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Dimensionality Reduction in Optimal Process Design with Many Uncertain Sustainability Objectives

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ABSTRACT

The study of sustainable design has gained prominence in response to the growing emphasis on environmental and social impacts of critical infrastructure. Addressing the different dimensions inherent in sustainability issues necessitates the application of many-objective optimization techniques. In this work, an illustrative four-objective design system is formulated, wherein uncertainties lie within two different socially-oriented objectives. A stochastic community detection approach is proposed to identify robust groupings of objectives. The findings reveal that the modularity of the optimal solution surpasses that of the average graph, thus demonstrating the efficacy of the proposed approach. Furthermore, a comprehensive exploration of the Pareto frontiers for both the robust and single-scenario best groupings is undertaken, demonstrating that using the robust grouping results in little to no information loss about tradeoffs.

Keywords: Sustainability, Multi-Objective Optimization, Network Theory

INTRODUCTION

Various global events over the past several years have made clear the importance of designing new infrastructure not only at low cost but also that does not negatively impact global climate, that is resilient against disruptive events such as pandemics and wars, and that provides positive social outcomes for all relevant stakeholders [1]. For many large industries, shareholders are increasingly concerned about the significance of environmental, social, and governance (ESG) considerations within the framework of sustainability. The chemical industry is no exception to this trend. Consequently, there exists a compelling impetus to investigate sustainable process designs which perform well both in traditional economic metrics, such as net present value, annualized cost, or payback period, while also achieving positive social and environmental outcomes [2]. Moreover, when such environmental and social outcomes are considered, it is important to consider tradeoffs between different aspects of these main pillars. For instance, a socially positive outcome will consist of outcomes such as added jobs, safe operation, equitable outcomes among relevant stakeholders, and community acceptance, some of which may be in conflict with one another when considering design alternatives. To evaluate the potential tradeoffs between these various goals, we employ many-objective optimization, an approach with widespread applicability in chemical process systems research. [3] The result of many-objective optimization is not a singular solution but a Pareto frontier, illustrating the tradeoffs between different objectives. All points along the Pareto frontier indicate the best one objective can do without hurting another one.

Unfortunately, for problems with large number of objectives, the time that is required to solve the sustainable design problem escalates significantly when the number of objectives increases, with problems of more than three objectives impractical to solve and interpret using rigorous solution methods such as the weighted sum or epsilon constraint approaches. Additionally, when Pareto frontiers can be obtained in these high dimensional spaces, they are challenging if not impossible for relevant stakeholders to interpret. To address these issues, our previous work developed a method for systematically reducing the dimensionality of a many-objective optimization problem on the basis of their competing or correlating nature using a network theoretic approach [4]. We then extended this framework to process operations problems where the underlying economic or environmental parameters inherently varied in time (due to, for example, varying costs and emissions associated with grid-purchased electricity), demonstrating that the time-varying natures of these signals can alter the appropriate grouping of objectives when repeatedly solving the operation problem over time [5]. This work builds upon our previous efforts in the many-objective optimization space by analyzing how to group objectives which inherently contain a large degree of uncertainty. This phenomenon is most commonly seen when considering social objectives, which are typically ill-defined and difficult to quantify, and thus can be subject to large ranges of uncertainty.

In this work, we focus on an illustrative four objective design problem formulated as a linear program (LP). The objectives to minimize include net present costs, carbon emissions, safety risk and social inequity. We assume the presence of uncertain parameters in the two social objectives, risk and equity. The design problem is straightforward and illustrative in nature, with all four objectives being linear combinations of design variables.

The dimensionality reduction approach is systematically applied in all different scenarios generated from uncertain parameters. We want to find out the most robust grouping of objectives among the scenarios identifying the grouping of objectives with the highest expected modularity over all scenarios. To achieve this, a novel approach is developed which treats the community detection of an uncertain graph as a stochastic optimization problem and employs a column generation approach to decompose the problem into several interconnected deterministic community detection problems with modified modularity objectives. The remainder of this paper is structured as follows: in the next section, we describe the many-objective optimal design problem considered in this work. Then, a novel approach for stochastic community detection of uncertain graphs is described. Next, we present results of solving applying our dimensionality reduction approach and solving the many-objective optimization design problem. Finally, concluding remarks and avenues for future work are presented.

PROBLEM FORMULATION

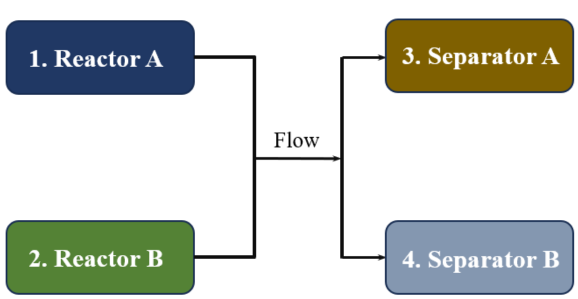

Figure 1. Two reactor, two separator superstructure considered in this work.

System description

In this study, we demonstrate a straightforward design problem with two reaction and two separators as shown in Fig. 1, which depicts the superstructure of the reactor/separator system. The chemical reaction design model considered has two reactants and one product, necessitating separation in the designated separators as part of the design problem. Flow with both reactants allows for reactions in either Reactor A, Reactor B or both. Additionally, there are two choices for separators, and all flow resulting from the chemical reaction is directed towards these separators. Each reactor and separator is characterized by a unique conversion for both the reaction and separation processes.

Moreover, specific carbon emission and operating cost parameters are assigned to each unit in the system. There are uncertain parameters in the system that are associated with safety risk and social equity objectives; in this problem, we assume that there are two possible realizations of this objective parameter for each unit considered.

Objective functions

The first objective that we consider is to minimize the annualized net present cost N that combines the capital cost and operating cost of the design system:

$$N = \sum_{i=1}^{4} cap_i * \frac{1}{\theta} + op_i \tag{1}$$

$$cap_i = c_i^{ref} (\frac{F_i}{F_i^{ref}})^{\gamma} \tag{2}$$

$$op_i = \alpha_i F_i \tag{3}$$

where θ is the NPC-scaled lifetime used to annualize the capital cost and F is the flow through the reactors or separators, which acts as a proxy for unit size. The capital cost as we can see in equation (2) is a nonlinear function,where c_i^{ref} and F_i^{ref} are the sizes and capital costs, respectively, of the reference for unit i, and γ is the scaling exponent. Unit subscripts i correspond to the four units shown in Fig. 1. In order to formulate the problem as an LP such that our objective reduction framework can be applied, we choose γ as 1; extension of our dimensionality reduction framework to nonlinear problems will be the scope of future work. The operating cost is given in equation (3) and it is proportional to the flow through each unit, where α_i are cost parameters and F_i are flow in each units.

Besides the traditional economic factors, we consider minimization of carbon emissions H, related to the usage of all the facilities in the system, where β_i represent emission parameter of different units:

$$H = \sum_{i=1}^{4} \beta_i F_i \tag{4}$$

The emission objective has similar structure with operating cost: it is linear combination of the flow through the different units. Moreover, two social objectives, risk and inequity, are analyzed in the optimization:

$$R = \sum_i \delta_{ri} F_i \quad (5)$$

$$E = \sum_i \delta_{ei} F_i \quad (6)$$

In this work, the coefficients for the two social objectives, δ_{ri} and δ_{ei}, are uncertain parameters. Note that for this illustrative example, the emissions, risk, and inequity objectives are a linear combination of all design variables, which for this problem are simply the flows. Thus, while it's uncommon to find that social objectives are determined by the same variables as cost and emission objectives in practical applications, the approach shown here is generalizable for linear objectives as variables which do not impact a given objective can have the corresponding coefficient set to zero. The extension of this approach to more realistic nonlinear problems is still ongoing work which is beyond the scope of this paper.

Model Constraints

The chemical design system should follow physical and practical limitations. First, we set a total amount of initial feed in the system (F_t) that equals to the sum of the flow in the reactors (F_1, F_2):

$$F_1 + F_2 = F_t \quad (7)$$

$$F_t \geq F_i \geq 0$$

Since an A+B->C reaction is assumed, total amount of flow (on a molar basis) will reduce after the reaction based on different conversions (E_1, E_2) of the reactors:

$$\left(1 - \frac{E_1}{2}\right) F_1 + \left(1 - \frac{E_2}{2}\right) F_2 = F_3 + F_4 \quad (8)$$

We assume that the separators can distinguish the specific product that we want but can't totally remove the product from the flow. Thus, here we use the flow from the reactors to the respective separators (F_3, F_4) and parameters for efficiency of the separators (E_3, E_4), which are all based on the mixture of reactants and products.

$$E_3 F_3 + E_4 F_4 \geq F_{min} \quad (9)$$

Equation (9) indicates that a minimum requirement of the product (F_{min}) needs to be satisfied in the reaction system.

Case study data

As this problem acts to serve as an illustrative example, problem parameters are chosen by the researchers and not necessarily meant to be representative of a real process. We aim to apply our method to analyze objective tradeoffs for different practical process designs from the literature as future work.

The conversions of the two reactors are 80% and 95% which means that 80% or 95% of the reactants are transformed into product. The two separators can obtain 25% and 40% of the product from the flow relatively. The total feed flow into the reactors is constrained as 100mol/h and the total flow goes into the separators is calculated from the conversions of the reactors.

For annualized net present cost, cost references of 2000, 5000, 700, 1200 dollars are set for the capital cost of the facilities. Operating cost and carbon emission parameters of all the facilities are set as 2, 0.9, 0.2, 0.15 dollar per mol/h and 80, 50, 80, 35 kg CO_2 per mol/h relatively.

Table 1: uncertain parameters in Risk and Equity objectives.

Facility	Risk parameter	Equity parameter
1	100 or 80	800 or 40
2	50 or 30	500 or 30
3	20 or 15	50 or 70
4	10 or 5	300 or 20

Risk and equity objectives are linear combination of the flow in each facility with uncertain parameters. Possible values of the parameters are shown in the Table 1. As social objectives such as equity can be difficult to quantify, we consider that these values can differ by a large amount. Each facility has two possible values of both risk and equity parameters, all 256 scenarios from their combinations are considered in the optimization. Despite having only two uncertain parameters, we note that the wide range of uncertainty and large number potential scenarios resulting from their combination showcases the ability of our proposed approach to deal with highly undertain objectives. We also note that our proposed approach also allows for the quantification of uncertain parameters with a larger number of values.

STOCHASTIC OBJECTIVE REDUCTION ALGORITHM

In this section, a process for systematically reducing the dimensionality of a MILP with many uncertain objectives into a problem with three or fewer objective functions is presented. The core of the algorithm, which considers deterministic objectives, was originally developed in our group's previous work and is summarized as follows [4]. First, cost vectors (the gradient vector of the objective function) are projected onto the constraint surfaces. Strength of interaction is defined as the inner product of the projected vectors and a weighted sum of the constraint interaction strengths is used to determine the total objective correlation strength. Objective correlation strength is scaled to be between 0 and 1. This information is embedded into an objective correlation graph, which consists of nodes corresponding to the different objectives and edges weighted by the objective correlation strength. Community detection is applied to identify groups of objectives that are strongly correlated within the group and competing with objectives in other groups. For more details about the objective reduction algorithm, please reference our previous works [4,5].

For problems with uncertain objective functions, this uncertainty will manifest itself as uncertainty in the edge weights of the objective correlation graph. For each realization of uncertainty, a different objective correlation graph can be obtained. Since the true realization of uncertainty is not known *a priori*, it is essential to identify a grouping of objectives that performs robustly well for all realizations of uncertainty to be able to obtain a full understanding of the tradeoffs between the many objectives.

Stochastic community detection

The community structure within a network manifests as a statistically significant configuration of edges which can be evaluated through the value of the modularity. [6] The modularity is described by the number of edges falling within groups minus the expected number in an equivalent network with edges placed at random, as depicted in formulation (10):

$$\max_z \ \sum_{i\epsilon I,\, i'\epsilon I} \left(\frac{A_{ii'}}{m} - \frac{a_i a_{i'}}{m^2}\right) z_{ii'} \tag{10a}$$

$$\text{s.t.} \quad z_{ii} = 1 \ \forall\, i \ \in I \tag{10b}$$

$$z_{ii'} + z_{ii''} - z_{i'i''} \ \leq \ 1 \ \forall\, i \ \in I, i' \in I\backslash\{i\}, i'' \in I\backslash\{i, i'\} \tag{10c}$$

$$z_{ii'} \in \{0,1\} \ \ \forall\, i \ \in I, i' \in I \tag{10d}$$

where I is the set of nodes in the graph, A is the graph adjacency matrix, $a_i = \sum_{i'\epsilon I} A_{ii'}$ is the degree of node i, $m = \sum_{i\epsilon I} a_i$ is twice of the total number of edges in the network, and $z_{ii'}$ is a binary partitioning variable that is one if nodes i and i' are assigned to the same community, and zero otherwise. The community detection is accomplished by maximizing modularity.

To apply this approach to uncertain graphs, such as those obtained from our objective reduction approach with uncertain objectives, the traditional community detection problem must be recast as a stochastic optimization problem. In this case, a reasonable goal is to pursue the most robust partition that has consistently high modularity across all realizations of uncertainty. Here, we use expected value of modularity to evaluate partitions:

$$\max_z \quad E_\Sigma\left[\sum_{i\epsilon I,\, i'\epsilon I} \left(\frac{A_{ii'}}{m} - \frac{a_i a_{i'}}{m^2}\right) z_{ii'}\right] \tag{11}$$

$$\text{s.t.} \quad (10b-d)$$

Note that other stochastic metrics, such as conditional value at risk, may also be used in place of expected value; we will assess how this proposed approach extends to other metrics in future work. To simply the equation, we assume all scenarios are equally likely and replace the expectation operator with an average over all scenarios:

$$\max_z \quad \frac{1}{|K|}\sum_{k\epsilon K} \sum_{i\epsilon I,\, i'\epsilon I} \left(\frac{A_{ii'k}}{m_k} - \frac{a_{ik} a_{i'k}}{m_k^2}\right) z_{ii'} \tag{12}$$

$$\text{s.t.} \quad (10b-d)$$

Set K indicates all the scenarios from the uncertain parameters. Unfortunately, fast algorithms for community detection such as spectral partitioning [7], fast unfolding [8], or the Leiden algorithm [9] are not directly applicable to the problem. However, this problem can be decomposed into a set of single-scenario community detection problems with a slightly modified objective. First, copy variables corresponding to each scenario are introduced to generate exploitable structure:

$$\max_z \quad \frac{1}{|K|}\sum_{k\epsilon K} \sum_{i\epsilon I,\, i'\epsilon I} \left(\frac{A_{ii'k}}{m_k} - \frac{a_{ik} a_{i'k}}{m_k^2}\right) z_{ii'k} \tag{13}$$

$$\text{s.t.} \quad z_{iik} = 1 \ \forall\, i \ \in I, k \ \in K$$

$$z_{ii'k} + z_{ii''k} - z_{i'i''k} \ \leq \ 1 \ \forall\, i \ \in I, i' \in I\backslash\{i\},$$

$$i'' \in I\backslash\{i, i'\}, k \ \in K$$

$$z_{ii'k} \in \{0,1\} \ \ \forall\, i \ \in I, i' \in I, k \ \in K$$

$$z_{ii'k} = z_{ii'k'} \ \ \forall\, i \ \in I, i' \in I, k \ \in K, k' \in K$$

In this problem, the non-anticipativity constraints $z_{ii'k} = z_{ii'k'}$ are complicating, such that if they were removed, the stochastic problem could be treated as $|K|$ independent community detection problems. Using column generation [10] can help to solve formulation (13). It can be transformed into the following master problem:

$$\max_{z,\lambda} \quad \frac{1}{|K|}\sum_{k\epsilon K} \sum_{c\epsilon C} \lambda_{ck} f_{ck}^* \tag{14}$$

$$\text{s.t.} \quad \sum_{c\epsilon C} \lambda_{ck} z_{ii'ck}^* = z_{ii'} \ \ \forall\, i \ \in I, i' \in I, k \ \in K \ \ (\pi)$$

$$\sum_{c\epsilon C} \lambda_{ck} = 1 \ \forall\, k \ \in K \ \ (\mu)$$

$$\lambda_{ck} \ \in \{0,1\} \ \forall\, k \ \in K, c \ \in C$$

where C is the set of columns generated which correspond to a specific partitioning of the graph into communities, f_{ck}^* is the modularity of column c in scenario k, $z_{ii'ck}^*$ is the partitioning variable in the corresponding modularity. π and μ are the dual variables corresponding to the constraints in the same line, which are used to generate new columns (potential partitions) via the following set of $|K|$ subproblems, one per scenario k:

$$\max_z \sum_{i\epsilon I,\, i'\epsilon I} \left(\frac{A_{ii'k}}{m_k} - \frac{a_{ik} a_{i'k}}{m_k^2} - \pi_{ii'k}\right) z_{ii'k} + \mu_k \tag{15}$$

$$z_{iik} = 1 \ \forall\, i \ \in I, k \ \in K$$

$$z_{ii'k} + z_{ii''k} - z_{i'i''k} \ \leq \ 1 \ \forall\, i \ \in I, i' \in I\backslash\{i\},$$

$$i'' \in I\backslash\{i, i'\}, k \ \in K$$

$z_{ii'k} \in \{0,1\} \; \forall \, i \in I, i' \in I, k \in K$

Formulation (15) is the modularity in scenario k with two Lagrangian terms resulting from the column generation decomposition. Since both are constants obtained from the dual solution of the master problem, only the πz term needs to be considered when implementing the objective change into a community detection algorithm. Doing so is straightforward: using Newman's spectral partitioning algorithm [7], which makes use of the eigenvalues and eigenvectors of the modularity matrix M, we modify the modularity matrix by subtracting the symmetric part of the π matrix:

$$\widehat{M}_{ii'} = \frac{A_{ii'k}}{m_k} - \frac{a_{ik}a_{i'k}}{m_k^2} - \frac{\pi_{ii'k}+\pi_{i'ik}}{2} \tag{16}$$

The eigenvalues and eigenvectors of the new matrix $\widehat{M}$ are then used to partition the graph in the same way as before. Alternatively, when using the fast unfolding (Louvain) [8] and Leiden [9] algorithms, we take grouping steps which give the largest increase in the modularity augmented with the Lagrangian πz terms, rather than just the modularity. As in any column generation approach, the algorithm proceeds by iteratively solving the master problem and subproblems until no subproblem returns a partition with positive objective value, indicating that no partition not already in the set of columns has the potential to improve the objective value.

RESULTS AND DISCUSSION

To study the stochastic design problem, objective correlation graphs are generated for all 256 possible scenarios of the social objective parameters. We then compare the results of community detection applied to each individual graph and show the resulting grouping frequencies are in Table 2. Notably, [[N, H], [R, E]] and [[N, E], [H, R]] emerge as the most common partitions, where the symbols N, E, H, and R refer to the four different objectives as introduced in the problem formulation section and defined again in Table 2. However, we observe that four different "best" objective groupings occur depending on which scenario is actually realized, and it is unclear which performs best, on average, over all possible scenarios with this approach. It's essential to highlight that there aren't any uncertain values in the annualized net present cost and emission objectives in our system, signifying a constant correlation strength between them. The established correlation strength, determined through our previous algorithm, is 0.813, a relatively but not overwhelmingly high value which explains the prevalence of 111 instances where annualized net present cost and emission fall within the same group.

In contrast, the introduction of uncertain parameters in risk and equity objectives brings variability to the correlation strengths between different objectives. For instance, with risk parameters set at [100, 50, 20, 10] and equity parameters at [800, 500, 70, 20], the correlation strength between risk and equity is notably high at 0.991, resulting in the grouping [[N, H], [R, E]]. Conversely, when using [80, 30, 20, 10] and [40, 500, 50, 20] as risk and equity parameters, the correlation strength significantly decreases to 0.094, leading to the grouping [[N, E], [H, R]]. Thus, the frequencies that risk and equity are in the same group or not depends on the realization of uncertain parameter set of the two objectives. In this case, these two objectives are in the same group over half of the scenarios.

Table 2: Community detection results of the uncertain system. N: annualized net present cost, H: carbon emissions, R: risk, E: Equity.

Grouping	Frequency
[[N, H], [R, E]]	94
[[N, E], [H, R]]	95
[[N], [H, R, E]]	50
[[R], [N, H, E]]	17

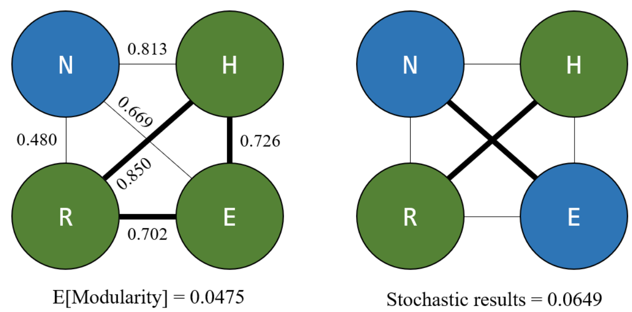

Figure 2. Grouping and expectation results of the average graph (left) and the most robust grouping (right)

Despite this variability, to address the tradeoffs within the uncertain design problem effectively, it is rational to identify the most robust partition across all scenarios as defined by the expected modularity over all scenarios. The results, as depicted in Fig. 2 through the application of the stochastic algorithm, reveal that the optimal grouping is, [[N, E], [H, R]]. It is important to note that this grouping differs from what one would find by just averaging the edge weights from the objective correlation graphs generated from all 256 scenarios, [[N], [H, R, E]]. The expectation of the modularity in the optimal solution is 0.0649, and the expectation of the second-best partition, [[N, H], [R, E]] is 0.0615. Both are higher than the partition of the average graph, which gives an expected modularity of 0.0475, suggesting that a

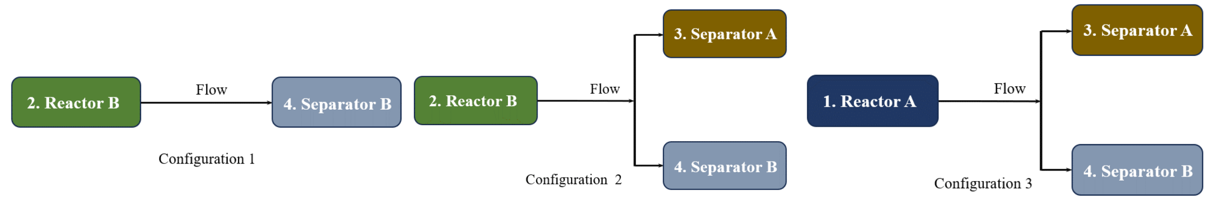

Figure 3: Illustration of different design configurations

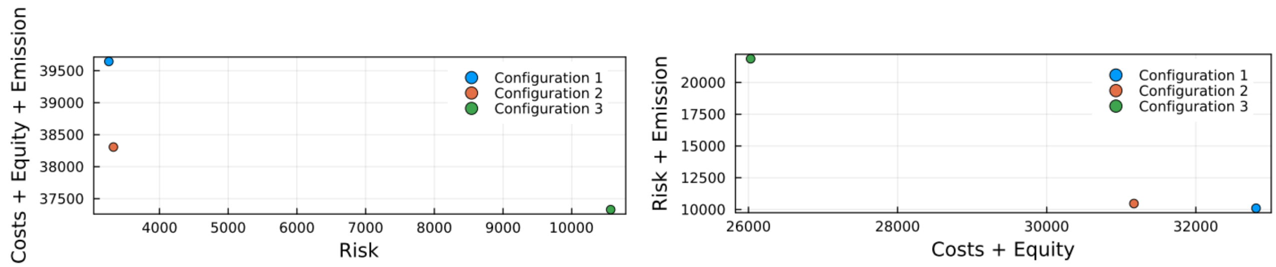

Figure 4: Weighted sum Pareto frontier between (left) risk and cost + equity + emission as well as (right) risk+ emission and cost + equity in the scenario of [[R], [H, N, E]] grouping.

deterministic approach of averaging edge weights is not an effective mechanism for identifying objective groupings that preserve tradeoff information in as many scenarios as possible.

For further study of the system, we compare the weighted sum Pareto frontiers for one scenario using both robust grouping found by community detection and the grouping that is "best" for the specific scenario considered, [R], [H, N, E]]. Fig. 3 illustrates all optimal design configurations occurring along the Pareto frontier. Pareto frontiers are depicted on the left side of Fig. 4 for the scenario which uses risk and equity parameters set at [100, 30, 15, 5] and [40, 30, 70, 300]. Points sharing the same color on the Pareto frontier represent the same optimal design configuration within the Pareto frontier. In configuration 1, the emphasis is on risk reduction, leading to the utilization of Reactor B and Separator B, both possessing the lowest risk parameters. Conversely, Configuration 3 aims to minimize the sum of costs, equity, and emissions. Only Reactor A is constructed due to its lower cost, emissions, and equity parameters. Separator A and B are both utilized with specific flow values to optimize the three objectives.

In the middle of the Pareto frontier, the tradeoff point results from balancing the sum of costs, equity, and emissions against risk. In this case, only Reactor B is employed compared to Configuration 3, and the flow values in the separators are also different. The Pareto frontier for the optimal result's grouping, [[N, E], [H, R]], is displayed on the right side of Fig. 4. The trade-off point using the [[R], [H, N, E]] grouping also appears in the Pareto frontier of [[N, E], [H, R]], suggesting that employing the most robust grouping can provide valuable insights in a certain extent, and demonstrating that tradeoff information can be preserved in the robust grouping even when it is not the same as the "best" grouping for a particular scenario.

However, in numerous other scenarios, the Pareto frontier of [[N, E], [H, R]] does lose a bit of information about design tradeoffs in comparison to the individual scenario's best grouping. This is not unexpected, as choosing a grouping of objectives with suboptimal modularity for a particular scenario inherently means that objectives with some degree of competition are being grouped together, which will result in loss of information regarding tradeoffs between the grouped objectives. The [[N, E], [H, R]] grouping with 95 times and other scenarios with no information loss in [[N, E], [H, R]] reveal that opting for the most robust grouping is a practical choice when attempting to understand tradeoffs in many-objective optimization problems with uncertain parameters.

CONCLUSIONS AND FUTURE WORK

Environmental and social considerations for sustainability are essential aspects of optimal design problems for modern chemical production infrastructure. However, they can be subject to a great deal of uncertainty making critical evaluation of tradeoffs between objectives challenging. In this work, we developed a method for systematically identifying groups of objectives that, on average, tend to be more correlating than competing, forming the basis of a dimensionality reduction in many-objective optimization problems that is robust to uncertainty. Through the use of an illustrative case study with a two reactors, two separators superstructure, the efficacy of our approach towards identifying an objective grouping with low loss of tradeoff information was demonstrated.

As future work, we aim to apply this framework to a set of more practically relevant design problems from the literature such as a hydrogen production process and green ammonia production system, in order to better understand the tradeoffs inherent in designing future chemical production infrastructure. This analysis will entail further development of our objective reduction algorithm, such that it can be applied to nonlinear, as well as linear, many-objective optimization problems.

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