Robustness Analysis for Adaptive Optimization

With Application to Industrial Decarbonization in the Netherlands

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Abstract

Robustness analysis assesses the performance of a particular solution under variation in the input data. This is distinct from sensitivity analysis, which assesses how variation in the input data changes a model's optimal solution. For risk assessment purposes, robustness analysis has more practical value than sensitivity analysis. This is because sensitivity analysis, when applied to optimization models, assumes that the solution is able to adapt to changes in the input data with perfect foresight, which may lead to an overly optimistic assessment. On the other hand, classical robustness analysis, which is intended for static optimization problems, assumes that the solution is entirely fixed and unable to adapt to changes in the input data, which may lead to an overly pessimistic assessment. In this paper we extend robustness analysis to deal with adaptive optimization problems in a more realistic manner. Furthermore, we propose an intuitive and computationally tractable method for applying robustness analysis to adaptive optimization problems and apply this method to the optimization of decarbonization pathways for heavy industry in the Netherlands. Here we find significant differences between the results obtained via (i) sensitivity analysis, (ii) classical robustness analysis (for static optimization) and (iii) robustness analysis for adaptive optimization. Our results demonstrate the importance of the methodology when analyzing the impact of uncertainty.

Keywords: Optimization; Uncertainty; Robustness Analysis; Decarbonization

1 Introduction

Mathematical optimization models have proven to be valuable for prescriptive analytics in, e.g., logistics, healthcare, finance and engineering. Due to advances in solution algorithms, computing power and availability of data, such models have become capable of tackling increasingly large and complex real-world problems. Yet, when modeling such problems, input data is required in the form of the model's "parameters" and this information is not always known with certainty. Parameter uncertainty can arise from various sources and ignoring this uncertainty may lead to faulty, or even disastrous, decisions to be made [1, pp. 2-5]. In response, many techniques have been proposed to deal with uncertainty. One highly popular technique is sensitivity analysis (SA), which the canonical textbook of Hillier and Lieberman refers to as "the most important of these techniques" [2, p. 225].

SA, in the context of optimization, analyzes how changes in the parameters of a model affect its *optimal* solution [3]. See Appendix A for a more elaborate description. The concept of SA is widely known and its usage is prescribed in national and international guidelines on uncertainty assessment, as seen in publications by the U.S. Environmental Protection Agency [4] and the European Commission [5]. As such, SA is considered by many to be an essential element of due diligence when faced with uncertainty.

Another technique for dealing with uncertainty is robustness analysis (RA). RA analyzes how changes in the parameters of a model affect the *performance* of a *particular* solution [6], where "performance" should be interpreted as an estimate of how well a solution would function if implemented in practice. The key difference with SA being that, in RA, the solution under analysis is (partially) fixed while the parameter values of the model are varied, whereas SA implicitly assumes that the solution is flexible and able to adapt to changes in the parameter values with perfect foresight. As such, when SA is used as a tool for risk assessment, the assessment tends to be overly optimistic. In most situations, RA more closely mirrors real-world conditions, where the uncertain parameters are unrealized at the moment that irreversible decisions must be made.

The methodology for performing RA in a static optimization setting, which refers to the setting where all decisions must be made "here-and-now" without any knowledge of the uncertain parameters, is well established [7]. This has been applied in many scientific articles within the field of robust optimization, see for example [8–10]. A notable example is the seminal work by Ben-Tal and Nemirovski [11], where they assess the feasibility of the "nominal solutions" (i.e. solutions that are optimal with respect to specific "nominal" parameter values) to problems from the `NETLIB` collection.

However, real-world problems often involve long time horizons with multiple time periods, where decisions are made sequentially over time as more information becomes known. Such problems are commonly referred to as "adaptive" optimization problems. A concrete example of an adaptive optimization problem is inventory planning, where one must determine inventory levels before customer demand is realized and can afterwards adjust replenishment decisions dynamically as more information becomes available. In this paper we consider problems of this nature, where time is discretized into a finite number of "decision stages". A visual sketch of a problem with K decision stages is presented in Figure 1. In the first stage, the decisions $\mathbf{x}_1$ are made without any realizations of the uncertain parameter vectors $\mathbf{z}_1, \dots, \mathbf{z}_K$. However, for the later stages $k = 2, \dots, K$, the decisions $\mathbf{x}_k$ are able to adapt to the set of realized parameter vectors $\mathbf{z}_1, \dots, \mathbf{z}_{k-1}$. Existing RA methodology assumes a static optimization setting, thus, when this is applied to adaptive optimization problems, the results are likely to be overly pessimistic.

In this paper, we extend RA to deal with adaptive optimization problems, which enables a more realistic assessment than classical RA. We note that the framework presented in [12] allows the operational decisions to be adaptive, however, their analysis is restricted to a two-stage setting, where the second stage decisions are optimized with full information. Our methodology is applicable to a wider range of problems as it allows for settings with more than two decision stages and does not require full information.

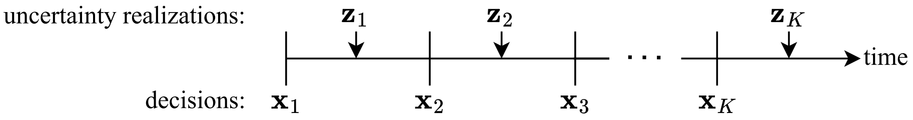


Figure 1: Visual aid for chronology of events in an adaptive optimization problem with K stages

As such, our extension of RA is a novel addition to the scientific literature.

Let $\mathcal{X}_k$ represent the feasible set for decision vector $\mathbf{x}_k$, for stages $k = 1, \ldots, K$. A generic mathematical formulation for K-stage adaptive optimization problems is as follows:

$$\max_{\mathbf{x}_1 \in \mathcal{X}_1} \max_{\mathbf{x}_2 \in \mathcal{X}_2(\mathbf{x}_1, \mathbf{z}_1)} \cdots \max_{\mathbf{x}_K \in \mathcal{X}_K(\mathbf{x}_1, \ldots, \mathbf{x}_{K-1}, \mathbf{z}_1, \ldots, \mathbf{z}_{K-1})} f(\mathbf{x}_1, \ldots, \mathbf{x}_K, \mathbf{z}_1, \ldots, \mathbf{z}_K). \tag{1}$$

At each adaptive decision stage $k \in \{2, \ldots, K\}$ the decision vector $\mathbf{x}_k$ is determined on the basis of previous decisions $\mathbf{x}_1, \ldots, \mathbf{x}_{k-1}$ and uncertainty realizations $\mathbf{z}_1, \ldots, \mathbf{z}_{k-1}$. Note that the problem as described above is not well defined as it does not specify how the unrealized uncertain parameters should be treated. In a stochastic optimization setting, the uncertain parameters are assumed to follow probability distributions and one typically optimizes the expectation of the objective function. In robust optimization, one optimizes for the worst-case over all possible realizations within deterministic “uncertainty sets”.

Solving adaptive optimization problems in a stochastic and/or robust manner can be computationally challenging [13]. We refer to [14] for a review on methods for solving multistage adaptive optimization problems. Given the challenging nature of these problems, a common approach is to simplify the problem by disregarding the uncertainty and solving for a particular sequence of realizations (i.e., a “scenario”). Let $\bar{\mathbf{z}}$ denote such a scenario, which is a vector constructed of K subvectors $\bar{\mathbf{z}}_1, \ldots, \bar{\mathbf{z}}_K$. This simplification reduces the problem complexity and allows one to solve a deterministic single-level optimization problem:

$$\begin{aligned} &\max_{\mathbf{x}} f(\mathbf{x}, \bar{\mathbf{z}}) \\ &\text{ s.t. } \mathbf{x} \in \mathcal{X}(\bar{\mathbf{z}}), \end{aligned} \tag{2}$$

where $\mathbf{x} = (\mathbf{x}_1, \ldots, \mathbf{x}_K)$ is a vector consisting of the decision variables across all stages. Here, $f(\mathbf{x}, \bar{\mathbf{z}})$ and $\mathcal{X}(\bar{\mathbf{z}})$ represent the objective function and feasible region under scenario $\bar{\mathbf{z}}$. Assuming that Problem (2) can be solved efficiently, this approach enables one to obtain a solution $\bar{\mathbf{x}}$ to a simplified version of the “true” adaptive optimization problem problem. In many cases such a simplification may be perfectly reasonable. In such cases, the effect of uncertainty may be limited and the solution $\bar{\mathbf{x}}$ may be sufficiently robust to deviations from $\bar{\mathbf{z}}$. However, we argue that one should verify whether this is the case and we suggest our methodology as the correct methodology for verification.

To apply RA in an adaptive optimization setting, one must specify an “adaptive decision policy”, which prescribes how the adaptive decisions should adapt to realizations of the uncertain parameters. Within the fields of robust and stochastic optimization, there exist solution methods that provide such a policy as part of their output, see [15] for a survey on the topic. For cases where such a policy is not readily available, we propose an intuitive and computationally tractable policy that involves re-solving Problem (2) in a folding horizon fashion, using predictions for the future based on realizations from the past.

We demonstrate our methodology by applying it to an illustrative toy problem[1] as well as a realistic case study on optimizing the decarbonization pathway for an energy-intensive industry cluster in the Netherlands. This case study was developed in collaboration with various companies and regional stakeholders as part of the HyChain 4 project, see [16, pp. 14-17] for more details. For this problem, we model decisions to be made over a long time horizon (2025 till 2050) and, because of this long term view,

[1] The source code is available at: `https://github.com/JustinStarreveld/robustness_analysis_adaptive_opt`

many of the model's parameters (e.g. the natural gas price and carbon emission tax) rely on forecasts that are highly uncertain. We use this case study to demonstrate the application of RA and find that the model's parameter settings can have a large effect on the outputs of interest, with significant differences between the results obtained via (i) SA, (ii) classical RA (for static optimization) and (iii) RA for adaptive optimization.

In summary, our unique contributions are as follows:

- we extend RA to multistage adaptive optimization problems, which enables a more realistic assessment for problems with two or more decision stages;
- we propose an intuitive and computationally tractable adaptive decision policy for RA in a multistage adaptive setting;
- we demonstrate our method via application to a realistic case study on optimizing decarbonization pathways for an industry cluster in the Netherlands.

The structure of this paper is as follows. In Section 2, we extend RA to an adaptive setting and highlight the difference between SA and RA using an illustrative toy problem. Then, in Section 3, we apply the methodology to a realistic case study. Finally, we provide concluding remarks in Section 4. The mathematical model formulation and additional details are relegated to the Appendix.

2 Robustness Analysis

This section extends RA to an adaptive optimization setting. To place this extension in context, we first describe the methodology of RA for a static optimization setting. After having described the extension, we highlight the difference using an illustrative toy problem.

In our notation we assume that there is a finite number of "outputs of interest" $Y_1, \ldots, Y_M$ in which one is interested. Furthermore, we assume that each output of interest $Y_j, j = 1 \ldots, M$ is a known function of the decision vector $\mathbf{x}$ and uncertain parameter vector $\mathbf{z}$. For example, if one is interested in the objective value and feasibility of a solution for Problem (2), one would define $Y_1(\mathbf{x}, \mathbf{z}) := f(\mathbf{x}, \mathbf{z})$ and $Y_2(\mathbf{x}, \mathbf{z}) := 1, \text{ if } \mathbf{x} \in \mathcal{X}(\mathbf{z})$, and $0, \text{ otherwise}$.

A common practice in stochastic optimization is to model the uncertain parameters $\mathbf{z}$ as random variables with probability distributions. In such cases, probabilistic conclusions can be derived from applying RA. However, we note that precise knowledge of the underlying probability distributions is rarely available in practice. Furthermore, estimating probability distributions is highly prone to errors (due to lack of historical data or deviations from historical trends). The approach we advocate (and utilize in the application in this paper) is to use a set of "plausible" scenarios without attaching probabilities to the scenarios. This can be seen as analogous to the idea of utilizing an "uncertainty set", as in robust optimization, which describes a set of scenarios for which we would like our solution to be robust. Such an approach implies that probabilistic conclusions cannot be derived from RA, however, one can still use RA to identify adverse scenarios that are considered to be plausible.

As such, throughout this paper we assume that the set of all possible realizations for the uncertain parameter vector $\mathbf{z}$ can be represented by a finite set of scenarios $\mathbf{z}^1, \ldots, \mathbf{z}^N$, where each scenario $\mathbf{z}^i$ is a vector constructed of K subvectors $\mathbf{z}_1^i, \ldots, \mathbf{z}_K^i$.

Static setting

When applying RA in a static optimization setting, it is assumed that all decisions are irrevocably fixed and unable to adapt to changes in the model's input. The situation is depicted in Figure 2, where the decision vector $\mathbf{x}$ is determined before the uncertain parameter vector $\mathbf{z}$ is realized.

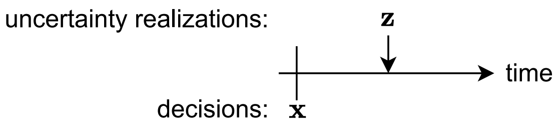


Figure 2: Visual aid for chronology of events in an uncertain static optimization problem

When dealing with problems of this nature, RA is rather straightforward. All one needs is a solution $\bar{\mathbf{x}}$ to analyze and a set of scenarios $\{\mathbf{z}^1, \ldots, \mathbf{z}^N\}$. See Algorithm 1 below for a procedural description.

Algorithm 1 Pseudo code for robustness analysis in a static setting

Input: Set of scenarios $\{\mathbf{z}^1, \ldots, \mathbf{z}^N\}$ and a solution $\bar{\mathbf{x}}$.
Output: Evaluation of performance of $\bar{\mathbf{x}}$ w.r.t. each scenario in $\{\mathbf{z}^1, \ldots, \mathbf{z}^N\}$.

```
for scenario $i \in \{1, \ldots, N\}$ do
    Evaluate outputs of interest $Y_j(\bar{\mathbf{x}}, \mathbf{z}^i), \quad \forall j = 1, \ldots, M$
end for
```

2.1 Adaptive setting

Here we consider a generic multistage adaptive problem with K decision stages as depicted in Figure 1. In an adaptive optimization setting, only the "first stage" decisions $\mathbf{x}_1$ are considered fixed, while the later stage decisions $\mathbf{x}_2, \ldots, \mathbf{x}_K$ are able to adapt to the realizations of the uncertain parameters. Thus, when determining the decision vector $\mathbf{x}_k$, the parameter vectors $\mathbf{z}_1, \ldots, \mathbf{z}_{k-1}$ have been realized and are no longer uncertain. A procedural description of RA for adaptive optimization is presented in Algorithm 2.

Algorithm 2 Pseudo code for robustness analysis for adaptive optimization

Input: Set of scenarios $\{\mathbf{z}^1, \ldots, \mathbf{z}^N\}$, first stage decisions $\bar{\mathbf{x}}_1$ and adaptive decision policy $\bar{\theta}$.
Output: Evaluation of performance of $(\bar{\mathbf{x}}_1, \bar{\theta})$ w.r.t. each scenario in $\{\mathbf{z}^1, \ldots, \mathbf{z}^N\}$.

```
Fix first stage decisions $\bar{\mathbf{x}}_1$
for scenario $i \in \{1, \ldots, N\}$ do
    for stage $k \in \{2, \ldots, K\}$ do
        Uncertain parameter vector $\mathbf{z}^i_{k-1}$ is realized
        Implement decision policy $\bar{\theta}$ to determine adaptive decision vector $\bar{\mathbf{x}}^i_k$
    end for
    $\bar{\mathbf{x}}^i \leftarrow (\bar{\mathbf{x}}_1, \bar{\mathbf{x}}^i_2, \ldots, \bar{\mathbf{x}}^i_K)$
    Evaluate outputs of interest $Y_j(\bar{\mathbf{x}}^i, \mathbf{z}^i), \quad \forall j = 1, \ldots, M$
end for
```

Note that in order to incorporate the ability for later stage decisions to adapt, the analysis requires additional input in the form of an adaptive decision policy $\bar{\theta}$. In certain cases, one may already have access to a policy via applying a multi-stage robust or stochastic optimization method. In case such a policy is not available, we propose an adaptive decision policy (see Algorithm 3), where, at each decision stage k, one determines $\mathbf{x}_k$ by solving an updated version of Problem (2). This is done in a folding horizon manner, where prior decisions $\mathbf{x}_1, \ldots, \mathbf{x}_{k-1}$ are fixed, realized parameter values $\mathbf{z}_1, \ldots, \mathbf{z}_{k-1}$ are known and future values $\mathbf{z}_k, \ldots, \mathbf{z}_K$ are predicted.

Algorithm 3 Pseudo code for folding horizon re-optimization with predictions

```
Input: Scenario $i$, decision stage $k$, known realizations $\mathbf{z}_1^i, \dots, \mathbf{z}_{k-1}^i$ and prior decisions $\bar{\mathbf{x}}_1, \bar{\mathbf{x}}_2^i, \dots, \bar{\mathbf{x}}_{k-1}^i$.
Output: Adaptive decision vector $\bar{\mathbf{x}}_k^i$.

Predict future realizations $\hat{\mathbf{z}}_k^i, \dots, \hat{\mathbf{z}}_K^i$ based on known realizations $\mathbf{z}_1^i, \dots, \mathbf{z}_{k-1}^i$
Determine adaptive decision vector $\bar{\mathbf{x}}_k^i$ by solving Problem (2) with $\bar{\mathbf{z}} = (\mathbf{z}_1^i, \dots, \mathbf{z}_{k-1}^i, \hat{\mathbf{z}}_k^i, \dots, \hat{\mathbf{z}}_K^i)$, $\mathbf{x}_1 = \bar{\mathbf{x}}_1$ and $\mathbf{x}_p = \bar{\mathbf{x}}_p^i$, for $p = 2, \dots, k-1$
return $\bar{\mathbf{x}}_k^i$
```

Our suggestion of Algorithm 3 to be used as $\bar{\theta}$ in Algorithm 2 is motivated by two reasons. First, assuming that Problem (2) can be solved efficiently and the number of decision stages K is not exceptionally large, the policy is computationally tractable, as it involves solving successively smaller versions of this problem $K-1$ times. (In Section 3.3 we show numerical experiments that provide evidence for the computational tractability of our policy.) Second, we believe that such a policy is commonly utilized in practice, where optimization models are frequently updated with new information and re-optimized. As such, using such a policy should provide realistic results when emulated in RA.

Determining predictions (Line 1 of Algorithm 3) can be done in a variety of ways. For example, in Section 2.2 we utilize knowledge of the true probability distribution and set the future predictions to their expected value, while in Section 3.3 we utilize predictive machine learning models that are trained on additional out-of-sample scenario data.

RA yields a set of values for each output of interest, reflecting the performance of a solution across multiple scenarios. These values can then be analyzed in several ways to evaluate the robustness of a solution. For example, a worst-case analysis can identify the most adverse scenario a solution may face, providing a conservative evaluation of robustness. Alternatively, cumulative distribution functions can estimate the probability of achieving a certain level of performance, providing a probabilistic evaluation. Additionally, performance profiles (see [17] for more details) can be useful when comparing multiple solutions. How to assess the robustness of a solution should depend on the problem at hand and the risk attitude of the stakeholders. In the application described in Section 3, we place emphasis on average regret, as this is a metric the stakeholders consider to be relevant for decision-making.

2.2 Illustrative toy problem

Consider the following problem. Product C can be sold at a fixed price per unit and is created by a process of conversion using either product A or product B as feedstock. However, investments must be made to enable the transportation and processing of each product. Products A and B are supplied at a particular cost per unit and the supply cost of product A is uncertain. The problem takes place over two time periods, the demand for product C is 100 units per time period and this demand must be satisfied. The goal is to determine which products (A and/or B) to use as feedstock, and therefore which investments to make, in order to maximize profit. We model the situation as a mixed-integer optimization problem, see Appendix B.1 for a mathematical formulation and Figure 3 for a visual aid.

For the parameters of the model, we assume the following. Each arc has an initial capacity of zero, but this can be increased by investment at a cost of 1 per 20 units of capacity. The processing nodes also start with an initial inflow capacity of zero, which can be increased by investment at a cost of 2 per 20 units of capacity. Product C can be sold at a price of 2 per unit. For the uncertain supply costs we assume that the unit cost of product B is known and fixed at 1.05, while the unit cost of product A is a uniformly distributed random variable. The cost per unit of A in time period 1, $c_{A,1}$, is uniformly distributed between 0.50 and 1.50. In time period 2, we assume that the supply cost is dependent on the

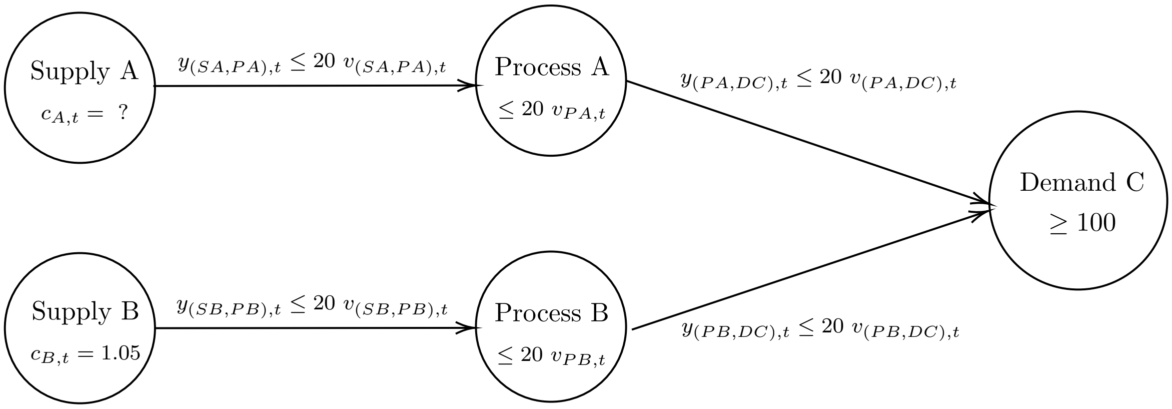

Supply A
$c_{A,t} = ?$
$y_{(SA,PA),t} \leq 20\ v_{(SA,PA),t}$
Process A
$\leq 20\ v_{PA,t}$
$y_{(PA,DC),t} \leq 20\ v_{(PA,DC),t}$
Demand C
≥ 100
Supply B
$c_{B,t} = 1.05$
$y_{(SB,PB),t} \leq 20\ v_{(SB,PB),t}$
Process B
$\leq 20\ v_{PB,t}$
$y_{(PB,DC),t} \leq 20\ v_{(PB,DC),t}$

Figure 3: Visualization of nodes and arcs used in illustrative toy problem

price in period 1, where $c_{A,2} \sim \mathcal{U}(\frac{1}{2}c_{A,1}, \frac{3}{2}c_{A,1})$. We set the nominal values of these two parameters equal to their expected values, thus: $\bar{\mathbf{z}} = (\bar{c}_{A,1}, \bar{c}_{A,2}) = (1.00, 1.00)$.

A "nominal solution" can then be obtained from solving the problem using the nominal parameter values $\bar{\mathbf{z}}$. This solution is depicted in Figure 4. As you might expect, our model advises us to solely utilize product A as feedstock in both time periods and only invest in the arc and processing capacities that are relevant to product A. Under the nominal parameter values, this is evidently the most profitable way to satisfy the demand of C, which achieves a total profit of:

$$\underbrace{2 \times 200}_{\text{revenue}} - \underbrace{(2 \times 5 \times 1 + 5 \times 2)}_{\text{investment costs}} - \underbrace{100 \times 1.00}_{\text{supply cost } t=1} - \underbrace{100 \times 1.00}_{\text{supply cost } t=2} = 180.$$

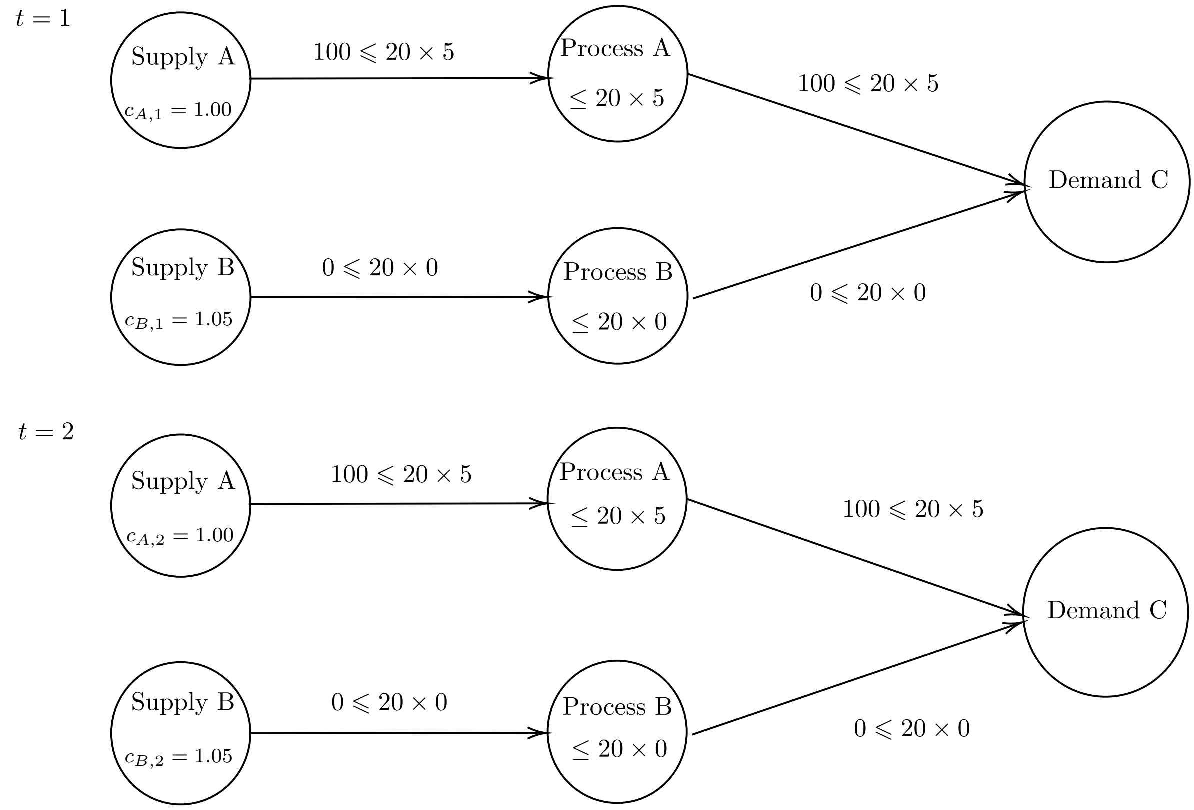
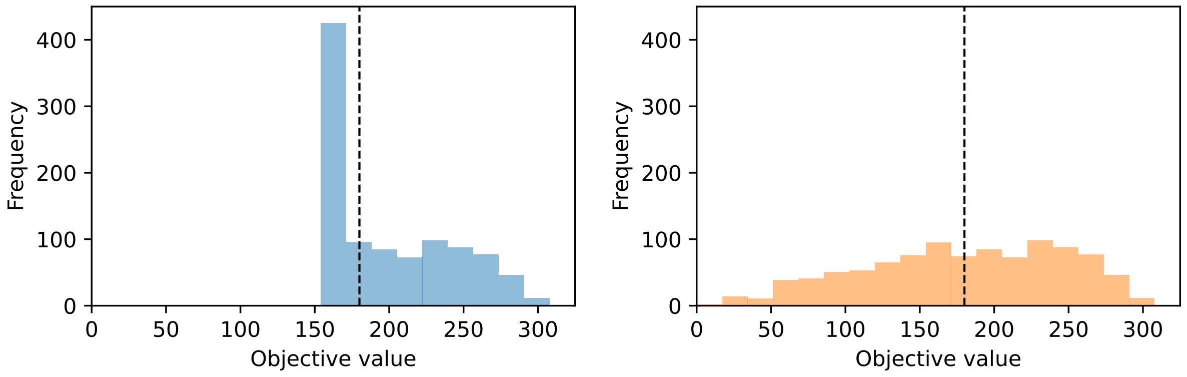


Figure 4: Depiction of nominal solution for illustrative toy problem

For this illustrative toy problem it is easy to see that the nominal solution is quite risky. Investing only in the arcs and processing capacity related to product A may not be wise given the uncertainty surrounding the supply cost of A. (An alternative solution, where one elects to solely utilize product B as feedstock and only invest in the arc and processing capacities that are relevant to product B, would achieve a certain profit of 170.) To determine the degree to which a solution is risky or robust, robustness analysis can be performed. In the following sections we apply SA and RA to this problem and show how the results differ.

For this illustrative toy problem there are no concerns regarding the feasibility of a solution, as the uncertain supply costs $c_{A,1}$ and $c_{A,2}$ do not affect any of the constraints of our problem. We assume that our only output of interest is the objective value, which is the total profit.

In this case, we can use our knowledge of the true distribution of $c_{A,1}$ and $c_{A,2}$ to generate a set of $N = 1{,}000$ randomly generated scenarios. In Figure 5a we show the results of SA and in Figure 5b we analyze the robustness of our nominal solution (see Figure 4) in a static setting.



(a) Sensitivity analysis

(b) Robustness analysis (static)

Figure 5: Comparison of results from applying SA and RA (for static optimization) to the setup described in Section 2.2. The dashed vertical line indicates the objective value for the nominal scenario.

Note that both analyses use the same set of possible scenarios $\{\mathbf{z}^1, \dots, \mathbf{z}^N\}$, yet yield starkly different results. Because SA assumes fully flexible decisions and perfect foresight, the analysis suggests that the total profit will never be less than 170. This is because, for adverse scenarios, the optimal solution changes to provide product C via the supply of product B, for which the unit cost is known and fixed.

On the other hand, RA (in a static setting) assumes that all decisions in our nominal solution are irrevocably fixed and that there is no ability to adapt to the scenario at hand. The results suggest that the total profit could range anywhere between 10 and 305. Depending on the situation, this may not be entirely realistic either and one should apply RA in an adaptive optimization setting.

Recall that we discretize our time horizon into two time periods $t \in \{1, 2\}$. During each time period t the (uncertain) cost $c_{A,t}$ for product A in period t is realized. At the start of each time period t, investment decisions $\mathbf{v}_t$ are made. The investment decisions made in the first period ($\mathbf{v}_1$) are considered static, however the investment decisions made in the second period ($\mathbf{v}_2$) are able to adapt to $c_{A,1}$. During each time period t, product flow decisions $\mathbf{y}_t$ are made. We assume that the flow variables for the first period $\mathbf{y}_1$ are adaptive with respect to $c_{A,1}$ and the flow variables for the second time period $\mathbf{y}_2$ are able to adapt to both $c_{A,1}$ and $c_{A,2}$.

Thus, we have a 3-stage problem (see Figure 6 for visual aid), with uncertain parameters $\mathbf{z}_1 = c_{A,1}$, $\mathbf{z}_2 = c_{A,2}$ and $\mathbf{z}_3 = \emptyset$, here-and-now decisions $\mathbf{x}_1 = \mathbf{v}_1$, second stage decisions $\mathbf{x}_2 = (\mathbf{y}_1, \mathbf{v}_2)$ and third stage decisions $\mathbf{x}_3 = \mathbf{y}_2$.

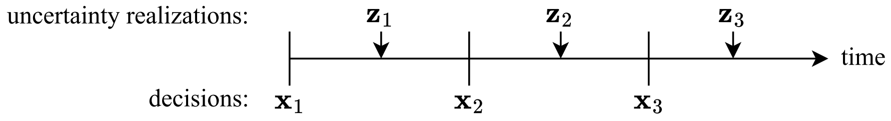
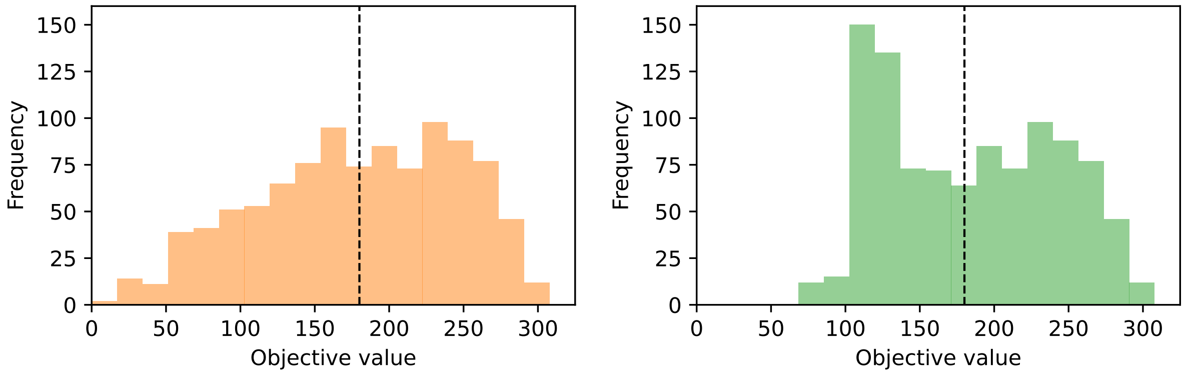


Figure 6: Visual aid for chronology of events for a 3-stage adaptive optimization problem

We can analyze the robustness of the first stage decisions of the nominal solution (as shown in Figure 4) and utilize Algorithm 3 as our adaptive decision policy, where our prediction of a future realization is set to its expected value (i.e., we set $\hat{c}^i_{A,2} = \mathbb{E}[c^i_{A,2}|c^i_{A,1}] = c^i_{A,1}$ for any scenario i). We then apply RA for adaptive optimization (Algorithm 2) and plot the results in Figure 7b. We compare this with the results from applying RA in a static setting (these results are the same as shown in Figure 5b, but with a different scale of the y-axis). The right-side of the distribution is similar for both analyses, these correspond with scenarios where the supply cost of A turns out lower than expected and the adaptive decisions $\mathbf{x}_2$ and $\mathbf{x}_3$ do not deviate from their values in the nominal solution. However, the left-side of the distribution differs as we have introduced the possibility to adapt some of our decisions, which occurs when the supply cost of product A is higher than expected.



(a) Robustness analysis (static)

(b) Robustness analysis (3-stage adaptive)

Figure 7: Comparison of results from applying RA (for static optimization) and RA (for adaptive optimization) to the setup described in Section 2.2. The dashed vertical line indicates the objective value for the nominal scenario.

3 Application

In this section we apply our methodology to a realistic case study. In this case study we focus on optimizing the decarbonization strategy for an energy-intensive industry cluster in the Netherlands. We refer to [16, pp. 14-17] for more details regarding the model. Three industrial sites are modeled in detail, on process unit level. These sites produce fertilizer, oil-products and various other chemical products. For the purpose of anonymity we only display aggregate data for the cluster as a whole.

The industry cluster requires large amounts of energy, which is currently primarily provided through carbon-emitting fossil-fuels. (For reference, approximately 9.5 Mton of CO_2 was emitted in 2020.) In accordance with the Dutch government's climate goals [18], the carbon emissions from this industry cluster must be reduced by 55% (relative to 1990 emission levels) by 2030 and entirely eliminated by 2050. These goals are included in the model as hard constraints on the annual aggregate amount of CO_2 emitted, where the required reduction is linearized over time. There is additional pressure to reduce carbon emissions in the form of a carbon emission tax. This is included in the model's objective function as a cost parameter and is expected to increase over time. As the future values for the emission tax are quite uncertain, we consider this input parameter in more detail in Section 3.2.

For the industrial sites, there are three primary options for reducing their carbon emissions, which are: (i) hydrogen usage, (ii) electrification and (iii) carbon capture and storage (CCS). Additionally, the model accounts for the surrounding infrastructure in the region. Via investment, the electricity grid can be expanded, new hydrogen pipelines can be built and existing natural gas pipelines can be retrofitted to transport hydrogen. The model is used to support long-term strategic decisions in regards to the decarbonization pathway for each industrial site, as well as the relevant infrastructure for the region.

3.1 Nominal model description and solution

A mathematical formulation of the optimization model is provided in Appendix B.2. The model determines when and which investments ought to be made to maximize the total (discounted) sum of margins for the industry cluster over the time horizon. To represent the relevant aspects of the problem, the model utilizes 31 time periods (representing $2020, 2021, \ldots, 2050$), 352 nodes, 825 arcs and 76 different "products" (which includes main energy carriers such as natural gas, electricity and hydrogen, but also includes subsidiary by-products). Note that the first 4 time periods ($2020 - 2023$) are included for backward compatibility of the model, but these time periods do not contain decision variables to be optimized. The resulting mixed-integer optimization model consists of 205,029 variables, 142,644 constraints and 753,151 parameters.

Of the 753,151 parameters we consider 6,231 to be uncertain, these are discussed in more detail in Section 3.2. However, we first assume some nominal/estimated values for these parameters and treat them as known in order to construct the nominal model, which is solved to obtain the nominal solution. For all parameters, the nominal values were determined in collaboration with industry partners as well as TNO (an independent statutory research organization in the Netherlands), see [16] for more details. The investment decisions of the nominal solution are summarized in Table 1.

Table 1: Overview of aggregate capital expenditure (in millions of EUR) for decarbonization pathway of the nominal solution. Note that, in the model formulation, these costs are annualized (i.e. converted to yearly payments) over the lifetime of the investments.

	2025	2026	2027	2028	2029	2030	···	2035	2036	2037	2038	2039	2040	2041	2042	2043	···	2049	2050
Hydrogen	1800							307			242			360		360			2817
Electrification	70		30			50													
CCS														304				31	25
Infrastructure	42					1		17	3				27						7

3.2 Uncertainty characterization

In characterizing and quantifying the uncertainty present in the input parameters of our optimization model, we follow the five criteria framework by [19]. Our quantification of uncertainty does deviate from the approach taken in [19], as we aim to generate scenarios instead of determining relative ranges.

For the analyses presented in Section 3.3 we utilize a set of 1,000 generated scenarios. Note that, we do not assign probabilities to the scenarios, the goal of our analysis is to provide insight into possible outcomes. Given that the uncertain parameters are continuous, the number of possible scenarios is infinite. Our choice of utilizing 1,000 scenarios is induced by our computational budget.

In our characterization we prioritize the use of historic data and external data sources in an effort to keep our characterization as objective as possible. However, due to lack of data, this is not possible for all parameters (such as the hydrogen price) and in such cases we are forced to make certain assumptions based on consultation with domain experts. When in doubt, we haven taken a conservative approach, preferring to overestimate rather than underestimate the magnitude of uncertainty. An overview of our characterization is presented in Table 2 below. In the following paragraphs we go over each of the uncertain parameters and discuss the characterization in more detail.

Table 2: Overview of uncertainty characterization

Uncertain Parameter	Characterization
Natural gas price	Historic EIA forecast data
Electricity price	Historic EIA forecast data
Hydrogen price	Expert opinion
Ammonia price	Expert opinion
CO_2 emission tax	Historic EU ETS data
CO_2 CCS tariff	Correlated with CO_2 emission tax
CapEx electrolyzers	Ranges from literature
Discount rate	Relative range from literature
Weighted average cost of capital	Relative range from literature
Annual OpEx as percentage of CapEx	Relative range from literature

Natural gas and electricity prices

To predict future forecast errors, we can use historic forecast error data. For this we use a data set provided by the annual energy outlooks (ranging from 1994 to 2022) of the U.S. Energy Information Administration [20]. This data is available for both the natural gas price and electricity price, the natural gas data is displayed in Figure 8.

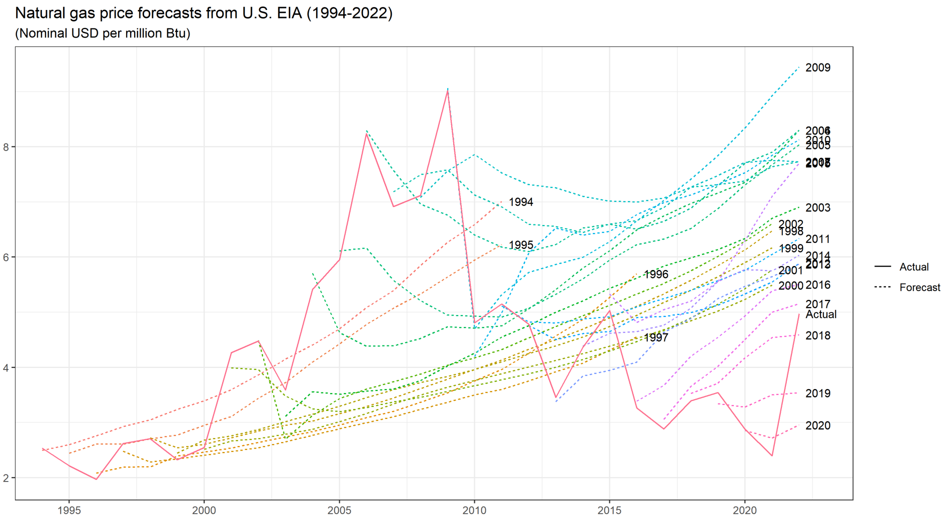


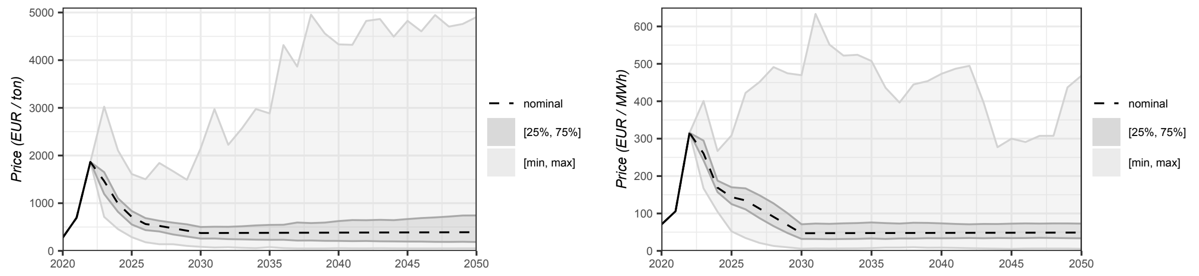
Figure 8: Historic natural gas price forecasts from [20].

We use the historical deviations between the actual price and the yearly forecasts to generate future forecast errors by fitting an ARIMA time series model to predict the log difference between the actual value c_t and forecasted value $\bar{c}_t$ for the years $t \in \{1993, \ldots, 2022\}$. The fitting was performed using the default settings of the `auto.arima` function of [21]. We use log difference as opposed to relative difference or absolute difference as it has the advantages of being symmetric, additive and enables use of linear time series models on exponential trends, which are often observed for economic price data [22]. This has also been observed in recent years (2020-2022) where European energy prices have been especially volatile.

Let the fitted ARIMA model be denoted by $\hat{f}$, we utilize $\hat{f}$ to generate possible future realizations for the natural gas and electricity prices by computing:

$$c_t = \bar{c}_t e^{\hat{f}(\ln(\frac{c_1}{\bar{c}_1}),\dots,\ln(\frac{c_{t-1}}{\bar{c}_{t-1}}))+\varepsilon_t},$$

for future years $t \in \{2023, \dots, 2050\}$, where ε_t is randomly sampled from $\mathcal{N}(0, \sigma_{\hat{f}})$. See Figure 9 for an overview of 1,000 generated scenarios for these two parameters.



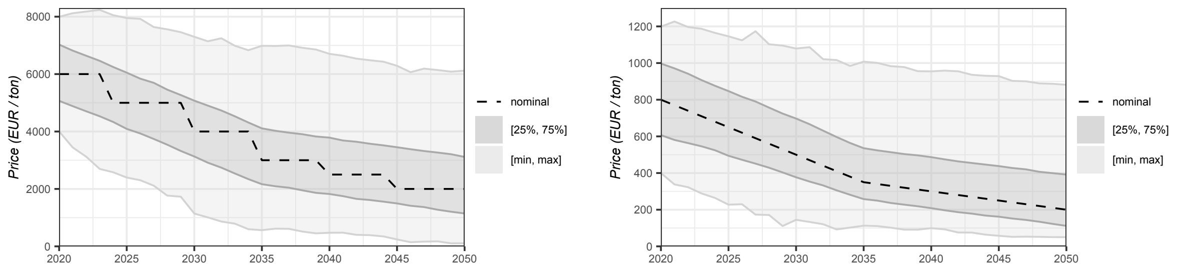
(a) Natural gas

(b) Electricity

Figure 9: Visual overview of 1,000 generated scenarios for natural gas and electricity prices.

Hydrogen and Ammonia price

Because hydrogen and ammonia have not yet been employed at scale as energy carriers, there is limited information available regarding their historic or even current price. Therefore, to characterize the uncertainty around this parameter, we have relied on consultation with domain experts and taken a conservative approach. See Figure 10 for an overview of the generated price scenarios.



(a) Hydrogen

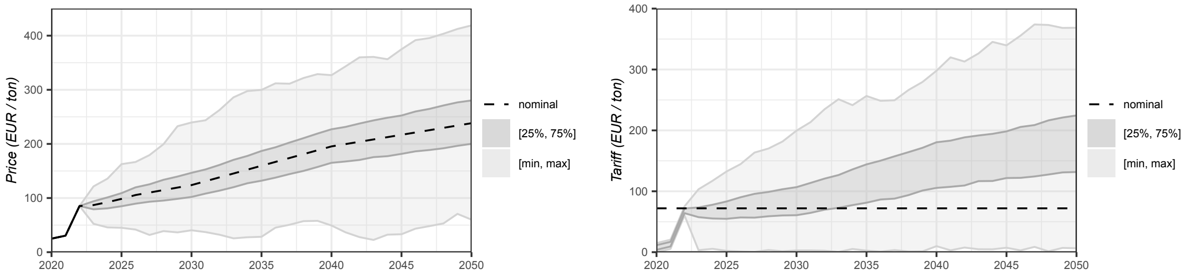
(b) Ammonia

Figure 10: Visual overview of 1,000 generated scenarios for hydrogen and ammonia prices.

CO_2 emission tax and CO_2 CCS tariff

Here we make use of historic EU emission trading system (ETS) data [23]. Due to a number of large policy changes the data pre-2015 is not representative of future volatility. Thus, in our analysis we only consider the data from 2015 onwards. Additionally, we aggregate the data to obtain yearly averages. Our scenario generation procedure for the CO_2 emission tax is identical to the procedure for the natural gas and electricity prices, where we fit an ARIMA time series model to the historic data and use the resulting residual distribution to emulate possible future deviations from our nominal forecast.

Another important CO_2-related parameter is the tariff paid for CCS. The forecast for this parameter is also highly uncertain, as captured CO_2 can play an advantageous role in enhanced oil recovery. However, it is generally expected to correlate with the CO_2 emission tax, as CCS is an alternative to emission. Let e_t^i and c_t^i represent the CO_2 emission tax and CCS tariff respectively for time period t in scenario i. We set $c_t^i = e_t^i - \gamma^i$ for $t = 2020, 2021, 2022$, where γ^i represents additional processing and transport costs ($\gamma^i \sim \mathcal{U}(10, 40)$ EUR/ton). For the later years, $t \in \{2023, \ldots, 2050\}$, we set $c_t^i = \min\{c_{t-1}^i + \epsilon_t^i, e_t^i - \gamma^i\}$, where $\epsilon_t^i \sim \mathcal{U}\left(-(e_t^i - e_{t-1}^i), 3(e_t^i - e_{t-1}^i)\right)$. An overview of the generated scenarios for these two parameters can be seen in Figure 11.



(a) CO_2 emission tax

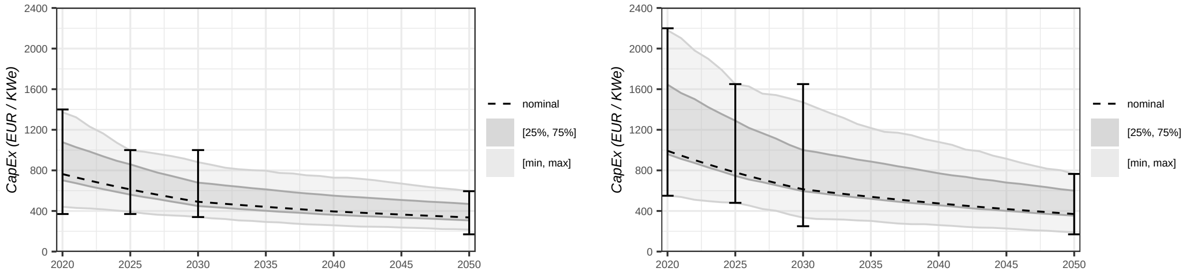
(b) CO_2 CCS tariff

Figure 11: Visual overview of 1,000 generated scenarios for the CO_2 emission tax and CO_2 CCS tariff.

Capital expenditure electrolyzers

The costs of producing hydrogen are dependent on the capital expenditure (CapEx) of electrolyzers. In our model we include two technology options for the production of electrolytic hydrogen, alkaline (ALK) and polymer electrolyte membrane (PEM) electrolysis. ALK electrolysis is generally considered to be more cost-effective than PEM electrolysis, however PEM electrolysis is more efficient in its energy conversion.

While there is still a lot of uncertainty surrounding the development of these technologies, there is scientific literature available on the topic. We have conservatively applied prediction intervals for 2020, 2025, 2030 and 2050 from [24–26]. Assuming that the realized CapEx for these technologies will be distributed uniformly within the ranges from the literature, we are able to generate possible scenarios, see Figure 12 for a visual overview.



(a) ALK

(b) PEM

Figure 12: Visual overview of 1,000 generated scenarios for the capital expenditure of electrolyzers. The error bars signify prediction intervals obtained from [24–26].

Other financial parameters

Finally, we consider the discount rate, weighted average cost of capital (WACC) and annual operating expense (OpEx), which is determined as a fixed percentage of the capital expenditure (CapEx). While the discount rate and WACC are both related to the time value of money, they are considered independently in our model to reflect potential differences due to particular capital funding schemes. A nominal value is chosen by domain experts and for the generated scenarios we assume that these will be situated within a certain range (see Table 3), which is derived using the relative ranges from [19].

Table 3: Overview for other financial parameters (in %)

	nominal	min	max
Discount rate	7.0	3.8	10.2
Weighted average cost of capital	7.5	4.0	11.0
Annual OpEx as percentage of CapEx	4.0	2.1	5.4

Note that in our optimization model, as described in Appendix B.2, these three financial parameters are time-independent (as this simplifies the annualization of costs). However, we still treat these uncertain parameters as if they are realized over time. We do this, per parameter, by generating scenarios where the value is varied over time and the value at the end of the time horizon ($t = 2050$) represents the actual parameter value. This final/actual value is assumed to be uniformly distributed between the ranges indicated in Table 3, and the yearly variations are assumed to be uniform within the interval $[-\frac{\max-\min}{3}, \frac{\max-\min}{3}]$. We do this to mimic the way in which the degree of uncertainty is reduced as a scenario is realized over time.

3.3 Robustness and Sensitivity Analysis

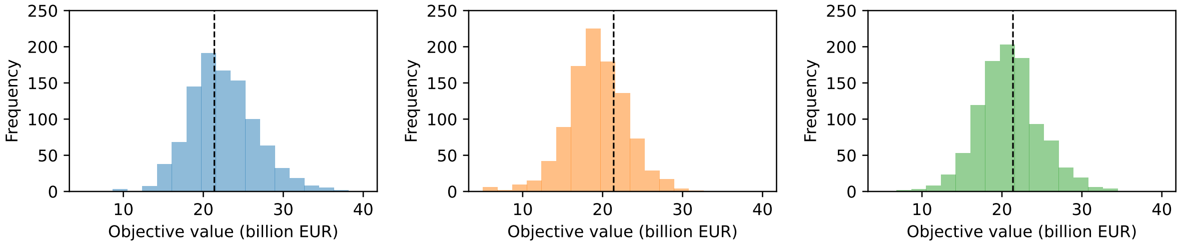
Now we will use our generated scenarios, along with sensitivity and robustness analysis, to gain insight into the potential impact of these uncertain parameters and obtain a more realistic depiction of our outputs of interest. Our main goal in this section is illustrate how RA can be used to determine whether the nominal solution (summarized in Table 1) is sufficiently robust with respect to the uncertain parameters (listed in Table 2).

We conduct three methods of analysis: (i) SA, (ii) RA for static optimization and (iii) RA for adaptive optimization. Note that for each analysis we utilize an identical set of 1,000 randomly generated scenarios. As such, the differences between the results arise purely from differences in methodology.

For the third method of analysis, RA for adaptive optimization, we assume that there are five decision stages, which occur at the start of time periods $t \in \{2020, 2031, 2036, 2041, 2046\}$. We further assume there to be two years between the realization of uncertainty and the implementation of adaptive decisions (e.g., for the decision stage at the start of $t = 2031$, we have access to the uncertainty realizations that occur in time periods $t \leq 2028$). Finally, in order to implement the adaptive decision policy described in Algorithm 3, we use neural networks (one per adaptive decision stage). These are trained, using 10,000 additional scenarios, to predict future parameter values based on the set of known realizations. Note that in practice a decision maker is unlikely to have access to training scenarios from the same distribution as the "test" scenarios. As a result, our adaptive analysis results could be considered overly optimistic. However, due to the high degree of randomness in our scenario generation process, the predictive power of our neural networks is limited. For instance, the model we utilize to make the predictions that are used in the second decision stage (this model makes predictions for $t \geq 2029$ based on realizations from $t \leq 2028$), achieves an R^2 value of 0.42 when evaluated on the 1,000 test scenarios.

All computations are conducted on a 64-bit Windows machine equipped with a 2.80 GHz Intel Core i7 processor with 32 GB of RAM. All mathematical programs are solved to a proven optimality gap of 1% using Gurobi 10.0.1. As the total computation time for each method depends on the degree of parallelization and other implementation details, we report the average accumulated solving time in seconds per scenario. These are: (i) 128, (ii) 0 and (iii) 20 for each method respectively. Interestingly, we find that solving smaller versions of the model 4 times (as we do in RA for adaptive optimization) is, on average, faster than solving the original model once (as we do in SA).

The first output of interest we consider is the objective value (recall that our objective is to maximize the total discounted sum or margins for the industry cluster). In Figure 13 we display the resulting histograms from our three methods of analysis. To further examine the differences between the histograms displayed in Figure 13, we plot the empirical cumulative distribution function for each method in Figure 14.



(a) SA (b) RA (static) (c) RA (adaptive)

Figure 13: Evaluations of the objective value from applying SA and RA. The dashed vertical line indicates the optimal objective value for the nominal model.

We cannot make valid probabilistic conclusions from these analyses. However, for the sake of exposition, assume that each scenario is equally likely and that we use the empirical frequency to estimate the true probability of an event occurring. Imagine that we would like to estimate the probability that our objective value will turn out to be lower than expected (our nominal model suggests an objective value of 21.4 billion EUR). For SA, the observed frequency with which this occurs is 43%. If we had instead chosen to apply RA for static optimization, we would observe a frequency of 72%. The former analysis is inclined to underestimate the true probability of this event occurring, while the latter analysis is inclined to overestimate this probability. Performing RA for adaptive optimization provides a more realistic assessment than either extreme, for which we observe a frequency of 57%.

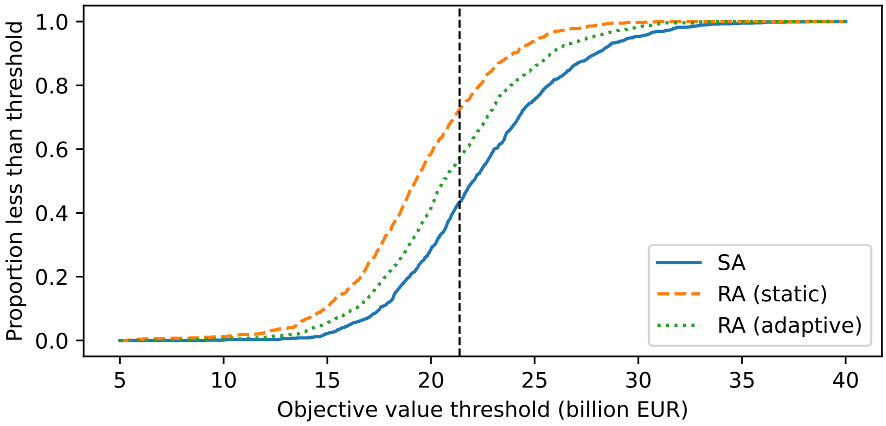


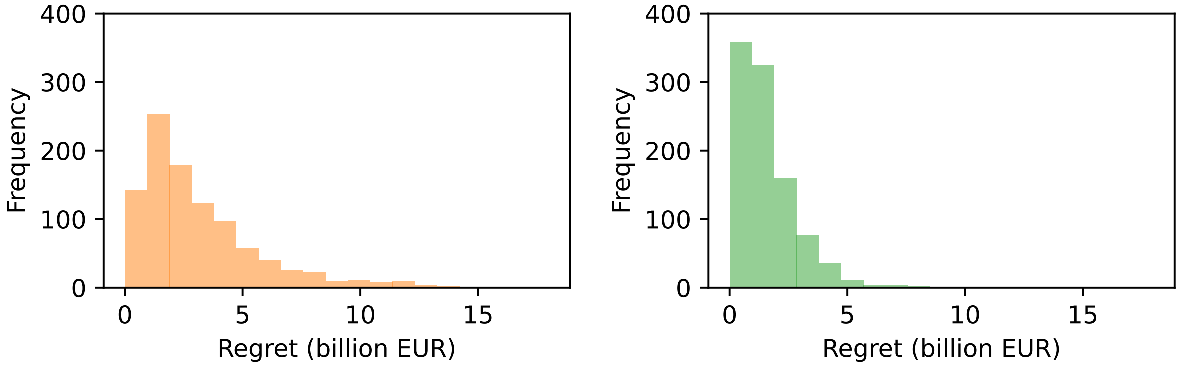
Figure 14: Empirical cumulative distribution function for objective value for each method of analysis. The dashed vertical line indicates the optimal objective value for the nominal model.

To highlight the importance of such differences, consider the following example. If one were to perform only SA, one may incorrectly conclude that the risk of obtaining an objective value of less than 15 billion

EUR is negligible (only 2.2%) and thus no action is required in order to mitigate this risk. However, if one were to perform RA for adaptive optimization, one would obtain a more accurate estimate of the risk (5.6%) and may instead conclude that a more robust solution is required.

Using SA in combination with RA to derive regret

Combining the results from SA and RA can provide valuable insight as it allows one to compute the possible regret associated with making specific decisions. In this context "regret" is defined as the ex-post difference between the achieved value and the best value that could have been obtained if the information had been known before making the decision. For each scenario we can compute the regret by taking the difference between the results from RA (which provides the "achieved value") and the results from SA (which provides the "best value that could have been obtained"). Knowing the potential regret of a decision is more informative than only knowing the achieved value as it provides evidence of the existence of alternative decisions that are preferable (for certain scenarios).



(a) Derived using RA (static)

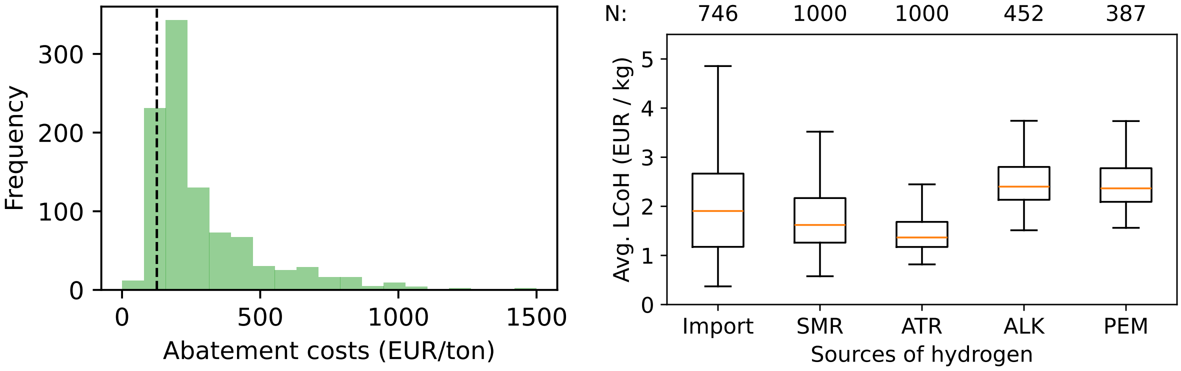
(b) Derived using RA (adaptive)

Figure 15: Comparison of potential regret with respect to the objective value. Obtained by comparing the results from SA with the results from RA (for static and adaptive optimization).

In Figure 15 we examine the potential regret of the nominal solution with respect to each scenario in our test set. The average regret (in billion EUR) for the static analysis is 3.1, while only 1.5 for the adaptive analysis. Again, we find a significant difference between the results due to the ability to adapt the later stage decisions when more information is realized.

Additional outputs of interest

So far, we have focused on the objective value as an output of interest. However, for real-world problems there may be multiple "key performance indicators" to consider in the analysis. For our case study, we are also interested in the following two metrics. First, the average CO_2 abatement costs, which is defined as the additionally incurred costs (calculated with respect to the corresponding scenario case without CO_2 emission penalties) divided by the avoided CO_2 emissions. Second, the average levelized cost of hydrogen (LCoH), which is defined as the net present value of the total cost of producing or importing hydrogen divided by the quantity. This metric is computed per source of hydrogen, which can either be imported, produced using steam methane reforming (SMR), autothermal reforming (ATR) or electrolysis (ALK and PEM). Note that this metric is computed over the time periods from 2025 up to 2050 and does not incorporate costs related to the CO_2 emission tax or CCS tariff. In Figure 16 we use RA (for adaptive optimization) to obtain an evaluation of these two outputs of interest.



(a) Average CO_2 abatement costs

(b) Average levelized cost of hydrogen

Figure 16: Two additional outputs of interest, evaluated using RA for adaptive optimization. The dashed vertical line in Figure 16a represents the abatement costs under the nominal scenario. Figure 16b displays a "box and whisker plot", where the whiskers extend to the farthest data point lying within 1.5x the inter-quartile range (represented by the box) and observations beyond the whiskers are omitted. The numbers reported at the top of the graph to the right of "N" represent the number of scenarios for which the quantity of hydrogen produced/imported is greater than zero.

Effect of altering the number of decision stages

While allowing for more decision stages may generate more realistic results (depending on how often decisions are re-evaluated in the real-world problem at hand), it comes at the cost of increased computation time. For RA in an adaptive setting, the number of decision stages K was set to 5. Here we consider alternative setups where we alter the number of decision stages to occur after 2031. All setups involve first and second stages at $t = 2020$ and $t = 2031$ respectively.

In Figure 17 we display the average accumulated solve time (per scenario) as a function of K. We find that this function is approximately linear in the number of decision stages, which provides empirical evidence that using our proposed adaptive decision policy (as described in Algorithm 3) is computationally tractable, even for a large number of decision stages.

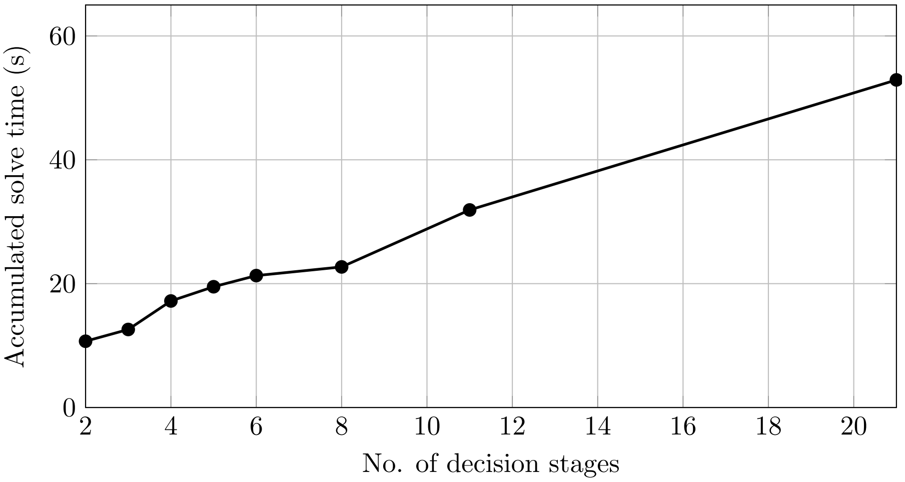


Figure 17: Average accumulated solve time of RA (in seconds per scenario) as a function of the number of decision stages.

Using RA to compare solutions

From the results presented in Figures 13c, 15b and 16 one may conclude that the nominal solution is insufficiently robust w.r.t. uncertainty regarding the parameter values of our model. Furthermore, Figure 15b suggests that there exist alternative solutions which perform better under certain scenarios. As such, one may look to apply techniques from stochastic programming and/or robust optimization in the hopes of obtaining a solution that is more robust in the presence of uncertainty. In order to test whether this is the case, one can apply robustness analysis to compare two (or more) solutions.

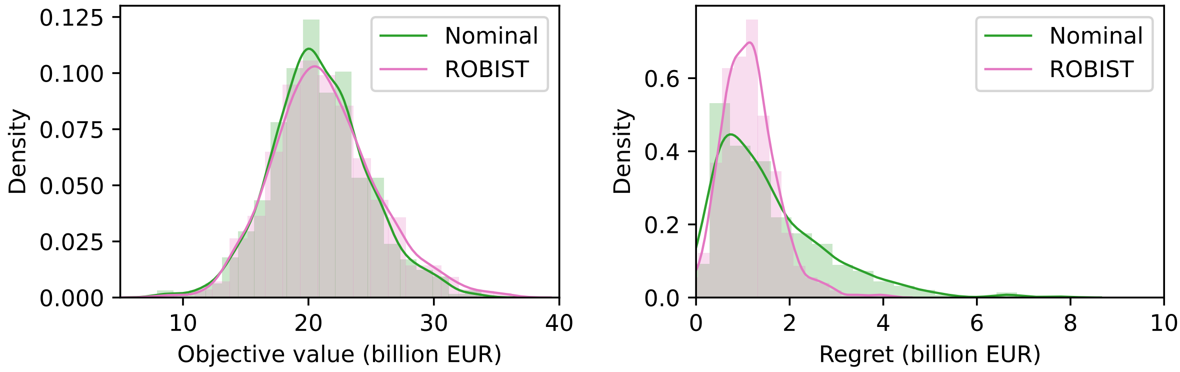
In this subsection we compare our nominal solution (as presented in Table 1), with an alternative solution obtained via application of the "ROBIST" algorithm [27]. See Appendix C for details regarding the application of ROBIST. The difference in first stage investment decisions is summarized in Table 4 below. The most striking difference we find is that the first stage decisions of the solution obtained via ROBIST involve less investment in hydrogen production and more investment in infrastructure.

Table 4: Overview of aggregate capital expenditure (in millions of EUR) for the first stage investment decisions. Nominal solution is summarized on the left, the solution obtained via ROBIST is depicted on the right, where the differences are highlighted in bold. Note that, in the model formulation, these costs are annualized (i.e. converted to yearly payments) over the lifetime of the investments.

	2025	2026	2027	2028	2029	2030
Hydrogen	1800					
Electrification	70		30			50
CCS						
Infrastructure	42					1

	2025	2026	2027	2028	2029	2030
Hydrogen	**1440**					
Electrification	70		30			**10**
CCS						**25**
Infrastructure	**87**					1

In Figure 18 we analyze and compare the performance of the first stage decisions of the two solutions using RA (in a 5-stage adaptive setting) in terms of objective value and regret. We find that, for our set of 1,000 randomly scenarios, the solution obtained via ROBIST performs better, on average, than the nominal solution. For the ROBIST solution, the average regret is 413 million euro lower and the percentage of scenarios for which the regret is larger than 2 billion is 7%, instead of 27.4% (for the nominal solution). This example demonstrates how RA can also be used to compare the performance of multiple solutions and assist in determining which solution is more robust to parametric uncertainty.



(a) Objective value

(b) Regret

Figure 18: Comparison of results from applying RA to two different solutions. We plot the results using histograms, and use kernel density estimation to visualize the data as continuous curves.

4 Conclusion

In this paper, we extend RA to deal with adaptive optimization problems, where decisions are made sequentially over time. By incorporating the ability for part of the solution to adapt once more information is known, the analysis can be made more realistic, which can ultimately lead to better decision-making in practice. Our proposed method is intuitive, computationally tractable and can be applied to a broad range of problems.

RA can be used to determine whether a particular solution is (or is not) sufficiently robust. Being able to properly verify such a conclusion is especially valuable when dealing with adaptive optimization problems, which are commonly encountered in practice, yet notoriously difficult to model and solve in a stochastic and/or robust manner.

We demonstrate our methodology by applying it to the optimization of decarbonization pathways for an industry cluster in the Netherlands. Here, we find that parametric uncertainty can have a large impact on the performance of a solution and that adverse outcomes can be mitigated via decreased investment in hydrogen production and increased investment in infrastructure.

We reiterate two recommendations made by Gorissen et al. [28]. First, that formulating and solving optimization problems in a stochastic and/or robust manner is not always necessary and that RA should be used as a screening method to identify cases where the nominal solution may already be sufficiently robust. Second, solving optimization problems in a stochastic and/or robust manner does not necessarily lead to superior solutions and RA should be used to analyze and compare multiple solutions before deciding which solution to implement.

While SA is often used to analyze the effect of uncertainty on optimization models, it may not provide an accurate assessment of risk. (However, performing SA in addition to RA can provide valuable insight into the amount of regret associated with particular decisions.) In [6] it is observed that all linear optimization textbooks cover SA extensively, and do not cover RA. Because RA can provide a more realistic risk assessment than SA, we plea for the inclusion of RA in these textbooks, both for static and adaptive optimization.

In terms of further research, it would be interesting to test alternative adaptive decision policies, to explore the usage of scenario reduction techniques and to further analyze the data obtained from RA in order to determine which parameters are the most impactful. Future work also envisions investigating the potential synergy between RA and modeling to generate alternatives as well as the usage of RA within simulation-based optimization.

Acknowledgments

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Appendix

A Sensitivity Analysis

Within SA there is a distinction made between "local" and "global" analysis [29]. While local SA is quite popular due its simplicity and ease of understanding [30], when analyzing the impact of uncertainty, one is typically more interested in global SA [31]. Within global SA, various methods have been developed (see [32, Chapter 1.2] for an overview), most of which involve numerical estimation by analyzing a finite number of model evaluations As such, this is the type of SA method we apply throughout this paper.

When SA is applied to optimization models, one analyzes how changes in the model's parameters affect its optimal solution. This is visualized in Figure 19 below, where the decision vector $\mathbf{x}$ is determined *after* the realization of the uncertain parameter vector $\mathbf{z}$. A procedural description of SA is presented in Algorithm 4.

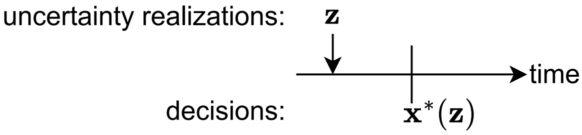

Figure 19: Visual aid for chronology of events in sensitivity analysis

Algorithm 4 Pseudo code for sensitivity analysis

Input: Set of scenarios $\{\mathbf{z}^1, \ldots, \mathbf{z}^N\}$.

Output: Evaluation of sensitivity of optimal solution $\mathbf{x}^*$ w.r.t. each scenario in $\{\mathbf{z}^1, \ldots, \mathbf{z}^N\}$.

```
for scenario $i \in \{1, \ldots, N\}$ do
    Determine optimal solution $\mathbf{x}^{i*}$ by solving Problem (2) with $\bar{\mathbf{z}} = \mathbf{z}^i$
    Evaluate outputs of interest $Y_j(\mathbf{x}^{i*}, \mathbf{z}^i), \quad \forall j = 1, \ldots, M$
end for
```

B Model Descriptions

B.1 Illustrative Toy Problem

In the illustrative toy problem presented in Section 2.2, we consider a supply chain network composed of supply nodes (SA and SB), processing nodes (PA and PB), and a demand node (DC). The network includes four arcs: $\mathcal{A} = \{(SA, PA), (SB, PB), (PA, DC), (PB, DC)\}$. The system operates over a discrete time horizon $T = \{1, 2\}$ and handles two products, A and B. Investments can be made to expand arc and processing capacities over time, while product flows determine how goods move through the network to satisfy demand.

Investment decision variables are integer and represented by v, where $v_{a,t}$ denotes investment in transport capacity on arc $a \in \mathcal{A}$ at time $t \in T$, and $v_{n,t}$ denotes investment in processing capacity at node $n \in \{PA, PB\}$ at time t. Product flow variables $y_{a,t}$ are non-negative and continuous, and represent the quantity transported along arc $a \in \mathcal{A}$ at time $t \in T$.

The objective is to maximize total profit, which is the revenue from selling product C minus investment and supply costs:

$$\max \sum_{t \in T} \Big[2(y_{(PA,DC),t} + y_{(PB,DC),t}) - \sum_{a \in \mathcal{A}} v_{a,t} - 2(v_{PA,t} + v_{PB,t}) - \big(c_{A,t} y_{(SA,PA),t} + c_{B,t} y_{(SB,PB),t}\big) \Big].$$

The constraints of the model are as follows. The demand (100 units) must be met in each time period:

$$y_{(PA,DC),t} + y_{(PB,DC),t} = 100, \quad \forall t \in T.$$

Flow conservation must hold at the processing nodes:

$$\begin{aligned} y_{(SA,PA),t} &= y_{(PA,DC),t}, \quad \forall t \in T, \\ y_{(SB,PB),t} &= y_{(PB,DC),t}, \quad \forall t \in T. \end{aligned}$$

Arc capacities limit the product flows, where the capacity can be increased via investment:

$$y_{a,t} \leq 0 + 20 \sum_{t'=1}^{t} v_{a,t'}, \quad \forall a \in \mathcal{A}, \forall t \in T.$$

Similarly, processing capacity constraints limit the inflows into processing nodes:

$$\begin{aligned} y_{(SA,PA),t} &\leq 0 + 20 \sum_{t'=1}^{t} v_{PA,t'}, \quad \forall t \in T, \\ y_{(SB,PB),t} &\leq 0 + 20 \sum_{t'=1}^{t} v_{PB,t'}, \quad \forall t \in T. \end{aligned}$$

Finally, the variable constraints:

$$\begin{aligned} & v_{a,t} \in \mathbb{N}_0, \quad \forall a \in \mathcal{A}, \forall t \in T, \\ & v_{n,t} \in \mathbb{N}_0, \quad \forall n \in \{PA, PB\}, \forall t \in T, \\ & y_{a,t} \geq 0, \quad \forall a \in \mathcal{A}, \forall t \in T. \end{aligned}$$

B.2 Industrial Decarbonization Problem

To optimize decarbonization pathways, we utilize a network flow mixed-integer optimization model. The network is made up of nodes and arcs, where the nodes represent supply, intermediary, and demand entities and the arcs represent connections between these entities. The flows over the arcs from one node to another represent units of energy, materials and emissions. The time horizon is discretized into 31 time periods, where the periods are connected through investment decisions and storage capability. The objective of the model is to maximize the total (discounted) sum of margins over the entire supply chain over the specified time horizon while adhering to a number of constraints, which enforce supply, storage, transport and processing capacities, as well as the balance of flows in and out of the nodes.

Here we present a mathematical formulation of this network flow model. To do this we must first introduce some notation. Let the set of time periods be represented by T. This set is made up of ordinal numbers, with initial time period $t_1 = 1$. Let P represent the set of products (e.g. forms of energy, emissions) and let Q represent the set of possible investment projects. We define the set of source/supply nodes as N_{sup}, the set of sink/demand nodes as N_{dem} and the set of intermediary nodes as N_{int}. These three combined give us the set of all nodes $N = N_{sup} \cup N_{int} \cup N_{dem}$. Additionally, we define a few special nodes, namely the set of processing nodes N_{pro} and the set of storage nodes N_{sto}. These are both subsets of the set of intermediary nodes N_{int}. We use A to represent the set of arcs between our nodes.

Proceeding with the variables and parameters, in summary, we model three types of flows. These are the flows in and out of nodes, flows to and from storage facilities and flows used in and produced from processing activity. For these flows the modeler is able to specify a minimum and/or maximum in order to emulate various types of restrictions. With such restrictions one is able to define the quantity of supply/demand, processing capacity, etc.

The notation is as follows, we use y_{ijpt} to represent the flow of material p over arc (i, j) in time period t and let U^{arc}_{ijpt} and L^{arc}_{ijpt} represent the maximum and minimum limits on the flow over arc (i, j) in period t. Additionally, we represent the flow into a node i with y^{in}_{ipt} and out of a node with y^{out}_{ipt}. We represent the maximum and minimum limits on the flow in/out of nodes by $U^{\text{in}}_{ipt}/U^{\text{out}}_{ipt}$ and $L^{\text{in}}_{ipt}/L^{\text{out}}_{ipt}$. Let s_{ipt} represent the storage level at node i of product p at the end of time period t. Let s^{-}_{ipt} represent the amount of product moved to storage and let s^{+}_{ipt} represent the amount procured from storage in time time period t. Additionally, we use s_{ip0} to represent an initial amount of product p in storage at node i. We denote the maximum and minimum storage capacity of product p at node i in time period t with U^{sto}_{ipt} and L^{sto}_{ipt}. Finally, we use r^{-}_{ipt} and r^{+}_{ipt} to represent the amount of product p consumed by and produced from the processing node i during time period t. Furthermore, let r_{it} represent a dimensionless quantity of processing activity at node i in time period t, and we use κ_{ipt} to denote the yield of product p at processing node i. The yield of a product is negative whenever that product is consumed in the processing activity and positive if it is produced from the activity.

Moving on to the investment component of the model, we use integer variable w_{qt} to represent the amount of capital invested in investment project q in time period t. We employ a supplementary variable v_{qt} to represent the amount of investment q that is active at time t, where "active" implies that the effect of the investment are realized during time period t. We use l_q to express the lifetime of investment q (expressed in number of time periods for which the effects persist). The effect of a unit of investment q on the maximum and minimum flow over arc (i, j) is expressed in units of product p and represented by $\delta^{arc,U}_{ijpq}$ and $\delta^{arc,L}_{ijpq}$. For the effect on the maximum and minimum over the flow in/out of a node i we use $\delta^{\text{in},U}_{ipq}/\delta^{\text{out},U}_{ipq}$ and $\delta^{\text{in},L}_{ipq}/\delta^{\text{out},L}_{ipq}$ respectively. The impact on maximum and minimum storage capacity is represented by $\delta^{sto,U}_{ipq}$ and $\delta^{sto,L}_{ipq}$.

Finally, using ψ as the discount rate, we determine the total net present value (Π_{NPV}) using the following equation:

$$\Pi_{NPV} = \sum_{t\in T} \frac{1}{(1+\psi)^{(t-1)}} \Bigg[\sum_{p\in P} \Bigg(\sum_{i\in N} \big[c^{rev}_{ipt} y^{in}_{ipt} - c^{sup}_{ipt} y^{out}_{ipt} - c^{hand}_{ipt} (y^{in}_{ipt} + y^{out}_{ipt}) - \sum_{j\in N^{out}_{i}} c^{arc}_{ijpt} y_{ijpt} \big] - \sum_{i\in N_{sto}} c^{sto}_{ipt} s_{ipt} \Bigg) - \sum_{q\in Q} c^{inv}_{qt} v_{qt} \Bigg].$$

Where c^{rev}_{ipt} reflects revenue gained per unit of product p at node i in time period t. Similarly, we introduce several cost parameters related to supply (c^{sup}_{ipt}), handling (c^{hand}_{ipt}), storage (c^{sto}_{ipt}), transportation (c^{arc}_{ijpt}) and investment (c^{inv}_{qt}). The investment costs c^{inv}_{qt} are the sum of two components, annualized capital expenditure costs (c^{AC}_{qt}) and operation and maintenance costs ($c^{O\&M}_{qt}$). The annualized capital expenditure associated with investment q is computed as follows: $c^{AC}_{qt} = \frac{c^{capex}_{qt}\phi}{(1-(1+\phi))^{-l_q}}$, where c^{capex}_{qt} and ϕ represent the capital expenditure of investment q at time t and weighted average cost of capital respectively. The operation and maintenance costs are computed as: $c^{O\&M}_{qt} = c^{capex}_{qt}\gamma$, where γ represents the annual OpEx as percentage of CapEx.

Using the notation described above, we arrive at the following mathematical formulation for our model:

$$
\begin{aligned}
&\max_{\mathbf{y},\mathbf{w},\mathbf{s},\mathbf{r}} && \Pi_{NPV} && \qquad (3a)\\
&\text{s.t.} && y^{\text{in}}_{ipt} + s^{+}_{ipt} + r^{+}_{ipt} = y^{\text{out}}_{ipt} + s^{-}_{ipt} + r^{-}_{ipt} && \forall i \in N_{pro} \cap N_{sto}, \forall p \in P, \forall t \in T \qquad (3b)\\
& && y^{\text{in}}_{ipt} + r^{+}_{ipt} = y^{\text{out}}_{ipt} + r^{-}_{ipt} && \forall i \in N_{pro} - N_{sto}, \forall p \in P, \forall t \in T \qquad (3c)\\
& && y^{\text{in}}_{ipt} + s^{+}_{ipt} = y^{\text{out}}_{ipt} + s^{-}_{ipt} && \forall i \in N_{sto} - N_{pro}, \forall p \in P, \forall t \in T \qquad (3d)\\
& && y^{\text{in}}_{ipt} = y^{\text{out}}_{ipt} && \forall i \in N_{int} - N_{pro} - N_{sto}, \forall p \in P, \forall t \in T \qquad (3e)\\
& && L^{arc}_{ijpt} + \sum_{q\in Q} \delta^{arc,L}_{ijpq} v_{qt} \le y_{ijpt} \le U^{arc}_{ijpt} + \sum_{q\in Q} \delta^{arc,U}_{ijpq} v_{qt} && \forall (i,j) \in A, \forall p \in P, \forall t \in T \qquad (3f)\\
& && L^{in}_{ipt} + \sum_{q\in Q} \delta^{in,L}_{ipq} v_{qt} \le y^{in}_{ipt} \le U^{in}_{ipt} + \sum_{q\in Q} \delta^{in,U}_{ipq} v_{qt} && \forall i \in N, \forall p \in P, \forall t \in T \qquad (3g)\\
& && L^{out}_{ipt} + \sum_{q\in Q} \delta^{out,L}_{ipq} v_{qt} \le y^{out}_{ipt} \le U^{out}_{ipt} + \sum_{q\in Q} \delta^{out,U}_{ipq} v_{qt} && \forall i \in N, \forall p \in P, \forall t \in T \qquad (3h)\\
& && L^{sto}_{ipt} + \sum_{q\in Q} \delta^{sto,L}_{ipq} v_{qt} \le s_{ipt} \le U^{sto}_{ipt} + \sum_{q\in Q} \delta^{sto,U}_{ipq} v_{qt} && \forall i \in N_{sto}, \forall p \in P, \forall t \in T \qquad (3i)\\
& && s_{ipt} = s_{ip(t-1)} + s^{-}_{ipt} - s^{+}_{ipt} && \forall i \in N_{sto}, \forall p \in P, \forall t \in T \qquad (3j)\\
& && r^{-}_{ipt} = -\kappa_{ipt} r_{it} && \forall (i,p,t) \in \{N_{pro} \times P \times T : \kappa_{ipt} < 0\} \qquad (3k)\\
& && r^{+}_{ipt} = \kappa_{ipt} r_{it} && \forall (i,p,t) \in \{N_{pro} \times P \times T : \kappa_{ipt} > 0\} \qquad (3l)\\
& && v_{qt} = \sum_{i=0}^{l_q} w_{q(t-i)} && \forall q \in Q, \forall t \in T \qquad (3m)\\
& && y^{\text{in}}_{ipt} = \sum_{j\in N^{in}_i} y_{jipt} && \forall i \in N, \forall p \in P, \forall t \in T \qquad (3n)\\
& && y^{\text{out}}_{ipt} = \sum_{j\in N^{out}_i} y_{ijpt} && \forall i \in N, \forall p \in P, \forall t \in T \qquad (3o)\\
& && y_{ijpt} \ge 0 && \forall (i,j) \in A, \forall p \in P, \forall t \in T \qquad (3p)\\
& && s_{ipt}, s^{+}_{ipt}, s^{-}_{ipt} \ge 0 && \forall i \in N_{sto}, \forall p \in P, \forall t \in T \qquad (3q)\\
& && r_{it} \ge 0 && \forall i \in N_{pro}, \forall t \in T \qquad (3r)\\
& && w_{qt} \in \mathbb{N}_0 && \forall q \in Q, \forall t \in T. \qquad (3s)
\end{aligned}
$$

The objective function of this optimization problem is to maximize the total net present value of margins over the entire supply chain. Constraints (3b), ..., (3e) form the backbone of our model and enforce the balance of all flows in and out of the intermediary nodes. Constraints (3f) restrict the arc flows such that they must satisfy the minimum and maximum requirements over the arc. These requirements, and thus the constraints, are dependent on the investment decisions. Constraints (3g), (3h) and (3i) serve a similar function for the flows in and out of nodes and for the amount of "product" kept in storage. Constraints (3j) ensure that the storage levels are derived correctly. Constraints (3k) and (3l) ensure that the in-feed and out-feed product flows from processing nodes is modeled correctly in accordance with the relevant yields. Here, the variable r_{it} plays an instrumental role in linking the different products together. Constraints (3m), (3n) and (3o) enforce the definitions which we have assigned to these variables. Finally, Constraints (3p), ..., (3s) enforce non-negativity and integer constraints on the decision variables.

C ROBIST Implementation Details

To obtain the alternative solution presented in the final paragraphs of Section 3.3, we utilize "Robust Optimization by Iterative Scenario Sampling" (abbreviated as ROBIST), see Sections 2 and 3 of [27] for more details on the method itself.

In summary, the ROBIST algorithm requires a set of scenarios, that is randomly split into a training data set $\mathcal{D}^{\text{train}}$, a validation data set $\mathcal{D}^{\text{valid}}$ and a test set $\mathcal{D}^{\text{test}}$. In our implementation we first generate 300 additional out-of-sample scenarios and randomly assign 100 scenarios to each of the three sets.

The algorithm is iterative, where at each iteration i, we generate a new solution by solving a scenario optimization problem for a finite set of sampled scenarios from $\mathcal{D}^{\text{train}}$. Let this set be denoted as $\mathcal{S}_i$. The scenario optimization problem we solve is a 2-stage variant of Problem (2), where we minimize the worst-case regret across all scenarios in $\mathcal{S}_i$:

$$\begin{aligned} \min_{\mathbf{x},\theta} \ & \theta \\ \text{s.t. } & f^\star(\mathbf{z}^j) - f(\mathbf{x}_1, \mathbf{x}_2^j, \mathbf{z}^j) \leq \theta, && \forall \mathbf{z}^j \in \mathcal{S}_i, \\ & \mathbf{x}_1 \in \mathcal{X}_1, \\ & \mathbf{x}_2^j \in \mathcal{X}_2(\mathbf{x}_1, \mathbf{z}^j), && \forall \mathbf{z}^j \in \mathcal{S}_i, \end{aligned} \tag{4}$$

where $\mathbf{x}_1$ represent the first stage decisions and $\mathbf{x}_2^j$ represent the adaptive "recourse" decisions, which are defined for each sampled scenario $\mathbf{z}^j \in \mathcal{S}_i$. Finally, $f^\star(\mathbf{z}^\mathbf{j})$ represents the best possible objective value under scenario $\mathbf{z}^j$, i.e., $f^\star(\mathbf{z}^j) := \max\{f(\mathbf{x}, \mathbf{z}^j) : \mathbf{x} \in \mathcal{X}(\mathbf{z}^j)\}$.

Solving (4) provides first stage decisions $\mathbf{x}_1^*$, which are then evaluated via robustness analysis using $\mathcal{D}^{\text{train}}$. We then select a scenario that is not already in $\mathcal{S}_i$, for which we find maximal regret. This scenario is then added to $\mathcal{S}_i$.

We initialize our scenario set with the nominal scenario $\bar{\mathbf{z}}$, i.e. $\mathcal{S}_0 = \{\bar{\mathbf{z}}\}$, and repeat the above procedure for a maximum of 8 iterations (for $|\mathcal{S}_i| > 9$, solving (4) becomes computationally prohibitive). After this, we use $\mathcal{D}^{\text{valid}}$ to analyze the robustness of the resulting 8 solutions to select the solution with the lowest average regret. Finally, the scenarios in $\mathcal{D}^{\text{test}}$ can be utilized to provide an independent estimate of the robustness of the selected solution.