added tax (VAT_j), enterprise income tax (EIT_j) and business tax and annex (BTA_j):

$$TOR_{tax}(j) = VAT_j + EIT_j + BTA_j \tag{A.14}$$

where VAT_j,EIT_j and BTA_j can be expressed as;

$$VAT_j = \begin{cases} 0, & \text{if } j \text{ is between 0 and 1} \\ 0.17 \times \frac{R_j}{1.17} - \frac{0.17 \times CAP}{29.25,} & \text{if } j \text{ is between 2 and 26} \end{cases} \tag{A.15}$$

$$EIT_j = \begin{cases} 0, & \text{if } j \text{ is between 0 and 1} \\ 0.25 \times (R_j - LP_j - OM_j - DP_j - BTA_j), & \text{if } j \text{ is between 2 and 26} \end{cases} \tag{A.16}$$

$$BTA_j = 0.11 \times VAT_j \tag{A.17}$$

where DP_j is the depreciation:

$$DP_j = \begin{cases} 0, & \text{if } j \text{ is between 0 and 1} \\ \frac{CAP \times 0.95}{25,} & \text{if } j \text{ is between 2 and 26} \end{cases} \tag{A.18}$$

The NPV represents an estimation of the future discounted cash flows back to the present moment using a discount rate k (k=8%).

$$NPV = -CF_0 + \sum_{1}^{j} \frac{CF_j}{(1+k)^j} \tag{A.19}$$

where CF_0 represents the initial cash outflow and CF_j represents the cash flow for the past 20 years.

A.2 CCUS model

Objective function (54)

$$Z = min(\sum_{a\in A} C_a^{cap} \times capture_a + \sum_{a\in A}\sum_{r\in R} c_{ar}^{tra} \times x_{ar} + \sum_{r\in R} c_r^{sto} \times b_r + p_c \times \sum_{a\in A}(E_r - a_r) - revenue) \tag{A.20}$$

$$\sum_{a\in A} capture_a \geq T \tag{A.21}$$

where C_a^{cap} is the unit cost of capture in location a;c_r^{sto} the unit cost of storage in storage site j; c_{ar}^{tra} is the unit cost of transportation from location i to storage site j; and c_r^{sto} and c_{ar}^{tra} are endogenous variables, which depend on specific engineering processes including pipeline construction and well drilling. $capture_a$,x_{ar}, and b_r are the amount of CO_2 capture, transportation, and sequestration, respectively; revenue is the income resulting from CO_2-enhanced oil recovery and CO_2-enhanced coal bed methane, which means this value is set to 0 when deep saline aquifers (DSAs) are selected, p_c is carbon price.

$$revenue = \sum_{r\in R}(p_{oil} \times \frac{b_r}{t} + p_{gas} \times \frac{b_r \times V_m}{M \times q}) \tag{A.22}$$

where p_{oil} and p_{gas} are the oil price and gas price in each site;t and q are the CO_2 replacement rates for oil and gas,respectively;M is the molar mass of CO_2, 44 g/mol; and V_m is the molar volume of ideal gas, 0.0224 m^3/mol.

Mass balance

$$\sum_{n\in Un\neq i} x_{in} - \sum_{n\in Un\neq i} x_{ni} - capture_a = 0, \forall i \in S \tag{A.23}$$

$$\sum_{n\in Un\neq j} x_{jn} - \sum_{n\in Un\neq j} x_{nj} + b_j = 0, \forall j \in R \tag{A.24}$$

Capture and storage capacity

$$E_a \times \eta - capture_a \geq 0, \forall a \in A \tag{A.25}$$

$$Q_r - B_r \times \tau \geq 0, \forall r \in R \tag{A.26}$$

$$N_r \times I_r - b_r \geq 0, \forall r \in R \tag{A.27}$$

where E_a and Q_r represent the annual CO_2 emissions and storage capacity;η is the capture efficiency, 95%;τ is the time lag for storage, 30 years;N_r is the number of injection wells at storage site r; and I_r represents the injectivity for one well at storage site r, which depends on the category of CO_2 storage.

Pipeline selection

$$\sum_{d \in D} v_{max}^d \times {N_{ar}}^d \geq x_{ar} \tag{A.28}$$

where v_{max}^d refers to the maximum flow rate of the pipe line with a diameter of d and N_{ij}^d is the number of pipelines (of the same diameter) on the same route.

Non-negativity

$$capture_a \geq 0 \tag{A.29}$$

$$b_r \geq 0 \tag{A.30}$$

$$0 \leq x_{ar} \leq x_{max} \tag{A.31}$$

APPENDIX B

KEY CONSTRAINT OF THE FRAMEWORK

B.1 Key constraint and framework implementation in material and electricity distribution model

For the framework implementation, the idea is like that, firstly, declare sets and variables.

```
model = ConcreteModel()
model.facility = Set(initialize = [n for n in range(4)], doc = 'set of facilities')
model.potential_facility_sites = Set(initialize = [n for n in range(4)], doc = 'set of potential sites')
model.source = Set(initialize = [n for n in range(4)], doc = 'set of sources')
model.potential_sources = Set(initialize = [n for n in range(4)], doc = 'set of potential sources')
model.demmand_sink = Set(initialize = [n for n in range(4)], doc = 'set of demmand sinks')
model.potential_demmand_sinks = Set(initialize = [n for n in range(4)], doc = 'set of potential demmand sinks')
model.time_scale = Set(initialize = [n for n in range(24)], doc = 'daily')
model.storage_technology = Set(initialize = [n for n in range(24)], doc = 'storage pathway')
```

Figure B.1: Sets declaration.

```
min_production_cap = {
    0: 200,
    1: 50,
    2: 123,
    3: 133
}


max_production_cap = {
    0: 2000,
    1: 500,
    2: 1230,
    3: 1300
}

max_material_supply = {
    0: 1000,
    1: 2000,
    2: 3000,
    3: 4000
}

efficiency = {
    0: 0.6,
    1: 0.7,
    2: 0.8,
    3: 0.9
}
```

Figure B.2: Parameter set up.

```
model.I_f = Var(model.facility, within=Binary)
model.material_sent = Var(model.source, model.facility, doc = 'Amount of material sent from sources to facility f')
model.material_sent_from_source_to_facility = Var(model.source, doc = 'Total amount of material sent from sources to facility f')
model.production_in_facility = Var(model.facility, doc = 'Amount of product made in facility f')
model.material_used_in_facility = Var(model.facility, doc = 'Amount of material used for production in facility f')
model.electricity_facility_to_sink = Var(model.facility, model.demmand_sink, doc = 'Amount of electricity sent from facility f to demmand sink ds')
model.total_electricity_facility_to_sink = Var(model.demmand_sink, doc = 'Total amount of electricity sent from facility f to demmand sink ds')
model.net_amount_electricity = Var(model.demmand_sink, doc = 'Net amount of electricity sent to demmand sink ds')
model.hourly_power = Var(model.storage_technology, model.time_scale, doc = "hourly power")
model.hourly_charge = Var(model.storage_technology, model.time_scale, domain = NonNegativeReals, doc = "hourly charge")
```

Figure B.3: Variables declaration.

The material and electricity distribution model constraint and framework implementation is shown below:

Either centralized or decentralized model, there is material production capacity constraint (55):

$$LB_f \times I_f \leq P_f \leq UB_f \times I_f, \forall f \in F \tag{B.1}$$

I_f is binary variables, P_f is production in facility f (f$\in F$)

```
def min_production_cap_rule(instance, facility):
    return min_production_cap[facility]* model.I_f[facility] <= model.production_in_facility[facility]

model.min_production_capacity_constraint = Constraint(model.facility, rule = min_production_cap_rule, doc = 'min production capacity cons')

def max_production_cap_rule(instance, facility):
    return model.production_in_facility[facility] <= max_production_cap[facility] * model.I_f[facility]

model.max_production_capacity_constraint = Constraint(model.facility, rule = max_production_cap_rule, doc = 'max production capacity cons')
```

Figure B.4: Framework implementation of constraint B.1 .

The total amount of the material for constructing wind farm cannot go beyond the amount of material available at the source:

$$\sum_{f}^{F} B_{s,f} \leq maxB_s, \forall s \in S \tag{B.2}$$

$B_{s,f}$ is amount of material sent from source s to facility, maxB_s is the maximum supply of the material in source s.

```
def material_sent_from_source_to_facility_rule(instance, facility):
    return model.material_sent_from_source_to_facility[facility] == sum(model.material_sent[source, facility] for source in model.potential_sources)

model.material_sent_from_source_to_facility_constraint = Constraint(model.facility, rule = material_sent_from_source_to_facility_rule, doc = 'material sent source cons')


Run Cell | Run Above | Debug Cell
#%%
def max_supply_rule(insatnce, facility, source):
    return model.material_sent_from_source_to_facility[facility] <= max_material_supply[source]

model.max_supply_constraint = Constraint(model.facility, model.source, rule = max_supply_rule, doc = 'max supply cons')
```

Figure B.5: Framework implementation of constraint B.2 .

The total amount of material for constructing in facility f is equal to the amount of material transport from every source to the facility.

$$\sum_{s}^{S} B_{s,f} = maxB_f, \forall f \in F \tag{B.3}$$

```
def material_sent_from_source_to_facility_second_rule(instance, source):
    return model.material_sent_from_source_to_facility[source] == sum(model.material_sent[source, facility] for facility in model.potential_facility_sites)

model.material_sent_from_source_to_facility_cnstraint = Constraint(model.source, rule = material_sent_from_source_to_facility_rule, doc = 'material sent facliity cons')


Run Cell | Run Above | Debug Cell
#%%
def max_supply_equal_constraint_rule(insatnce, source):
    return model.material_sent_from_source_to_facility[source] == max_material_supply[facility]

model.max_supply_equal_constraint_constraint = Constraint(model.facility, model.source, rule = max_supply_equal_constraint_rule, doc = 'max supply equal cons')
```

Figure B.6: Framework implementation of constraint B.3 .

Efficiency is the ratio between amount of production made and amount of used:

$$P_f = \eta \times B_f, \forall f \in F \tag{B.4}$$

The total amount of electricity sent from f cannot exceed the amount of electricity made by the

```
def efficiency_rule(instance, facility):
    return model.production_in_facility[facility] == efficiency[facility] * model.material_used_in_facility[facility]

model.efficiency_constraint = Constraint(model.facility, rule = efficiency_rule, doc = 'eff cons')
```

Figure B.7: Framework implementation of constraint B.4 .

facility

$$\sum_{ds}^{Ds} P_{f,m} \leq P_k + P_k^d, \forall f \in F \tag{B.5}$$

ds=demand sink

```
def max_electricity_rule(instance, time_scale):
    return sum(model.total_electricity_facility_to_sink[demmand_sink] for demmand_sink in model.demmand_sink)<= sum(model.hourly_power[storage_technology, time_scale] + model.hourly_charge[storage_technology, time_scale] for storage_technology in model.storage_technology)

model.max_electricity_constraint = Constraint(model.time_scale, rule = max_electricity_rule, doc = 'max electricity cons')


Run Cell | Run Above | Debug Cell
#%%
def electriity_from_facility_rule(instance, facility):
    return model.total_electricity_facility_to_sink[facility] == sum(model.electricity_facility_to_sink[facility, demmand_sink] for demmand_sink in model.potential_demmand_sinks)

model.electriity_from_facility_constraint = Constraint(model.facility, rule = electriity_from_facility_rule, doc = 'electriity from facility cons')
```

Figure B.8: Framework implementation of constraint B.5 .

The total amount of electricity received by demand sink is equal to the amount of electricity transport from every facility to the demand sink.

$$P_{ds}^{net} = \sum_{f}^{F} P_{f,ds}, \forall ds \in Ds \tag{B.6}$$

```
def electriity_from_facility_rule(instance, facility):
    return model.total_electricity_facility_to_sink[facility] == sum(model.electricity_facility_to_sink[facility, demmand_sink] for demmand_sink in model.potential_demmand_sinks)

model.electriity_from_facility_constraint = Constraint(model.facility, rule = electriity_from_facility_rule, doc = 'electriity from facility cons')


Run Cell | Run Above | Debug Cell
#%%
def equal_electricity_rule(instance, facility, demmand_sink):
    return model.net_amount_electricity[demmand_sink] == model.total_electricity_facility_to_sink[facility]

model.equal_electricity_constraint = Constraint(model.facility, model.demmand_sink, rule = equal_electricity_rule, doc = 'equal electricity cons')
```

Figure B.9: Framework implementation of constraint B.6 .

B.2 Nomenclature of sets

L	locations (l)
R	resources (r)
Y	years (y)
D	days (d)
H	hours (h)
P	processes (p)
Scale	scale (h,d,y)
M	material (m)

B.3 Nomenclature of parameters

$Store^{max}$	max storage capacity
$Store^{min}$	min storage capacity
$Prod_{max}$	max production capacity
$Prod_{min}$	min production capacity
$land^{p}_{dict}$	dictionary of land requirement for each process per capacity size
$land_{restriction}$	upper bound of land requirement
$C^{max}(l,r)$	upper bound of resource (r) or material (m) consumption
$r_{GWPdict}(l,r)$	GWP dictionary of resource (r) at location (l)
$material_{GWPdict}(l,m)$	GWP dictionary of material (m) at location (l)
$WF_{materialdict}(WF,m)$	material dictionary of Wind Farm

$GWP_{dict}(l, WF)$	GWP dictionary of process (WF) at location (l)
$maxC_p$	upper bound capacity for storage process (p)
$minC_p$	lower bound capacity for storage process (p)

B.4 Nomenclature of variables

$Inv(l, r, y, d, h)$	inventory in hour (h) and day (d) of year (y)
$Cap^S(l, r, y)$	storage capacity for resource (r) at location (l) of year (y)
$Prod(l, p, y, d, h)$	total production of process (p) in hour (h) and day (d) of year (y)
$Cap^P(l, p, y)$	production capacity of process (p) at location (l) of year (y)
$Land_p(l, p, y)$	land requirement of process (p) at location (l) of year (y)
$Land_l(l, y)$	land requirement at location (l) of year (y)
$Land_n(y)$	land requirement in network (n) of year (y)
$cluster_{wt}(y, d, h)$	weighted cluster in hour (h) and day (d) of year (y)
$C(l, r, y, d, h)$	amount of resource (r) or material (m) consumed at location (l) in hour (h) and day (d) of year (y)
$R(l, r)$	price of resource (r) purchased in location (l)
$P^l(l, p, y)$	amount of resource (r) or material (m) production via process (p) at location (l) of year (y)
$P^l(l, p, scale)$	amount of resource or material production via process (p) at location (l) in hour (h) and day (d) of year (y)
$S^l(l, r, y)$	amount of resource (r) or material (m) discharged in year (y)
$S(l, r, scale)$	amount of resource (r) or material (m) discharged in hour (h) and day (d) of year (y)
$C^l(l, r, y)$	amount of resource (r) or material (m) consumed at location (l) of year (y)

$C(l, r, scale)$	amount of resource (r) or material (m) consumed at location (l) in hour (h) and day (d) of year (y)
$B^l(l, r, y)$	amount of resource (r) or material (m) purchased at location (l) of year (y)
$B(l, r, scale) \& B(l, r, y, d, h)$	amount of resource (r) or material (m) purchased at location (l) in hour (h) and day (d) of year (y)
$P^n(p, y)$	amount of resource (r) or material (m) produced in network (n) by process (p) in year (y)
$P^l(l, p, y)$	amount of resource (r) or material (m) produced at location (l) by process (p) in year (y)
$S^n(r, y)$	amount of resource (r) or material (m) discharged in network (n) of year (y)
$C^n(r, y)$	amount of resource (r) or material (m) consumed in network (n) of year (y)
$B^n(r, y)$	amount of resource (r) or material (m) in network (n) of year (y)
$GWP_{WF}(l, WF, y)$	GWP of process (WF) at location (l) of year (y)
$Cap^P(l, WF, y)$	production capacity of process (WF) at location (l) of year (y)
$GWP_{material}(l, WF, y)$	GWP of material (m) of process (WF) at location (l) of year (y)
$GWP_r(l, r, y)$	GWP of resource (r) at location (l) of year (y)
$Cap^P(l, r, y)$	production capacity of process (WF) at location (l) of year (y)
$GWP_l(l, y)$	GWP at location (l) of year (y)
GWP_{WF}	total GWP of process (WF)
GWP_r	total GWP of resource (r)
GWP_m	total GWP of resource (m)
$GWP_n(y)$	total GWP in network (n) of year (y)

$GWP_p(l, r, y)$	GWP of process (p) using resource (r) at location (l) of year (y)
$GWP_p(l, m, y)$	GWP of process (p) utilizing material (m) at location (l) of year (y)
$GWP_{nr}(y)$	GWP network reduction of year (y)
$GWP_{reductionpercentage}$	reduction scale of GWP
CAP_y^{total}	total capital cost of year (y)
$OPEX^{total}$	total operational and management cost of year (y)
p_y^{total}	annual purchase expenditure for resource (r) or material (m) in year (y)
$transport_y^{total}$	annual transportation expenditure for resource (r) or material (m) in year (y)
$CAP_{penalty}$	penalty for capital cost
$C_{l,r}$	capacity for storage process (p) using resource (r) or material (m) at location (l)
$y_{l,r}$	binary variable, 1 if storage process (p) is chosen, 0 otherwise