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Resilient-aware Design for Sustainable Energy Systems

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ABSTRACT

To mitigate the effects of catastrophic failure while maintaining resource and production efficiencies, energy systems need to be designed for resilience and sustainability. Conventional approaches such as redundancies through backup processes or inventory stockpiles demand high capital investment and resource allocation. In addition, responding to unexpected “black swan” events requires that systems have the agility to transform and adapt rapidly. To develop targeted solutions that protect the system efficiently, the supply chain network needs to be considered as an integrated multi-scale system incorporating every component from individual process units all the way to the whole network. This approach can be readily integrated with analogous multiscale approaches for sustainability, safety, and intensification. In this work, we bring together classical supply chain resilience with process systems engineering to leverage the multi-scale nature of energy systems for developing resilience enhancement strategies that are resource-efficient. In particular, we adapt qualitative risk analysis methods to uncover critical system components and major vulnerabilities to guide resource allocation decisions. To account for these vulnerabilities, we explore the feasible region of operation around each node of the supply chain. An optimization formulation is devised to generate multiscale alternative. The approach is demonstrated through a case study involving the production of biofuels, demonstrating the range of adaptation strategies possible when process-level strategies are incorporated into overall supply chain design.

Keywords: Supply Chain, Multiscale Modelling, Planning & Scheduling, Renewable and Sustainable Energy, Energy Systems

INTRODUCTION

The study of energy system resilience, which is typically defined as the ability of systems to manage possible disturbances and recover from them, has increased in importance over the last decade as energy systems become more complex and disturbances become more frequent and severe [1, 2]. The integration of multiple energy sources, including intermittent and geographically-dispersed renewables, facilitates the transition to a more sustainable energy system, but also introduces complexity and vulnerability [2]. Therefore, energy systems need to be designed and operated in such a way that they are prepared to adapt and recover from future disturbances whether or not these disturbances are expected.

In minimizing the impact that a particular disturbance has on energy system infrastructure, resilience contributes to the sustainability of the energy system in that less waste in the form of broken equipment and unused raw material or product is generated [3, 4, 5]. Additionally, systems that are better able to withstand disturbances are also able to continue operating for a longer period of time, maximizing their useful lifetimes. However, commonly-deployed resilience strategies center around reserving resources (either raw materials or finished products) as safety inventory to maintain high production output for as long as possible [6]. This strategy is useful, but relying solely on storing large amounts of unused inventory also raises its own sustainability and safety concerns [3]. For example, large-scale storage of hydrogen for energy currently relies on artificially-built salt caverns or depleted natural gas reservoirs, but there may be possible reactions between the stored hydrogen with the microorganisms and mineral constituents of the reservoir, leading to deterioration of the hydrogen storage or unwanted deposits of reaction products [7]. Furthermore, long-term backup inventory storage can represent a financial drain on companies, which may make it economically unattractive. Therefore, cost-effective targeted resilience enhancement strategies need to be considered to balance the issues of resilience, sustainability, and economic cost.

Consideration of energy system resilience (and adjacent concepts) independently and alongside sustainability has been demonstrated in the open literature. Panteli et al. [8] proposed that power system resilience consists of two separate characteristics: operational resilience, which corresponds to the ability to ensure uninterrupted power supply, and infrastructure resilience, which refers to the physical strength of the power system to mitigate faulty portions of the system. Moreno-Sader et al. [9] proposed the use of a modified return-on-investment (ROI) metric that includes safety, sustainability, resilience, and reliability weights to screen process alternatives early in the design process. The weights are calculated based on whether a proposed design reaches a desired target value for each of the four desired objectives. Hosseini-Motlagh et al. [10] designed a power supply chain to minimize unmet electricity demand as well as pollution emission under uncertainty.

The complexities within an energy system not only come from supply chain dynamics such as material flow, customer energy demand, and transportation linkages, but also in the chemical reactions that occur within manufacturing facilities. Harnessing the physical and chemical synergies in energy systems through multi-scale systems engineering could be key to unlocking a variety of targeted resilience strategies that do not require significant resource or capital investments [11]. With a multi-scale approach, tools and methods built for supply chain, process, unit operations, and reaction-scale optimization are integrated to provide an accurate representation of the interactions across spatio-temporal scales [11, 12]. The approach allows bespoke models to be constructed that contains appropriate levels of detail at relevant spatio-temporal scales to open up the possibility for targeted resilience strategies.

Multi-scale approaches have been utilized in the design and optimization of energy systems to achieve economic and/or sustainability goals. Demirhan et al. [12] developed a multi-scale model for an energy system which uses solar and wind resources to supply electricity via various storage technologies at the lowest possible cost. The model accounts for renewable resource availability, storage technology constraints, as well as demand fluctuations. Shao et al. [13] proposed a multi-scale model for a hydrogen-based off-grid microgrid to generate both power and heat for rural areas. A two-stage stochastic formulation was used to derive optimal capacity sizing and scheduling for both normal and on-emergency scenarios. Lin [14] explored the life-cycle impact of different technology pathways to develop future energy systems that integrate renewable resources, battery storage, and dense energy carrier production.

For a holistic consideration of energy system resilience, a multi-scale modeling approach can be beneficial to integrate risk factors and resilience enhancement strategies on the supply chain level and on the component level. This paper, therefore, aims to illustrate how process-level considerations contribute to overall supply chain resilience in a cost-competitive and sustainable manner. A qualitative resilience analysis is conducted to identify critical model variables that directly affect overall system performance. Next, an integrated system model is constructed around key variables and optimized. What-if scenarios are applied on the optimized network to demonstrate its resilience against several supply chain disturbances. The proposed methodology is demonstrated through a small regional biofuel supply chain.

METHODOLOGY

Consideration of Process Feasible Regions

In a typical supply chain optimization formulation, the manufacturing facilities that produce goods to sell are modeled as nodes with a fixed production rate; that is, given some quantity of raw materials, the quantity of products made is known [3, 6]. Responding to disruptions involves adding redundancies into the supply chain superstructure through alternate suppliers or transport routes, excess inventory, and overdesign of manufacturing capacity. Conversely, in process systems literature, a manufacturing facility is modeled as a set of processes (chemical or physical) that can be described by their operating parameters. Given a process design, it is well-known that there exists a region of feasible operation where different operating parameters will yield a different amount of product [15].

In our previous work, we demonstrated the benefits of designing processes with high reliability on enhancing overall supply chain resilience under disruptions [16]. Reliability is achieved through choosing to install process equipment with low failure rates and high repair rates. In this work, we expand on the concept of implementing process-level strategies to enhance supply chain resilience by considering the process feasible region within the supply chain optimization problem [17]. In effect, each manufacturing facility will be represented as a node with operational parameters that can be optimized for different scenarios. This necessitates a mathematical model for the process node that is then integrated into the supply chain optimization formulation.

To formulate a mathematical model of each process, computer-aided simulation software (e.g. Aspen Plus) and functional equations of key units within the module are first used to generate a computer model of the module. Next, the operating parameters that are most critical to process output are identified. A surrogate model for each critical unit is then generated to represent the relationship between the critical parameters with process output. These surrogate models are then integrated as additional constraints in the supply chain formulation. A generalized form of the surrogate model is shown in Eq. 1, where the unit-level parameter realizations $\boldsymbol{x_{u,f,t}}$ determine the unit efficiency $Q_{u,f,t}$.

$$Q_{u,f,t} = \Phi(\boldsymbol{x_{u,f,t}}) \tag{1}$$

Integrated Model

In this work, the energy system is assumed to be composed of a set of supplier cities that contain a set amount of raw material and could also contain modular refineries of a fixed nameplate capacity for production of a dense energy carrier (DEC). Finally, the product is transported to market cities to fulfill the required demand. Mass balance constraints for a similar system is available in Chrisandina et al. [11]. Additional constraints to include process information are outlined in this section.

Nomenclature

The symbols used for the rest of the paper are defined in Table 1 below.

Table 1: Symbols and definitions for sets, parameters, and variables

Notation	Description
	Sets
$\mathcal{F}$	Set of manufacturing sites
S	Set of supplier sites
M	Set of market sites
T	Set of scheduling time periods
U	Set of process units
	Parameters
$yield_f$	Yield of product in site f
$\mathrm{Gmax}_{\mathrm{m,t}}$	Demand for product in market m at time t
$d_{i,j}$	Distance between two locations i and j
$\mathrm{service}_{\mathrm{m}}$	Minimum service rate for market m
x_u^{Nom}	Nominal parameter value for unit u
Ct	Cost of shipping feedstock [$/mile-ton]
Cb	Cost of feedstock [$/ton]
Cp	Cost of shipping product [$/mile-ton]
	Variables
$G_{f,t}$	Production from site f at time t
$G'_{f,m,t}$	Product delivered from site f to market m at time t
$\mathrm{B}_{s,f,t}$	Raw material from supplier s consumed by site f at time t
$\boldsymbol{Q_{f,t}}$	Efficiency of process modules in site f at time t
$\boldsymbol{x_{u,f,t}}$	Realized parameter value for unit u in site f at time t
$Q_{u,f,t}$	Efficiency for unit u in site f at time t
$\mathrm{mod}_{f,t}$	Number of process modules in site f at time t
	Generalized functions
$\Phi(\boldsymbol{x_{u,f,t}})$	Correlation between unit-level parameters and unit efficiency
$\Lambda_{\mathrm{u}}(\mathrm{Q}_{u,f,t})$	Correlation between unit efficiency and overall process module efficiency
$\Psi_f(\mathrm{mod}_{f,\lvert T\rvert})$	Correlation between number of process modules and capital expense

Constraints

These constraints are modified from the original mass balance constraints to include process efficiency information.

The product yield at each manufacturing site is governed by the amount of raw material supplied to the site and the efficiency of the process modules placed on site.

$$G_{f,t} = \mathrm{yield}_f \times \sum_s^S B_{s,f,t} \times \mathrm{Q}_{f,t} \tag{2}$$

The efficiency of a process module is defined as a multiplier on the nominal process output which depends on the operating conditions to which the process module is set. The process module efficiency is governed by the efficiencies of the critical units within the process module. The specific function that relates unit efficiency with process module efficiency depends on the exact configuration of the module.

$$Q_{f,t} = \Lambda_{u\in U}(\mathrm{Q}_{u,f,t}) \tag{3}$$

Objectives

The main objective of the optimization problem is to minimize total annual cost. This includes the annualized fixed cost in the purchase of process modules, as well as the operating cost (raw material purchase and transportation). The purchase cost is a function of the number of process modules deployed in the supply chain, and the specific function depends on how capacity scales with cost. The annualized fixed cost (AFC) is calculated by dividing the total capital cost across the lifetime of the process modules.

$$Cost = AFC + OPEX \tag{4a}$$
$$CAPEX = \Psi_{f\in F}(\mathrm{mod}_{f,t=\lvert T\rvert}) \tag{4b}$$
$$AFC = \frac{\mathrm{CAPEX}}{years} \tag{4c}$$

$$OPEX_t = \sum_{f}^{F}\sum_{s}^{S} B_{s,f,t} \times Cb + \sum_{f}^{F}\sum_{s}^{S}(B_{s,f,t} \times d_{s,f} \times Ct) + \sum_{f}^{F}\sum_{m}^{M}(G'_{f,m,t} \times d_{f,m} \times Cp) \quad (4d)$$

To represent system resilience, we include a constraint on the target demand fill rate required at every scheduling time step.

$$\sum_{f}^{F} G'_{f,m,t} \geq \mathrm{Gmax}_{\mathrm{m,t}} \times \mathrm{service}_{\mathrm{m}} \quad (5)$$

CASE STUDY

In this work, we adapt the case study introduced by Lopez-Molina et al. [18] where refuse-derived fuel (RDF) is converted to methanol and then sold as fuel. Gasification-based technology is used, and a modular biorefinery is assumed for each manufacturing site. The goal of this case study is to compare the resilience of the supply chain to various external disruptions with and without the incorporation of process surrogate models in the supply chain formulation.

Background Information

The RDF-to-methanol conversion process occurs via gasification to produce syngas as an intermediary, purification of the syngas, and methanol synthesis as a final step. Technical and operational details of the process are given in the literature [19, 20], and key process inputs and outputs are shown in Fig. 1. A simplified process flow diagram is shown in Fig. 2. In this work, linear surrogate models (see Eq. 6) are generated for each critical parameter of the process, as listed in Table 2. Linear surrogates are chosen due to the small range of possible values for each critical parameter.

$$Q_{u,f,t} = m_u \frac{x_{u,f,t}}{x_{u,0}} + b_u \quad (6)$$

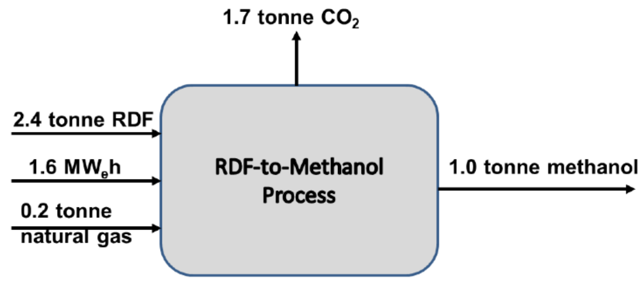

Figure 1: Key process inputs and outputs [18]

We consider the case of six cities: three producer cities which act as suppliers and manufacturers (A, B, C), and three market cities which purchase methanol (D, E, F). The specific supply availability and demand requirements are given in Fig. 3, and as a base-case scenario a 90% target demand fill rate is assumed. A planning horizon of one year with monthly schedules is assumed. The strategic decision to be made is where to locate process modules, and the operational decisions to be made are how many process modules to deploy, tuning of process

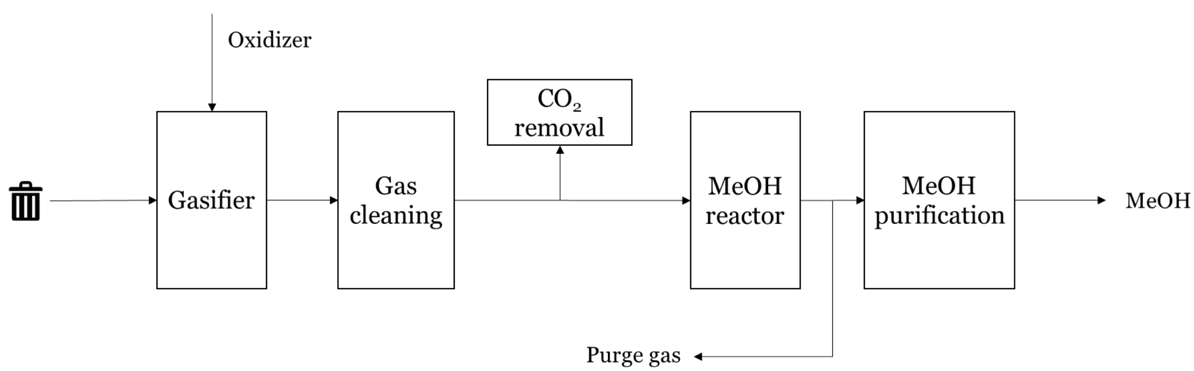

Figure 2: A simplified process flow diagram of the methanol synthesis process

Table 2: Critical parameters for methanol synthesis and their feasible operating range [20]

	Nominal operating condition ($x_{u,0}$)	Minimum	Maximum	Gradient (m)	Intercept (b)
MSW moisture content [%]	25	15	40	-0.24	1.23
Gasifier temperature [^{o}C]	850	700	900	1.72	-0.72
Gasifier equivalence ratio	0.42	0.35	0.6	-1.31	2.25
Reactor pressure [bar]	60	40	90	0.68	0.28
Recycle ratio	4.75	4.05	5.5	0.26	0.73

parameters in a location (listed in Table 2), and the connection between supplier and market cities.

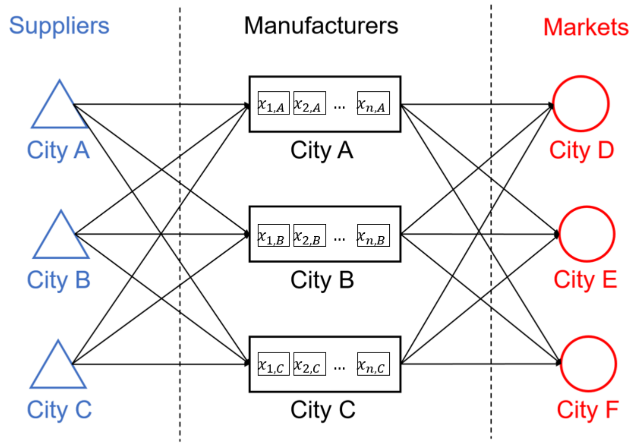

Figure 3: The supply chain superstructure

RESULTS AND DISCUSSION

Qualitative Resilience Analysis Results

In order to identify major risks to the supply chain, a table of potential failure modes and mitigation strategies has been constructed (see Table 3). Failure modes on supply chain entities (suppliers, logistic providers, manufacturing sites, and markets) as well as on process components (gasifier, syngas purifier, methanol reactor) are considered. It can be seen that there are multiple potential mitigation strategies for each entity failure mode and that in many cases operational changes on the process module level (a sub-entity of a manufacturing site) can help in failure mitigation. It is expected, therefore, that simultaneous optimization of process and supply chain parameters will yield a supply chain schedule that is more resilient to these failure modes. The next sub-section will aim to quantify these benefits.

Impact of Process Tuning on Supply Chain Performance

In the base-case scenario, processes are operated at their nominal parameter values ($Q_{f,t} = 1$) with a total cost of $317MM. Several failure scenarios are tested to see if the supply chain is able to adjust. Table 4 shows the feasibility of different failure scenarios that occur in the beginning of the planning horizon. It can be seen that reacting to deviations away from the base-case scenario without process tuning increases the total cost of the supply chain, as more process modules are needed to compensate for additional production. However, process-level tuning allows for existing modules to increase production within their feasible regions as needed, which significantly reduces the additional capital investment needed to meet the new demand. In these cases, raw material and utility costs contribute to the increase in total economic cost but no new process modules were

Table 3: Potential failure modes and mitigation strategies

Entity	Sub-entity	Potential failure mode	Mitigation strategies
Supplier		Decline in supply availability	Multiple suppliers Tune process module to increase yield Forecasting – storage for future
Logistics provider		Technical problems with vehicle	Vehicle maintenance Investment in updated vehicles
		Delivery delays	Reroute vehicles
Manufacturing site	Geographical location	Location experiences natural disaster event	Relocate process modules to other manufacturing locations
	Process module	Module temporarily unavailable	Surge production in other manufacturing sites Repair/replace module
	Gasifier	Temperature Moisture content	
	Syngas scrubber	Absorption failure	
	Methanol reactor	Low yield	
Market		Increase in demand	Acquire new modules Surge production in manufacturing sites
		Demand concentrated in one location	Relocate process modules to manufacturing sites in proximity Ship raw material to manufacturing sites in proximity

purchased. Table 5 shows the process parameter realizations that correspond to various service fill rates, which demonstrates how different process units are operated to meet specific market demands. Furthermore, the deployment of additional process modules represents an increase in material consumption that is used to construct the process modules, meaning that process-level tuning also opens up the possibility for lower emission footprint across the supply chain while delivering the same level of service throughout the year.

Table 4: Total economic cost of different supply chain scenarios – comparison between supply chain-only design and supply chain design with process surrogate model included

Scenario	Supply chain only	Supply chain + process
Target fill rate increases to 95%	\$357MM (+13%)	\$330MM (+4%)
Target fill rate increases to 100%	\$367MM (+16%)	\$342MM (+8%)
City E demand increases to 110%, start of year	\$357MM (+13%)	\$332MM (+4%)
City E demand increases to 110% for one month	\$343MM (+8%)	\$318MM (+0%)
City B is partially disrupted	\$344MM (+8%)	\$318MM (+0%)

Table 5: Process parameter realization for various service fill rates

Process parameter	Base case	Fill rate 95%	Fill rate 100%
MSW moisture content [%]	25	25	25
Gasifier temperature [^{o}C]	850	850	900
Gasifier equivalence ratio	0.42	0.42	0.42
Reactor pressure [bar]	60	66	66
Recycle ratio	4.75	5	5.2

Some scenarios are also tested where failure modes happen in the middle of the planning horizon. Without process tuning, supply chain operational decisions are updated to address failure. With process tuning, however, process module operational decisions are also updated which provides additional options for failure mitigation. Taking Scenario #4 from Table 4 as an example, if the demand increase occurs in the middle of the year the process module in City C (the closest manufacturing site) slightly increases its capacity temporarily to meet the additional demand without affecting the operations of the other manufacturing sites or investing in additional process modules. This temporary capacity increase is achieved by increasing the reactor pressure by 10% and recycle ratio by 5%. When the demand level lowers, the process module in City C adjusts its operation again to its baseline level.

A scenario where process-level failure occurs is also tested, where the process module in City B experiences a failure that lowers its production capacity until recovery efforts have concluded. In this scenario, City B experiences a partial failure that affects 50% of its capacity and recovery efforts are concluded at the end of the planning horizon. The other manufacturing sites respond to this failure by increasing their production so that demand can still be met, alleviating the need to invest in a replacement process module.

CONCLUSION

To achieve a resilient and sustainable energy system, incorporating targeted strategies to mitigate potential failures while maintaining efficient resource utilization and low capital investment is critical. A multi-scale approach to design and optimization of energy systems enables a holistic assessment of potential failure modes and mitigation strategies that operate on multiple spatio-temporal scales. In this work, we have demonstrated a first attempt at simultaneous optimization of supply chain and process design by including critical process parameters as additional constraints within a supply chain model formulation. We showed that the consideration of the feasible region around each process allows the energy system design to operate in various disruption scenarios with low additional capital investment and no additional process module constructions, limiting the economic and environmental cost of these mitigation strategies. Furthermore, we also demonstrated that targeted changes can also be implemented in the middle of the planning horizon on specific nodes without affecting the overall system design or other nodes' operations. To further develop this methodology, more bespoke process surrogate models that account for the relationship between multiple critical parameters will be beneficial. Additionally, the emissions footprint of establishing or transporting additional process modules to a different manufacturing site can be incorporated to further elucidate the environmental cost of these resilience strategies. Finally, the effects of running processes at the boundary of their feasible regions on the reliability of the modules themselves need to be studied, as this may lead to an increased need for maintenance.

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