A framework for reliability-embedded design of multi-scale energy systems

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Abstract

The incorporation of renewable energy solutions into the global value chain is vital to the decarbonization of energy systems. However, the additional complexity may also lead to increased vulnerability in the face of disruptive events. It is therefore imperative that future energy systems are resilient to these vulnerabilities. In this work, we propose a multi-scale design methodology in the design of resilient energy systems that integrates supply chain network decisions with individual process reliability analysis. A two-step procedure is utilized where a network is first designed to optimize for economic objectives, and then scenario analysis is conducted to study how the network behaves under discrete disruptions. Agglomerative hierarchical clustering (AHC) is used to reduce problem size and increase computational efficiency. The use of this procedure is demonstrated through a simultaneous design and scheduling case study for the hydrogen supply chain. It is shown that a single process was chosen to meet 100% of demand if no failure scenarios are applied, but redundancies are favored when discrete disruptions are introduced. Furthermore, the quantitative levels at which investing in system reliability becomes cost-effective towards avoiding a penalty for unfulfilled demand can be identified.

Keywords

Process Optimization and Control, Planning & Scheduling, Supply Chain Management, Uncertainty & Stochastic Systems, Energy & Environment

Introduction

To support the decarbonization of energy systems, a suite of renewable energy solutions are being investigated for their potential incorporation into the global value chain. However, with this increase in complexity also comes an increase in vulnerability, as more parts of the system are exposed to potentially disruptive events (Sarma and Zabaniotou, 2021). Cyberattacks, natural disasters exacerbated by climate change, as well as other global upheavals such as pandemics have massively destructive effects that could ripple through the value chain, impacting the lives and livelihoods of people around the world. It is imperative, therefore, that energy systems are designed to withstand and adapt to disruptive events. However, a major challenge in achieving resilient energy systems is the occurrence of 'unknownunknown' events – where both the time and the impact of the disruption are unknown (Golan et al., 2020). While it is possible to optimize energy system resilience against a wide array of possible scenarios to account for the possibility of unknown-unknown events, it is highly inefficient and may

result in blind spots where a particularly destructive potential scenario is not included in the set of test scenarios.

A potential methodology to overcome this difficulty is to optimize energy system design in a multi-scale manner; taking into account not only the supply chain network but also the reliability of processes involved in the system and the components of these processes (Chrisandina et al., 2022). Multi-scale engineering has been applied to energy systems due to its ability to incorporate information from the multiple spatiotemporal scales that are at play in energy systems, and therefore this methodology is well-suited to analyze and optimize energy system performance against disruptions (Floudas et al., 2016; Kakodkar et al., 2022). Integrating equipment-level quantitative risk analysis into supply chain network design facilitates the consideration of system resilience on economic objectives without specifying a disruption scenario a priori (Al-Douri et al., 2021). A trade-off between investing in reliability and cost minimization strategies can thereby be investigated, dependent on the penalties imposed by customers for unmet energy demand. Therefore, this work aims to propose a framework for the multi-scale design and integration of energy systems considering the tradeoff between resilience and cost-efficiency through the use of quantitative risk analysis and supply chain network optimiza-

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tion. This framework will guide decision-makers in making cost-effective decisions when planning investments in energy system resilience, equipping energy systems to face an increasingly uncertain future.

To this end, the presented work demonstrates a multi-scale framework for the design on systems with network reliability considerations to bridge operational and strategic decisions across spatiotemporal scales. The application of the framework is demonstrated through a computational case study involving planning and scheduling to meet daily hydrogen demand.

Problem Statement

Given the at-scale introduction of renewables into the energy mix, as well as the higher incidence of weather-related and social disruptions, it is desirable to design energy systems which perform better in terms of reliability. The multiple available modes of production with disparate temporal dynamics, resource consumption, and scaling limitations, can be computationally challenging to resolve.

It is understood that in modern energy systems, redundancies can provide a degree of resilience. It should be noted that despite the additional cost incurred through the implementation of larger process capacities or newer processes, the investment could be justified if there is a high penalty enforced on unmet demand.

To this end, a framework for the design of energy systems which consider the reliability of process components implicitly can help decision-makers design resilient energy systems.

Methodology

Modeling and optimization of energy systems frameworks are able to provide solutions to optimize network configurations, process design, and scheduling decisions. Nevertheless, mathematical programming frameworks constructed as mixed integer programs (MIPs) assume perfect explicit knowledge of the temporal horizon over which they are resolved. Naturally, addressing discrete events such as systemic disruptions or temporary constraints under such a modeling paradigm is computationally impractical for large-scale problems. As a consequence, there is a gap in addressing optimal design under the influence of discrete uncertainties.

In this work, a two-step procedure is presented wherein: 1) a base-case network is designed through the implementation of a multi-scale MIP framework where every process is assumed to be functional 100% of the time and there is no penalty incurred for unmet demand, 2) process failure probabilities and penalties for unmet demand are introduced to the system and a new network is designed for different penalties. At every realization of the procedure, the failure probability indicates the likelihood that the process is completely nonoperational.

To reduce the problem size in each step of the procedure, the agglomerative hierarchial clustering (AHC) algorithm as described by Tso et al. (2020) is used to provide a sample of representative days that can sufficiently capture the intermittency of weather-related phenomena and varying natural gas prices. Component failure rates are provided through sampling from a randomly generated distribution as a measure of the probability of failure.

Model Formulation

The framework is modeled as a mixed-integer linear program (MILP) which allows for integrated design, planning, and scheduling. In this section, we summarize some of the key constraints of the framework. The full set of equations and parameters are provided in the supplementary section.

Subsection "Network design" describes the network problem which is resolved at the temporal scale of a year. The planning and scheduling decision constraints are determined for each hour of the planning period. The demand constraints are presented in Subsection "Demand constraints". The annual production costs are determined using the constraints described in Subsection "Annual production cost". The constraints to evaluate the expenditure on resource purchase are shown in Subsection "Resource purchase expenditure". Lastly the objective is described in Subsection "Objective".

Nomenclature

The nomenclature used in the rest of this section is outlined below.

Table 1: Sets

Notation	Description
\mathcal{I}_p	Set of all resources used
I_p	Set of all processes
${\mathcal H}$	Set of hours in one year
\mathscr{Y}	Set of years in the planning horizon
S	Set of cost scenarios

Table 2: Parameters

Notation	Description
$Cap_{i,y}^{P-max}$	Max. production capacity for process i at
	year y
$Cap_{j,y}^{S-max}$	Max. storage capacity for resource j at
0.0	year y
$\eta_{i,j}$	Conversion efficiency for resource j by
	process <i>i</i>
$LOSS_i$	Storage loss factor for resource j
ζ^p	Disruption pattern for production capacity
ζ^s	Disruption pattern for storage capacity
$Demand_{j,h,y}$	Demand for resource j at time period h in
	year y
demand d_{ihv}^{slack}	Demand slack for resource j at time period
J 7 7,5	<i>h</i> in year <i>y</i>
$Cost_{j,i,y}^{purchase}$	Purchase cost of resource j for process i in
/2	year y
Ψ	Penalty for unmet demand

Table 3: Continuous decision variables

Notation	Description
$cap_{i,y}^P$	Production capacity of process i in year y
$cap_{i,y}^{S}$	Storage capacity for resource <i>j</i> in year <i>y</i>
$p_{i,h,y}$	Realized production for process i in time
	period h within year y
$inv_{j,h,y}$	Inventory level for resource j in time pe-
	riod <i>h</i> within year <i>y</i>
$c_{j,h,y}$	Amount of resource j purchased in time
	period h within year y
$opex_{i,y}^{var}$	Variable O&M expenditure for process i in
~	year y
$Opex_{i,y}^{var}$	Variable O&M expenditure for process i in
	year y
$opex_{i,v}^{fix}$	Fixed O&M expenditure for process i in
- 10	year y
$Opex_{i,v}^{fix}$	Fixed O&M expenditure for process i in
- 1.7	year y
capexi,y	Capital expenditure for process <i>i</i> in year <i>y</i>
$capex_{i,y}$	Capital expenditure for process <i>i</i> in year <i>y</i>
$b_{i,v}^{annual}$	Annual purchase expenditure for resource
312	<i>j</i> in year <i>y</i>

Table 4: Binary decision variables

Notation	Description
$x_{i,y}^P$	1 if production facility <i>i</i> is built in year <i>y</i> , 0
	otherwise
$x_{i,v}^S$	1 if storage facility i is built in year y , 0
5.0	otherwise

Scenario reduction

The temporal scale is clustered using agglomerative hierarchical clustering (AHC) (Tso et al., 2020), using the normalized solar and wind profiles as well as varying natural gas spot prices. It should be noted that AHC maintains temporal chronology which makes it easier to relay information between the time periods in the scheduling model. However, it was inferred by (Tso et al., 2020) that minimizing the within cluster variance does not necessarily lead to a reduction in the objective error. Hence, the model is run over the time period of a year for various cluster sizes to gain insight into how the objective error scales with an increase in cluster sizes (see Figure 1). Notwithstanding the absence of a formal methodology to identify the optimal number of clusters from the perspective of objective error, a cluster number of 20 (288 hours) is chosen based on the trade-off with computational time. Moreover, the solution is validated with the full-scale solution across the planning horizon.

Network design

Binary variables $(x_{i,y}^{P} \text{ for production facilities and } x_{j,y}^{S} \text{ for storage facilities})$ are assigned to each node. The binary equals to 1 if the facility is built in a particular year, 0 otherwise. Note that distinction between storage and production facilities is only for the ease of representation. Moreover, we do not impose a mathematical distinction between energy



Figure 1: Trade-off between within cluster sum of squares (WCSS) and number of representative days.

and material conversion processes.

Production capacity sizing

Qualitatively, these constraints allow the model to account for capital invested in establishing infrastructure in the preceding planning periods.

$$cap_{i,y}^{P} \leq Cap_{i,y}^{P-max} \cdot x_{i,y}^{P}, \quad \forall i \in I_{p}, \quad \forall y \in \mathcal{Y}$$

$$(1)$$

The storage capacity and facility location decisions are determined using the following constraint:

$$cap_{j,y}^{S} \leq Cap_{j,y}^{S-max} \cdot x_{j,y}^{S}, \quad \forall j \in \mathcal{I}_{p}, \quad \forall y \in \mathcal{Y}$$

$$(2)$$

where $cap_{i,y}^{P}$ is the production capacity of process *i* in year *y*, $cap_{j,y}^{S}$ is the storage capacity for resource *j* in year *y*, $Cap_{i,y}^{P-max}$ and $Cap_{j,y}^{S-max}$ are the maximum production capacities for process *i* and storage capacities for resource *j* respectively in year *y*.

Resource balance

We assume that all processes in the superstructure function on a continuous basis. For each process *i*, the realized production $(p_{i,h,y})$ in a time period (h) of year (y) is constrained to the capacity of the production facility as determined by Constraint 1. Similarly, the inventory level $(inv_{j,h,y})$ in a time period (h) of year (y) is constrained to the storage capacity as determined by Constraint 2. Furthermore, we restrict the amount of resource that can be purchased from outside the system $(c_{j,h,y})$ to the maximum resource availability. Note that the maximum resource availability will be non-zero only for resources that serve as raw materials in the system, e.g.: natural gas and water.

Nameplate production capacity

The realized production rates for each hour are determined using Constraint 3 below. To account for the intermittent availability of solar and wind, the solar direct normal irradiance (DNI) and wind speed power outputs are normalized to generate capacity utilization factors. ζ^p and ζ^s are disruption Variable O&M expenditure patterns sampled based on the mean-time-to-failure.

$$p_{i,h,y} \leq \zeta_{i,h,y}^{p} \cdot Cap_{i,h,y}^{f} \cdot cap_{i,y}^{P}, \quad \forall i \in I_{p}, h \in \mathcal{H}, y \in \mathcal{Y}$$
(3)

Nameplate storage capacity

The inventory levels at every hour are restricted to the nameplate storage capacity using the following constraint:

$$inv_{j,h,y} \leq \zeta_{i,h,y}^s \cdot cap_{j,y}^s, \quad \forall j \in \mathcal{I}_p, \quad \forall h \in \mathcal{H}, \quad \forall y \in \mathcal{Y}$$
(4)

Resource consumption capacity

This constraint restricts the amount of resource that can be consumed.

$$c_{j,h,y} \leq C_{j,h,y}^{max}, \quad \forall j \in \mathcal{J}_p, \quad \forall h \in \mathcal{H}, \quad \forall y \in \mathcal{Y}$$
 (5)

Inventory balance

The inventory balance constraint is applied over the planning horizon to determine both the resource flow through the network, and account for inventory cycling:

$$inv_{j,h,y} = (1 - Loss_j) \cdot inv_{j,h-1,y} + \sum_{\forall i \in I_p} \eta_{i,j} \cdot p_{i,h,y} + c_{j,h,p} - s_{i,h,y}$$
$$\forall j \in \mathcal{J}_p, h \in \mathcal{H} \setminus \{\underline{h}\}, y \in \mathcal{Y} \quad (6)$$

Where $\underline{h}, \underline{d}$ are the first elements in the sets of time periods (\mathcal{H}) and seasons (\mathcal{D}) respectively, whereas \bar{h} , \bar{d} are the last. The conversion efficiencies for each resource (j) by each process (*i*) is given by the factor $\eta_{i,j}$. The model accounts for storage losses using the factor $LOSS_j$.

Demand constraints

The demand constraint ensures that the daily demand for hydrogen is satisfied:

$$\sum_{\forall h \in \mathcal{H}} s_{j,h,y} = demand_{j,h,y} - demand_{j,h,y}^{slack},$$

$$\forall j \in \mathcal{J}_{H_2-demand} \cap \mathcal{J}_p y \in \mathcal{Y} \quad (7)$$

Annual production cost

We consider three costing components. Variable operational and maintenance (O&M) costs are calculated based on the amount of basis resource produced by a process (Constraint 8). Annualized capital expenditure(Constraint 10) and fixed (O&M) costs (Constraint 9), on the other hand, are evaluated based on the capacity sizing of the processes.

$$opex_{i,y}^{var} = Opex_{i,y}^{var} \cdot p_{i,y}^{annual}, \quad \forall i \in I_p, y \in \mathcal{Y}$$
 (8)

Fixed O&M expenditure

$$ppex_{i,y}^{fix} = Opex_{i,y}^{fix} \cdot cap_{i,y}^{P}, \quad \forall i \in I_p, y \in \mathcal{Y}$$
(9)

Capital expenditure

$$capex_{i,y} = A^f \cdot Capex_{i,y} \cdot cap_{i,y}^P, \quad \forall i \in I_p, y \in \mathcal{Y}$$
(10)

Resource purchase expenditure

The annual expenditure on resource purchase is evaluated using Constraint 11:

$$b_{j,y}^{annual} = Cost_{j,i,y}^{purchase} \cdot c_{i,y}^{annual}, \quad \forall i \in I_p, y \in \mathcal{Y}$$
(11)

Objective

The objective of the model is to minimize the total cost incurred by the system. If the hydrogen demand is met, the objective value divided by the total hydrogen production indicates the levelized cost of hydrogen (LCOH).

The cost objective minimizes the levelized total cost borne by the system. The total cost consists of the annualized capital expenditure $(capex_{a,y}^{total})$, operational expenditure $(opex_{a,y}^{total})$, and material purchase cost $(b_{j,y}^{total})$. Notably, capital and operational expenditures as well as purchase costs are minimized in the system.

This objective minimizes the cost while meeting a daily hydrogen demand. A penalty (ψ) is added to penalize unmet demand.

$$\min \sum_{y \in \mathcal{Y}} cost_{y}^{total}$$

$$cost_{y}^{total} = capex_{y}^{total} + opex_{y}^{total} + b_{y}^{total}$$

$$+ \sum \Psi \cdot demand_{i,h,y}^{slack} \quad (12)$$

Computational studies

The framework is applied towards the simultaneous design and schedule optimization of an energy system to meet a daily demand for hydrogen. 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. Of key interest is the trade-off between incurring a cost penalty for unmet demand versus the cost of investing in redundancies to increase the overall reliability of the system.

The implemented case study considers both wind and solar energy for the generation of power; steam methane reforming (SMR) and alkaline water electrolysis (AWE) for the production of hydrogen; lithium ion batteries for energy storage, and geological storage for produced hydrogen. The weather data for capacity factors is taken from the National Solar Radiation Data Base (NSRDB) (Sengupta et al., 2018), and the natural gas prices are from the Henry Hub Spot Price Index (Energy Information Administration, 2022). The costing data is taken from Demirhan et al. (2020).

First, a base case is implemented sans the consideration of process failure. It should be noted that failure can be experienced by various systems that can have real world implications. For example, in the case of the failure of hydrogen storage, it would imply that while hydrogen is produced it cannot be accessed. Similarly, weather-related disruptions can affect the grid causing failure of wind and/or solar farms. The generality of the framework allows it to be applied towards the analysis of myriad cost and reliability scenarios.

In the subsequent case studies, the model is provided with both an economic penalty for not meeting demand and process failure realizations. In principle, the application of the framework should allow for determination of designs wherein the additional cost towards redundant facilities is justified depending on the penalty that is imposed on unmet demand.

Results and Discussion

In the base case, it can be observed that the entirety of the production is met through the cheaper SMR process. There is no failure imposed, and hence there are no redundancies observed. It can be seen in Figure 2 that the cost objective remains constant in the base case and this is due to the fact that the SMR process is capable of meeting 100% of network demand and thus the penalty does not affect network design.

Trade-off between penalty and cost objective

In the case where process failure realizations are introduced to the system, it can be seen in Figure 2 that the system willfully accepts the penalty until the cost incurred surpasses the cost of the base case. At a cost point above the base case cost (above the dotted line in Figure 2), it is more costeffective to install additional capacity despite the additional investment costs incurred as the penalty for unmet demand is high. Penalty on unmet demand can serve as a proxy for the loss of business due to non-fulfillment of expected system output.

It should, however, be noted that the results are highly dependent on the consideration of the failure probabilities, and also how the process failure is realized. In the illustrative results as shown in Figure 3, the model chooses to augment the production of hydrogen by setting up other process units such as alkaline water electrolysis units and additional hydrogen storage. Moreover, the discharge capabilities of stored electricity is also augmented. Furthermore, it is also possible to conduct sensitivity analysis on the failure probabilities to determine which processes display outsized economic gains



Figure 2: Trade-off between penalty on unmet demand and cost objective

relative to investments in process reliability.



Figure 3: illustrative results for a penalty factor of $0.75/kg.H_2$. Here, change in installed capacity is calculated on the basis of the new scenario.

Scenario Analysis

In essence, the framework can be used for scenario analysis through the consideration of myriad values for the component failure probabilities. For example, the scenario presented in Figure 4 only differs from the scenario as described in Figure 3 in the failure probability of the energy storage (lithium-ion) batteries. In this scenario, it can be observed that the capacity of wind farms is augmented and the reliance on energy storage is curtailed. Furthermore, the increase in power generation potential also translates to a lower requirement for hydrogen storage at scale. In both cases the discharging capacities are improved. It is understood that under the influence of process disruption, a larger amount of demand will need to be met directly through stored product or by in-time production by utilizing stored energy.

Conclusion and future work

Real world systems vary greatly in terms of reliability. Reliability is notably influenced by exogenous factors, and is thus suspect to localized factors such as weather patterns and



Figure 4: Illustrative results for a penalty factor of $0.75/kg.H_2$ - with risk assigned to energy storage. Here, change in installed capacity is calculated on the basis of the new scenario.

events, as well as factors which may be influenced by dynamics outside the system boundaries such as the cost of natural gas which is dependent on global trade factors and social events. Quantifying the overall reliability of a system can thus be challenging. Nonetheless, in the absence of a realizable perfectly reliable system, networks need to be analyzed under the context of a penalty assigned to the failure to meet a set demand target. Here, it can be noted that a high penalty could justify investment towards redundancies and larger capacities to increase system reliability.

The proposed MIP framework can be implemented for the analysis of various energy transition scenarios to design optimal energy systems models with embedded reliability. The appetite for risk and non-fulfillment of demand can be described through the different levels of penalty. While the framework can also be applied towards the curtailment of carbon emissions, a multi-objective study is not presented in this article.

In future iterations of the framework, the downtime of processes in the face of disruption will also be considered. Longer downtime during repair negatively impacts revenuemaking potential, and it may be desirable to invest in more capital-intensive processes to limit idle time in the future. This becomes particularly important for the comparison of modular processes (viz. water electrolysis) as compared to larger facilities (methane reforming). Depending on the nature of failure, modular facilities may be able to reconfigure quickly to more rapidly bring a section of installed capacity back online, which would change the configuration of the energy system to incorporate more modular technologies as opposed to larger ones.

Additionally, in the presented work, failure is considered as a complete disruption of the process. In reality, however, failures may only partially reduce the production capacity of the process. To address this limitation, different levels of failure need to be sampled by fitting available data. Moreover, lower down the scale failure could be limited to the equipment level as opposed to the entire process, thus motivating the integration of process-level dynamics within the framework. This may also provide valuable information on specific bottlenecks and vulnerable components in the process, which could lead to targeted investment opportunities to enhance system reliability at large.

References

- Al-Douri, A., V. Kazantzi, N. Currie-Gregg, and M. M. El-Halwagi (2021). Integrating uncertainty quantification in reliability, availability, and maintainability (ram) analysis in the conceptual and preliminary stages of chemical process design. *Chemical Engineering Research and De*sign 167, 281–291.
- Chrisandina, N., S. Vedant, E. Iakovou, E. Pistikopoulos, and M. El-Halwagi (2022). Multi-scale integration for enhanced resilience of sustainable energy supply chains: Perspectives and challenges. *Computers & Chemical Engineering 164*, 107891.
- Demirhan, C. D., W. W. Tso, J. B. Powell, C. F. Heuberger, and E. N. Pistikopoulos (2020). A multiscale energy systems engineering approach for renewable power generation and storage optimization. *Industrial & Engineering Chemistry Research* 59(16), 7706–7721.
- Energy Information Administration (2022). Henry hub natural gas spot price.
- Floudas, C. A., A. M. Niziolek, O. Onel, and L. R. Matthews (2016). Multi-scale systems engineering for energy and the environment: Challenges and opportunities. *AIChE Journal* 62(3), 602–623.
- Golan, M. S., L. H. Jernegan, and I. Linkov (2020). Trends and applications of resilience analytics in supply chain modeling: systematic literature review in the context of the covid-19 pandemic. *Environment Systems and Deci*sions 40(2), 222–243.
- Kakodkar, R., G. He, C. Demirhan, M. Arbabzadeh, S. Baratsas, S. Avraamidou, D. Mallapragada, I. Miller, R. Allen, E. Gençer, et al. (2022). A review of analytical and optimization methodologies for transitions in multi-scale energy systems. *Renewable and Sustainable Energy Reviews 160*, 112277.
- Sarma, G. and A. Zabaniotou (2021). Understanding vulnerabilities of renewable energy systems for building their resilience to climate change hazards: Key concepts and assessment approaches. *Renewable Energy and Environmental Sustainability* 6, 35.
- Sengupta, M., Y. Xie, A. Lopez, A. Habte, G. Maclaurin, and J. Shelby (2018). The national solar radiation data base (nsrdb). *Renewable and sustainable energy reviews 89*, 51–60.
- Tso, W. W., C. D. Demirhan, C. F. Heuberger, J. B. Powell, and E. N. Pistikopoulos (2020). A hierarchical clustering decomposition algorithm for optimizing renewable power systems with storage. *Applied Energy* 270, 115190.