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Stochastic optimization of Power-to-Methanol: Production cost sensitivity to process design vs. scheduling

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Abstract

Under time-varying electricity prices, the production costs of Power-to-X processes with intermediate storage can be reduced by simultaneously optimizing the process unit design and size with their scheduling and operation. However, the production cost sensitivity to optimal process design or scheduling is unclear, especially when several scheduling scenarios are considered to address uncertainty. To answer this question, we consider a grid-connected Power-to-Methanol process with intermediate storage and compare: (i) optimal process design under steady-state operation, (ii) optimal scheduling for several randomly generated process designs, and (iii) combined design and scheduling optimization. We show that optimal scheduling is, on average, more important than optimal design (within the considered variable bounds), since it can mitigate the effects of poor design choices. As a consequence, very different process designs, especially with oversized electrolysis and methanol synthesis units, can lead to similar objective function values when flexible operation is enabled and scheduling is optimized.

KEYWORDS
battery and hydrogen storage, combined design and scheduling, Power-to-Methanol, process design correlation analysis, two-stage stochastic programming

1 | INTRODUCTION

The cost of hydrogen-based chemicals and fuels produced via Power-to-X (PtX) processes is generally dominated by the high investment costs for water electrolyzers as well as high operating costs. For grid-connected PtX processes under time-varying electricity prices, the economic competitiveness against fossil-based alternatives can be improved by operating them flexibly as well as taking advantage of intermediate storage.[1–3]

To minimize production costs, the design of PtX processes, including both design variables and unit sizing, should be optimized while considering process scheduling so that the process units are optimally designed and (over-)sized while meeting the production goals. Most works that simultaneously optimize the design and scheduling of PtX processes consider single specific power generation or electricity price profiles, for example, in the case of Power-to-Ammonia,[4,5] Power-to-Gas[6,7] and Power-to-Methanol.[2,8] Especially for the sustainable production of methanol, several studies have recently looked at the interplay between flexible operation and intermediate storage via optimization. For instance, Chen et al.[9,10] and Akram and Kienberger[11] optimized a Power-to-Methanol process model with hydrogen storage. In our previous work,[8] we investigated the combined role of flexible operation and intermediate storage (battery and hydrogen storage) in Power-to-Methanol. Maggi et al.[12] optimized the design of a Power-to-Methanol process with battery and hydrogen storage via multi-period optimization. Taslimi and Khosravi[13] optimized the design and scheduling of a Power-to-Methanol process with battery and hydrogen storage, also considering optimal participation in ancillary markets. Further, even more heat and work storage technologies were considered in support of a Power-to-Methanol process by Svitnič and Sundmacher.[2] Nonetheless, fewer works account for uncertainty on the input profiles, for example, electricity prices[14,15] and renewable power generation[16,17] for grid-connected and stand-alone processes, respectively, especially when process design is also optimized as, for example, in microgrids,[18] organic Rankine cycles,[19] energy systems,[20,21] and PtX processes.[16,22,23]

An approach to account for such uncertainty is formulating the deterministic equivalent of risk-neutral stochastic combined design and scheduling (S-CDS) optimization problems.[24–29] In these two-stage stochastic programming problems, the uncertainty is generally addressed by simultaneously considering several scheduling scenarios. However, these problems can become extremely challenging to solve within reasonable CPU times depending on factors such as the model type, for example, LP vs. MINLP, number of scheduling scenarios, and length and time discretization of the scheduling horizons.

To tackle the numerical complexity directly on the solver side, several optimization strategies based on either black-box optimizers, for example, a genetic algorithm to identify first-stage variables,[18] sample average approximation performed within the solver,[30] or decomposition approaches to exploit the problem structure have been proposed, mainly for stochastic LPs and MILPs.[25,27,31] For instance, L-shaped methods based on generalized Benders decomposition iteratively identify first-stage variables in a master problem, which are then fixed to solve a stochastic scheduling problem that is used to introduce feasibility and optimality cuts into the master problem.[25,27,32] Lagrangean or scenario decomposition[25,27,31] is also used to generate simpler (non-stochastic) independent two-stage subproblems, which embed penalty terms into the objective function to enforce the equality of the first-stage variables across the subproblems through the iterations. Further, beyond improving the above-mentioned optimization strategies, for example, introducing stronger Benders cuts,[33,34] dedicated branching strategies[35,36] have also been proposed.

For cases where these optimization strategies still cannot solve two-stage problems or are not implemented in conventional solvers, several tailored optimization algorithms have been proposed, especially for energy system applications. For instance, Liu et al.[37] proposed a decomposition algorithm based on optimality cuts for two-stage stochastic programs reformulated as large-scale multi-period MINLP problems by applying a sampling and integration technique. Heo et al.[38] proposed a decomposition algorithm for CDS problems that first identifies a design candidate with a simplified model and then tests the design candidate's performance by solving an optimal scheduling problem with a linearized model. Furthermore, Baumgärtner et al.[39] proposed RiSES[4], an algorithm for CDS problems based on time series aggregation (TSA), whose time resolution is iteratively increased until the desired optimality gap is reached. RiSES[4][39] was later extended to account for nonlinearities (RiNSES[4][40]). However, some of these tailored approaches,[38,40] which can be applied in stochastic problems, can generate infeasible design candidates for the original problem due to linearization.[40]

To tackle the numerical complexity without the need for tailored optimization algorithms, S-CDS optimization problems can be simplified, for example, via model relaxation,[14] scenario clustering,[20,22,23] and TSA[41–43] or degrees of freedom (DoF) reduction.[23,44] Further approximation strategies can be applied to the original S-CDS problems, such as only optimizing the process design considering steady-state operation or only optimizing the process scheduling for given process designs. Nonetheless, it remains unclear whether these approximations of S-CDS problems are sufficiently accurate for stochastic optimization of Power-to-X processes. Moreover, the literature has not considered whether optimal process design versus optimal process scheduling is more important for reducing the production cost when accounting for the uncertainty of scenario realization.

Furthermore, the impact of process design variables on the production cost in Power-to-X processes is generally unknown, particularly when several scheduling scenarios are considered. In fact, several process designs can potentially lead to similar objective function values, for example, with a difference below the optimality tolerance. This situation can occur, for instance, when the objective function is not particularly sensitive to certain design variables[45] or because of the economic trade-offs captured by the objective function when optimized under uncertainty.[26,46,47]

To answer these questions related to the sensitivity of the objective function to optimal stochastic design and scheduling and to the design variables, we solve S-CDS problems for a MINLP model of a grid-connected Power-to-Methanol (PtMeOH) process with intermediate storage based on our previous work.[8,23] In particular, we first investigate how sensitive the methanol production cost is to optimal design, mainly the size of the key process units, and optimal scheduling under uncertainty when enabling flexible operation for different process units. We then analyze the optimization results statistically to identify general trends between the process design variables and the production cost. Finally, we benchmark the optimization results by solving a simplified S-CDS problem as in our previous work.[23]

In the following, Sections 2 and 3 describe the methodology, the model, and the considered case studies, Section 4 presents the results, while the conclusions are drawn in Section 5.

2 | METHODOLOGY

To investigate how sensitive grid-connected Power-to-Methanol processes are to optimal design (mainly unit sizing) and scheduling when several scenarios are considered, we formulate and solve the deterministic equivalent of the corresponding stochastic optimization problems.

In the following subsections, we describe the optimization problems, the statistical analysis, as well as their implementation.

2.1 | Stochastic programming

The PtMeOH process is optimized while considering uncertainty related to the realization of electricity price scenarios, which represent an input to the S-CDS problem. In contrast, the full sequence of N_{TS} values within each scenario n is assumed to be known (assumption of perfect information on the scenario time series) and is collected in a vector $\boldsymbol{c}_n \in \mathbb{R}^{N_{TS}}$. For simplicity, for the most general cases, we assume uniform probability across scenarios, that is, each scenario n has a probability $p_n = 1/N_{scen}$, where N_{scen} is the number of scenarios. In the case of scenario clustering (performed to reduce the numerical complexity[22,23,43]), we identify representative scenarios from each cluster and calculate their probability accounting for the cluster sizes.

For each scenario n, the levelized cost of methanol $LCOM_n$ accounts for both investment and operating costs. The weighted sum of the scenario objective functions ($LCOM_n$) is minimized subject to equality and inequality constraints:

$$\begin{aligned} \min_{\boldsymbol{d},\,\boldsymbol{s}} \quad & \left(\sum_{n=1}^{N_{scen}} p_n \cdot \mathrm{LCOM}_n(\boldsymbol{d}, \boldsymbol{s}_n(\boldsymbol{c}_n)) \right) \\ s.t. \quad & \\ & h_n(\boldsymbol{d}, \boldsymbol{s}_n(\boldsymbol{c}_n)) = 0 \quad n = 1,\ldots,N_{scen} \\ & g_n(\boldsymbol{d}, \boldsymbol{s}_n(\boldsymbol{c}_n)) \leq 0 \quad n = 1,\ldots,N_{scen}, \end{aligned} \tag{OP1}$$

where $\boldsymbol{d} \in \mathbb{R}^{N_{\text{design var}}}$ are the first-stage variables (design) and $\boldsymbol{s} \in \mathbb{R}^{N_{scen} \times N_{\text{scheduling var}} \times N_{TS}}$ the accumulated second-stage variables (scheduling). Accordingly, $N_{\text{design var}}$ is the number of design variables and $N_{\text{scheduling var}}$ the number of distinct scheduling variables for each scenario instance.

The considered PtMeOH model is a MINLP due to the presence of integer decision variables as well as nonlinearities in the process unit efficiencies and cost correlations (Section 3). This model is particularly challenging to solve when used in S-CDS problems, especially for long and finely discretized scheduling horizons and high scenario numbers.

Depending on the considered case study (Section 3), the original S-CDS problem (OP1) is simplified. For instance, when only the process design is optimized, steady-state operation for the scheduling variables $\boldsymbol{s}_n$ is assumed, thus reducing the complexity of the original S-CDS problem significantly, since the number of optimization variables does not scale with N_{TS}. When only the stochastic scheduling is optimized, the process design is fixed. This reduces the problem complexity and also allows solving every instance of the stochastic problem independently.

To benchmark these results, we solve both the original and a reduced S-CDS problem. The reduced S-CDS problem is obtained by applying a complexity reduction technique that combines feature-based scenario clustering and selective DoF reduction[23] (see Section S1 in Supporting Information for additional details). To sufficiently represent the original scenario space, we consider 15 scenario clusters, that is, ca. 30% of the original scenario space. Further, after fixing the design obtained in the reduced S-CDS problem, we solve a stochastic scheduling problem being interested in the objective function in the original scenario and DoF spaces. As the objective function value of the original S-CDS problem is worse than the one obtained through the reduced S-CDS problem (the optimizer could not find the global optimum or a better local optimum within the considered computational time limit due to the significantly higher numerical complexity), we do not report these results.

2.2 | Statistical analysis

To analyze the complex relationship among the process design variables and the objective function, we carry out a statistical analysis based on the results obtained by solving stochastic scheduling problems for several process designs. In particular, the process designs have been identified via latin hypercube sampling (LHS), a frequently used sampling approach that allows covering multi-dimensional design spaces with relatively low numbers of samples.[48] For these samples, a correlation analysis is performed by calculating distance correlation coefficients,[49] which can capture nonlinear correlation trends for single variables and their combinations.

The correlation direction is estimated via the sign of the Spearman coefficient between single design variables and the objective function. Nonetheless, given the nonlinear, not-strictly monotonic relationship between the design variables and the objective function, the correlation coefficients and directions represent an average trend over the considered design variable range rather than an absolute indication.

2.3 | Implementation

A Matlab script calls GAMS to solve the implemented deterministic equivalent of the two-stage stochastic programming problems with BARON 23.6.22[50] to global optimality as in our previous work.[23] Moreover, the data processing, scenario clustering, DoF reduction, and data exchange file generation are performed in Matlab before solving the optimization problems in GAMS. Also, the stochastic scheduling problems are solved in parallel by splitting the problem into four smaller subproblems to reduce the numerical complexity; the optimization results are combined afterward.

A relative optimality tolerance and a CPU time limit were set to 2% and 6 h, respectively, for most optimization runs. Global optimality was achieved for most optimal design and optimal scheduling problems within this CPU time. In contrast, global optimality was not achieved for the reduced S-CDS optimization problem within the CPU time limit despite setting a higher optimality tolerance (5%) and CPU time limit (12 h). For the cases where global optimality was not achieved within the CPU time limit, the locally optimal solution found by BARON was considered.

The statistical analysis is also performed in Matlab.

3 | PROCESS MODEL AND CASE STUDIES

A grid-connected Power-to-Methanol process with intermediate storage is considered and modeled as in our previous work.[23] In particular, the PtMeOH process is composed of a PEM water electrolysis (PEM-WE) unit, a hydrogen compression unit, a methanol synthesis (MeOH) unit, as well as a Li-based battery and pressurized vessel for hydrogen storage.

In the considered process, pure hydrogen is produced by the PEM-WE unit at 40 bar and then compressed to reach the pressure inside the hydrogen storage, ranging from 75 bar to 140 bar, in a single compression stage. The hydrogen taken from the hydrogen storage is then mixed with a pure CO_2 stream, which is pressurized from 1 bar to 75 bar in the methanol synthesis plant. The CO_2-H_2 mixture is then converted into methanol in a two-stage catalytic reactor with intermediate product removal,[8] which is then purified via distillation. The methanol synthesis reactor is operated at ca. 75 bar, a pressure in the typical operating range (50-100 bar[51]) that generally provides a good trade-off between investment cost and reactant conversion. Moreover, some works suggest that lower methanol synthesis pressures, for example, 50 bar[52] and 65 bar,[53] are more suitable. These differences in the optimal operating pressure are most likely due to the fact that it depends on the considered process units and configuration, catalyst, modeling assumptions, and boundaries. However, identifying the optimal operating pressure for the considered methanol synthesis process was beyond the scope of this work.

The considered model is quasi-steady-state, that is, modeled in discrete time, due to the fast process dynamics compared to the considered time discretization (hourly).[3,54,55] The model includes nonlinearities due to process unit efficiency and cost correlations as well as integer variables, for example, the electrolysis unit size and the variables to enforce part-load operating constraints, thus resulting in an MINLP problem.

The levelized cost of methanol (LCOM) is optimized with respect to design and scheduling variables. The considered process design variables are the sizes of the process units, namely, the battery, electrolyzer, hydrogen storage, and methanol synthesis plant, and the maximum pressure that can be reached within the hydrogen storage. These design variables directly affect the investment costs of each process unit and enable investigation of trade-offs between process unit oversizing and intermediate storage needs (see Section S2 in Supporting Information for more details on the economic assumptions). A summary of the considered design variables and their respective bounds is displayed in Table 1. The scheduling variables, that is, the power and mass flow rates (in an aggregate level) of the process units that directly affect the operation of the PtMeOH process are defined accordingly (for further details, refer to our previous work[23]). Also, a fixed yearly methanol production rate of 50 kt is considered to enable the comparison among the case studies. This plant size is assumed to be representative of PtMeOH plants in the short-term future, as it requires an electrolysis unit with a nominal size ranging between 50 MW and 100 MW. Further, note that the chosen bounds and assumptions always ensure problem feasibility.

To investigate how sensitive the LCOM of grid-connected PtMeOH processes is to optimal design or scheduling when accounting for uncertainty of scenario realization and different levels of process flexibility, we considered 52 weekly scheduling scenarios with hourly discretization (day-ahead electricity price data for Germany in the year 2023[56]), and evaluated the following case studies, also summarized in Table 2:

- ***Random designs and optimal scheduling—Flexible: No unit***: 100 process designs are generated via LHS within the design variable bounds (see Table 1) to explore the solution space. These process designs are then fixed in the optimization problems, thus defining the operating constraints and investment cost of the process units. For these process designs, the scheduling of the process units is optimized to meet the yearly methanol production target (50 kt) for each scenario instance. However, for each scenario instance, steady-state operation is assumed for the PEM-WE and methanol synthesis units within the scheduling horizon. In this simplified case that does not allow any flexible operation, the generated design values of the battery, compression unit, and the hydrogen storage are discarded: the hydrogen compression unit is sized to reach 75 bar (the operating pressure of the methanol production plant[8]), and the battery and hydrogen storage are removed from the model, since they cannot be properly exploited given the enforced operating strategy.
- ***Random designs and optimal scheduling—Flexible: Battery***: For the 100 generated process designs, the scheduling of the process units is optimized assuming steady-state operation only for the PEM-WE and methanol synthesis units. In contrast, the battery can be operated flexibly. While the battery size is now determined as part of the generated random designs, the design

TABLE 1 Design variables of the optimization problem for the grid-connected case study with their upper and lower bounds.

Unit	Variable name	Variable description	Lower bound	Upper bound
Battery	Battery	Energy capacity	5 MWh	150 MWh
PEM-WE	Modules	Number of electrolysis modules	25	35
H_2 compression	Pressure ratio	Maximum pressure ratio	1.88	3.50
H_2 storage	Volume	Volume of the vessel	50 m^3	1000 m^3
MeOH plant	H_2 flow	Nominal H_2 flow rate for the methanol synthesis plant	1.18 t/h	1.60 t/h

TABLE 2 Summary of the case studies investigated for the stochastic optimization of a grid-connected Power-to-Methanol process with intermediate storage. Note that, when the process design is not optimized, a generated process design is fixed and only optimal stochastic scheduling is performed.

		Scheduling optimization		
	Design optimization	Battery	PEM-WE	MeOH
Random designs and optimal scheduling—Flexible: No unit	No*	—	Steady state	Steady state
Random designs and optimal scheduling—Flexible: Battery	No**	Flexible	Steady state	Steady state
Random designs and optimal scheduling—Flexible: Battery & PEM-WE	No	Flexible	Flexible	Steady state
Random designs and optimal scheduling—Flexible: Battery, PEM-WE, & MeOH	No	Flexible	Flexible	Flexible
Optimal design and scheduling—Flexible: No unit	Yes*	—	Steady state	Steady state
Optimal design and scheduling—Flexible: Battery	Yes**	Flexible	Steady state	Steady state
Optimal design and scheduling—Flexible: Battery & PEM-WE	Yes	Flexible	Flexible	Steady state
Optimal design and scheduling—Flexible: Battery, PEM-WE, & MeOH	Yes	Flexible	Flexible	Flexible

*Neither battery nor intermediate hydrogen storage are considered.
**No intermediate hydrogen storage is considered.

values for the compression unit and the hydrogen storage are discarded, as in the previous case: the hydrogen compression unit is sized to reach 75 bar and the hydrogen storage is removed from the model, since it cannot be exploited given the enforced operating strategy.

- ***Random designs and optimal scheduling—Flexible: Battery & PEM-WE***: For the 100 generated process designs, the scheduling of the process units is optimized assuming steady-state operation of only the methanol synthesis unit, thus meaning the battery and the electrolyzer can be operated flexibly.
- ***Random designs and optimal scheduling—Flexible: Battery, PEM-WE, & MeOH***: For the 100 process designs generated via LHS, all process units can be operated flexibly, and their scheduling is optimized.
- ***Optimal design and scheduling—Flexible: No unit***: The PtMeOH process design is optimized while simultaneously optimizing the process scheduling. Therefore, the process design is decided by the optimizer and is not preliminarily fixed. For this case study, steady-state operation of the PEM-WE and methanol synthesis units is considered. No battery and intermediate hydrogen storage are considered.
- ***Optimal design and scheduling—Flexible: Battery***: The PtMeOH process design is optimized while considering steady-state operation only of the PEM-WE and methanol synthesis units and no intermediate hydrogen storage. The battery can be operated flexibly, and its scheduling is optimized.
- ***Optimal design and scheduling—Flexible: Battery & PEM-WE***: The PtMeOH process design is optimized while considering steady-state operation only of the methanol synthesis unit. In contrast, the other process units can be operated flexibly, and their scheduling is optimized.
- ***Optimal design and scheduling—Flexible: Battery, PEM-WE, & MeOH***: Both the design and scheduling of all process units are optimized. Moreover, all process units can be operated flexibly. To ensure numerical tractability, we solve an approximated version of the original S-CDS problem (OP1) by applying feature-based scenario clustering (15 scenario clusters) and selective DoF reduction (see Section S1 in Supporting Information). The resulting process design is then fixed to solve a stochastic scheduling problem in the original scenario and DoF spaces, so that the objective function value can be compared with those from the other case studies.

4 | RESULTS AND DISCUSSION

In the following sections, we first evaluate how optimal design and scheduling affect the methanol production cost. The relationship between the considered designs and the objective function is then analyzed to identify data correlation and the sensitivity of the objective function to the design variables. Finally, we further discuss the results of the stochastic combined design and scheduling optimization problems.

4.1 | Optimal design vs. scheduling

The LCOMs obtained for the 100 randomly generated designs show different values and data distributions depending on which units can be operated flexibly when scheduling is optimized (Figure 1). In particular, the average LCOM values decrease and the data distribution skewness increases when the hydrogen storage is used and the key process units, that is, electrolysis and methanol synthesis units, are operated flexibly.

When assuming steady-state operation of all (or some) process units for the 100 random designs, the LCOM ranges are quite wide: 1.46-1.52 € kg^{-1}, 1.46-1.54 € kg^{-1}, and 1.44-1.54 € kg^{-1} (three violin plots on the left in Figure 1, respectively). As expected, these results indicate that optimal design plays a significant role in reducing the production cost (black, green, and cyan markers in Figure 1).

When the electrolysis and methanol synthesis units are operated in steady state, the results suggest that battery storage is not

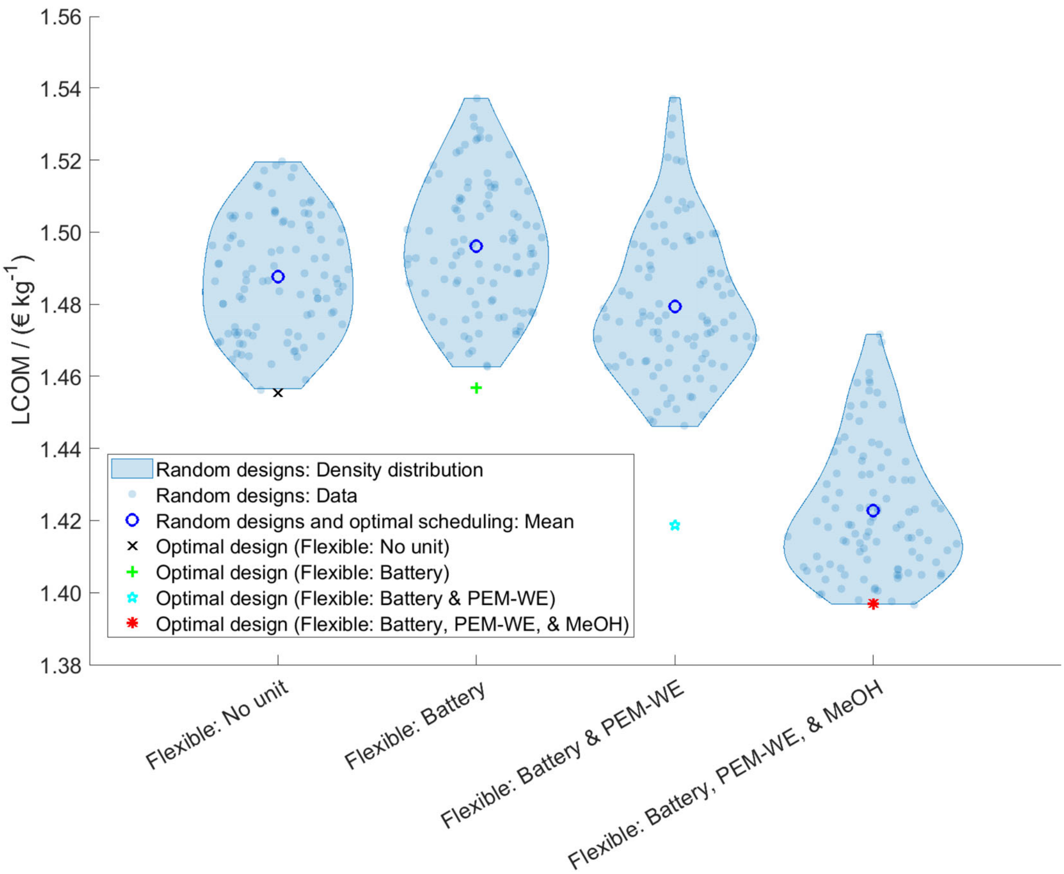

FIGURE 1 Violin plots displaying the levelized cost of methanol (LCOM) data points and their density distribution for the 100 randomly generated designs. Note that the density distribution is displayed only within the obtained LCOM ranges. The LCOMs for the "Flexible: No unit" case are calculated by assuming no battery and hydrogen storage and steady-state operation for the electrolysis and methanol synthesis units; the LCOMs for the "Flexible: Battery" case are calculated by assuming no hydrogen storage and steady-state operation for the electrolysis and methanol synthesis units; the LCOMs for the "Flexible: Battery & PEM-WE" case are calculated by considering flexible operation for the battery and the electrolysis unit and steady-state operation for the methanol synthesis unit; the LCOMs for the "Flexible: Battery, PEM-WE, & MeOH" case are calculated by assuming flexible operation of all process units. Additionally, the LCOMs of the Power-to-Methanol processes optimized with respect to the design (black, green, cyan, and red markers) are displayed; these values are not displayed in all violin plots since they were obtained for different process configurations, namely, storage technologies.

economically viable (compare the two violin plots on the left in Figure 1). In fact, the savings in the operating expenditures due to the battery are not sufficient to repay the investment expenditures under the considered economic assumptions.

When the electrolysis unit is operated flexibly differently from the methanol synthesis plant (and hydrogen storage is present), the data distribution is skewed toward lower LCOM values (compare the violin plots in the middle in Figure 1). This suggests that the use of hydrogen storage combined with the flexible operation of the PEM-WE unit reduces, on average, the methanol production cost. This is again confirmed by comparing the LCOMs obtained via optimal design: LCOM of 1.42 € kg^{-1} instead of 1.46 € kg^{-1} thanks to the possibility of exploiting price fluctuations to reduce the hydrogen production cost, and thus the LCOM.

When flexible operation of the methanol synthesis unit is enabled, the LCOMs are on average ca. 4% lower still (compare the two violin plots on the right in Figure 1). The LCOM reduction is due to the savings in the operating expenditures, which range between −1% and −12% for the considered process designs (also see Figure S.1 in Supporting Information), thus confirming the importance of flexible operation. Also, the LCOM range obtained when optimizing the scheduling for the same generated process designs is slightly lower than for the case with no methanol process flexibility: 1.40–1.47 € kg^{-1} vs. 1.44-1.54 € kg^{-1} (compare the two violin plots on the right in Figure 1). Furthermore, the LCOM data distribution is more skewed toward low LCOMs, thus meaning that several process design combinations lead to similar objective function values, as also mentioned in previous works[26,46,47] (this aspect will be investigated in more detail in Section 4.2). These results show that the enhanced process flexibility related to the methanol process operation helps mitigate economic losses caused by poor process design choices. Nonetheless, the relatively wide LCOM range highlights that making sufficiently good process design choices matters even when methanol process flexibility is enabled.

Further, the best LCOM obtained for a randomly generated process design when allowing methanol process flexibility is better than the LCOM obtained by optimizing the PtMeOH design while considering steady-state operation of the methanol synthesis unit, thus highlighting that these processes should be operated flexibly. Moreover, the average of the LCOMs in the violin plot on the right is quite close to the cyan marker that indicates the LCOM of the PtMeOH with the process design optimized when assuming steady-state operation of the methanol synthesis unit (Figure 1). This suggests that optimal scheduling (when allowing flexible operation and assuming perfect information on the scenario time series) is, on average, more important than optimal design (when assuming steady-state operation of the process units) in PtMeOH processes. This is most likely due to the high share of the operating costs on the LCOM in Power-to-X processes.[8]

Finally, the best LCOM obtained for a randomly generated process design is similar to the LCOM obtained by solving a stochastic scheduling problem by fixing the design obtained by solving the reduced S-CDS problem (the optimal stochastic scheduling results are reported in Supporting Information). Nonetheless, the wide range of LCOMs suggests that the design and scheduling should still be optimized simultaneously, especially when considering flexibility for all process units (also see Section 4.3).

4.2 | Data correlation analysis

As several process designs can lead to similar objective functions (Section 4.1), we analyze the optimization results to identify patterns among these variables. In particular, we investigate the impact of the process design variables on the LCOM.

For this analysis, we consider the results obtained by optimizing the stochastic scheduling for the 100 generated process designs, while allowing flexible operation of all process units (violin plot on the right of Figure 1). The considered data set is suitable for this correlation analysis since the design variables, that is, the only input that is varied in the solved stochastic scheduling problems, show weak-to-no cross-correlation because of the LHS (Figure S.4 in Supporting Information). The correlation analysis between the process design variables and the objective function is conducted by examining the design variables first independently and then together.

4.2.1 | Correlation between single design variables and objective function

In analyzing the distance correlation coefficients (Table 3), either weak or moderate negative correlation with the LCOM emerges across the considered design variable ranges. In particular, the sizes of the electrolysis and methanol production units exhibit the strongest effect on the methanol production cost. While intermediate storage can also contribute positively to LCOM reduction, its impact remains relatively minor compared to oversizing the electrolysis and methanol production units under the considered economic assumptions.

TABLE 3 Signed distance correlation coefficients between the design variables and the objective function.

Variable	Distance correlation	Sign
Battery	0.191	–
Modules	0.405	–
Pressure ratio	0.199	–
Volume	0.199	–
H_2 flow	0.417	–

Note: The distance correlation coefficient ranges from 0 (independent) to 1 (strongly dependent). The correlation direction indicated via the sign is estimated from the Spearman coefficient. Note that, given the nonlinear relationship between the design variables and the objective function, the displayed metrics represent only average trends over the considered design variable ranges.

These general trends are confirmed by analyzing the objective function values (LCOMs) plotted against the single design variables (Figure 2). The LCOM is quite sensitive to the electrolyzer module number and the nominal hydrogen flow rate supplied to the methanol synthesis unit. In contrast, a less sensitive behavior is experienced for the other design variables, since low and high objective function values are obtained for all design variable ranges. However, the process performance with those design variables depends on the combination of the others. A relatively low sensitivity to certain key design variables was already shown in other processes, for instance, a pressurized oxy-coal combustion process.[45]

The low sensitivity to certain design variables was further explored by fixing the sizes of the electrolysis and methanol synthesis units equal to the ones of the random design leading to the lowest objective function. In this case, the LCOM is nearly insensitive to battery and hydrogen storage sizes (Figure 3), its variation being lower than the optimization tolerance for wide variable ranges. Similar results were obtained for different maximum pressure ratios for the compression unit (see Figure S.5 in Supporting Information). This is most likely due to the high flexibility of the electrolysis and methanol plants, which can largely offset the lack or presence of storage when scheduling is optimized. Nonetheless, solving S-CDS optimization problems remains necessary because this exemplary case study cannot be generalized, and the relationship between design variable values and LCOM is not known across the entire solution space (see Section 4.2.2).

4.2.2 | Correlation between multiple design variables and objective function

Identifying clear patterns between combinations of design variables is, in general, more complicated, especially because of the problem nonlinearities and the fact that the objective function does not always have a monotonic behavior with respect to the process design variables in the considered variable ranges (Figure 2). For instance, large hydrogen storage volumes can be either economically favorable or

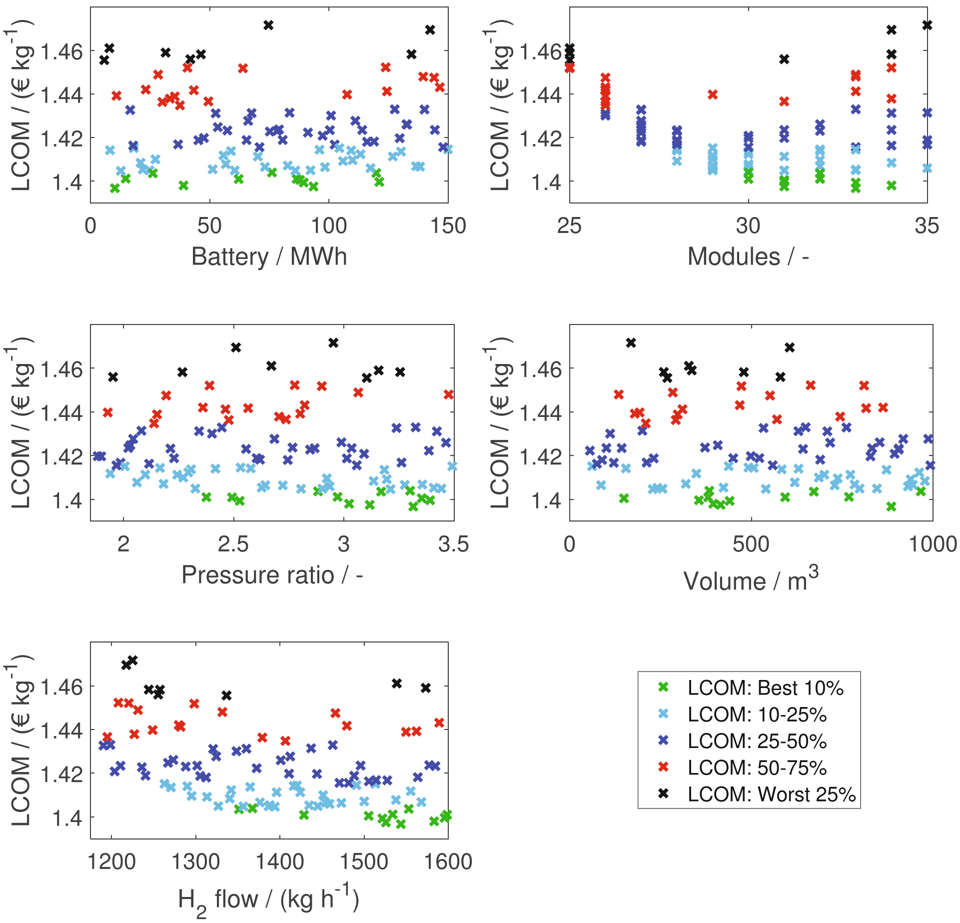

FIGURE 2 Objective function (LCOM) value obtained when optimizing the scheduling of all process units for the 100 randomly generated process designs plotted against the design values. The color of the crosses is based on the LCOM value.

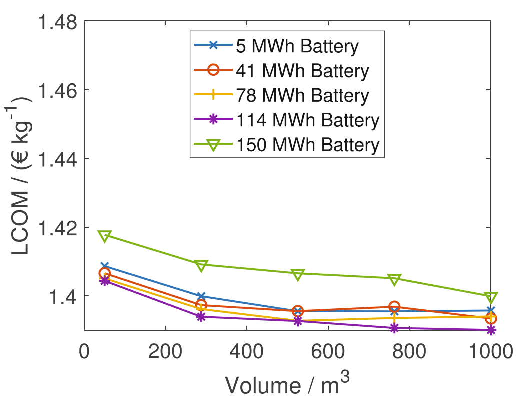

FIGURE 3 Sensitivity analysis of the objective function (LCOM) calculated by optimizing the stochastic scheduling for fixed process designs. In particular, the storage sizes were varied, while the electrolysis modules, maximum pressure ratio of the compression unit, and nominal hydrogen flow rate supplied to the methanol synthesis plant were set equal to 33, 3.5, and 1.54 t h^{-1}, respectively. For these sizes of the electrolysis and methanol synthesis units, the storage sizes only have a minor impact on the LCOM.

unfavorable based on the other design variable values. Nonetheless, a few trends can be extracted.

Increasing the number of modules of the electrolysis unit helps reducing the levelized cost of methanol (Figure 4). However, excessively oversized electrolysis units, for example, with 35 modules, can again lead to high LCOMs, most likely because of the high investment costs and the set yearly methanol production constraint (50 kt). Furthermore, installing battery or hydrogen storage of any size is beneficial when the electrolyzer is moderately oversized to enable a flexibility margin (Figure 4, top row). Similarly, relatively large storage capacities are preferred when the methanol synthesis unit is oversized. Also, an oversized methanol synthesis unit should be combined with an oversized electrolysis plant to increase the flexibilization potential further.

For the other design variable combinations, there is no clear trend. For instance, the relationship between the H_2 storage volume and the pressure ratio of the compression unit, which determines how much hydrogen can be stored within the volume, is unclear. Similarly, whether and when having both storage technologies is beneficial depends on the other design variables.

4.3 | Optimal stochastic combined design and scheduling

As previously shown, the spread of the objective function values when solving optimal stochastic scheduling problems (Figure 1) indicates that having a good process design matters. Also, the lack of clear

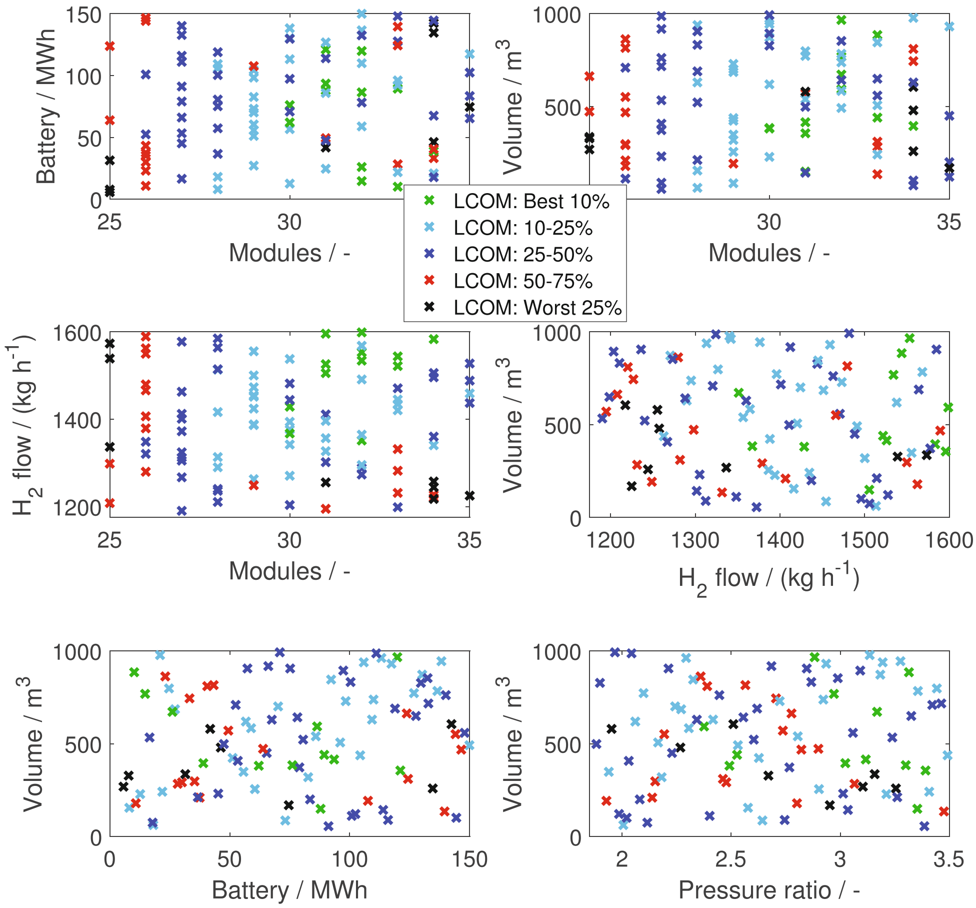

FIGURE 4 Comparison of key couples of the 100 randomly generated design variables colored according to the objective function value (LCOM) obtained when allowing scheduling of all process units. The color of the crosses is based on the LCOM value.

trends for all design variables when exploring the design space (Figure 4) highlights the need for optimizing design and scheduling simultaneously. However, these S-CDS optimization problems generally suffer from numerical intractability.

As described in Section 2, we solved a reduced S-CDS problem with 15 scenario clusters, and then fixed the resulting process design to solve an optimal stochastic scheduling problem in the original scenario and DoFs spaces (red marker in Figure 1). The reduced S-CDS problem can identify a promising design candidate (Figure S.1 in Supporting Information). This is probably due to two concurrent reasons: 1) several process designs lead to similar LCOMs when scheduling is optimized and 2) the numerical complexity reduction techniques applied to generate the reduced S-CDS problem can preserve the key characteristics of the original S-CDS problem, thus identifying good design candidates.[23]

Furthermore, the LCOM in the original scenario and DoF spaces is also close to the best objective function value obtained via stochastic scheduling for random designs: the difference is below the optimization tolerance, as it can be noticed in Figure 1. This might suggest that developing strategies to solve S-CDS optimization problems is not necessary. However, random design generation does not account for any information about the relationship between the process design and the objective function of the S-CDS problem itself. Therefore, the number of stochastic scheduling optimization problems that need to be solved before identifying a good process design is not known in advance, thus potentially requiring extremely high computational costs.

5 | CONCLUSIONS

For a grid-connected PtMeOH process with intermediate storage, we investigated the effect of optimizing the design, the scheduling, and their combination on methanol production cost under scheduling scenario uncertainty.

By solving stochastic scheduling optimization problems with perfect information on the scenario time series for randomly generated designs, we show that a significant methanol production cost reduction can be achieved by enabling flexible operation, especially of the methanol synthesis unit. Moreover, optimal scheduling by assuming flexible operation of all process units seems to be, on average, more important than optimal design performed by assuming steady-state operation of the methanol synthesis unit, since process flexibility can mitigate economic losses due to poor design choices.

The operating strategy of the methanol synthesis process affects the optimal process design. However, very different process designs lead to similar objective function values. Moreover, the objective function seems to be quite insensitive to certain design variables, for example, storage capacity, for wide variable ranges under the considered economic assumptions, thanks to the high flexibility enabled by the other process units. Also, no clear patterns in well-performing process designs were found via statistical analysis, besides the fact that oversizing the water electrolysis and methanol synthesis units seems the most relevant design choice.

These results also highlight the need for optimizing the design and scheduling simultaneously. For the cases where the numerical complexity cannot be handled within reasonable computational times, solving simpler but representative S-CDS problems can help identify well-performing process designs.

Future work might include considering other optimization variables, for example, the operating pressure of the methanol synthesis reactor, to capture additional economic trade-offs. Furthermore, the assumption of perfect information on the scenario time series could be relaxed to investigate its effect on the optimal stochastic process design. Finally, since several process design leads to similar methanol production costs, identifying an optimal design space instead of a single optimal design could provide valuable insights. Approaches like modeling-to-generate-alternatives[57] could be applied to obtain such optimal design variable ranges, which could be particularly valuable when process unit sizes are modular or standardized.

AUTHOR CONTRIBUTIONS

Simone Mucci: conceptualization; methodology; software; investigation; visualization; writing – original draft. **Dominik Bongartz:** conceptualization; methodology; supervision; funding acquisition; writing – review and editing.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflicts of interest.

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DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available in the Supporting Information of this article.

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REFERENCES

1. Zhang Q, Grossmann IE. Enterprise-wide optimization for industrial demand side management: Fundamentals, advances, and perspectives. *Chem Eng Res Des*. 2016;116:114-131. doi:10.1016/j.cherd.2016.10.006
2. Svitnič T, Sundmacher K. Renewable methanol production: Optimization-based design, scheduling and waste-heat utilization with the FluxMax approach. *Appl Energy*. 2022;326(11):120017. doi:10.1016/j.apenergy.2022.120017
3. Mucci S, Mitsos A, Bongartz D. Power-to-X processes based on PEM water electrolyzers: A review of process integration and flexible operation. *Comput Chem Eng*. 2023;175:108260. doi:10.1016/j.compchemeng.2023.108260
4. Allman A, Palys MJ, Daoutidis P. Scheduling-informed optimal design of systems with time-varying operation: A wind-powered ammonia case study. *AIChE J*. 2019;65:e16434. doi:10.1002/aic.16434
5. Schulte Beerbühl S, Fröhling M, Schultmann F. Combined scheduling and capacity planning of electricity-based ammonia production to integrate renewable energies. *Eur J Oper Res*. 2015;241(3):851-862. doi:10.1016/j.ejor.2014.08.039
6. Gorre J, Ruoss F, Karjunen H, Schaffert J, Tynjälä T. Cost benefits of optimizing hydrogen storage and methanation capacities for Power-to-Gas plants in dynamic operation. *Appl Energy*. 2020;257:113967. doi:10.1016/j.apenergy.2019.113967
7. Mößle P, Herrmannsdörfer T, Welzl M, Brüggemann D, Danzer MA. Economic optimization for the dynamic operation of a grid connected and battery-supported electrolyzer. *Int J Hydrogen Energy*. 2025;100:749-759. doi:10.1016/j.ijhydene.2024.12.216
8. Mucci S, Mitsos A, Bongartz D. Cost-optimal power-to-methanol: Flexible operation or intermediate storage? *J Energy Storage*. 2023;72:108614. doi:10.1016/j.est.2023.108614
9. Chen C, Yang A. Power-to-methanol: The role of process flexibility in the integration of variable renewable energy into chemical production. *Energy Convers Manag*. 2021;228:113673. doi:10.1016/j.enconman.2020.113673
10. Chen C, Yang A, Bañares-Alcántara R. Renewable methanol production: Understanding the interplay between storage sizing, renewable mix and dispatchable energy price. *Adv Appl Energy*. 2021;2:100021. doi:10.1016/j.adapen.2021.100021
11. Akram N, Kienberger T. A combined investment and operational optimization approach for power-to-methanol plants. *Energies*. 2024;17(23):5937. doi:10.3390/en17235937
12. Maggi A, Bremer J, Sundmacher K. Multi-period optimization for the design and operation of a flexible power-to-methanol process. *Chem Eng Sci*. 2023;281:119202. doi:10.1016/j.ces.2023.119202
13. Taslimi M, Khosravi A. Flexibility and profitability in power-to-methanol plants: Integrating storage solutions and reserve market participation. *Energy*. 2025;327:136438. doi:10.1016/j.energy.2025.136438
14. Raheli E, Werner Y, Kazempour J. A conic model for electrolyzer scheduling. *Comput Chem Eng*. 2023;179:108450. doi:10.1016/j.compchemeng.2023.108450
15. Germscheid SH, Mitsos A, Dahmen M. Demand response potential of industrial processes considering uncertain short-term electricity prices. *AIChE J*. 2022;68(11):e17828. doi:10.1002/aic.17828
16. Martín M. Methodology for solar and wind energy chemical storage facilities design under uncertainty: Methanol production from CO2 and hydrogen. *Comput Chem Eng*. 2016;92:43-54. doi:10.1016/j.compchemeng.2016.05.001
17. Lee J, Ryu KH, Lee JH. Optimal design and evaluation of electrochemical CO_2 reduction system with renewable energy generation using two-stage stochastic programming. *J CO2 Util*. 2022;61:102026. doi:10.1016/j.jcou.2022.102026
18. Han D, Lee JH. Two-stage stochastic programming formulation for optimal design and operation of multi-microgrid system using data-based modeling of renewable energy sources. *Appl Energy*. 2021;291:116830. doi:10.1016/j.apenergy.2021.116830
19. Langiu M, Dahmen M, Mitsos A. Simultaneous optimization of design and operation of an air-cooled geothermal ORC under consideration of multiple operating points. *Comput Chem Eng*. 2022;161:107745. doi:10.1016/j.compchemeng.2022.107745

20. Jürgens B, Seele H, Schricker H, Reinert C, von der Assen N. Decision-Based vs. Distribution-Driven Clustering for Stochastic Energy System Design Optimization. ArXiv, 7. 2024. http://arxiv.org/abs/2407.11457
21. Akülker H, Alakent B, Aydin E. A two-stage stochastic MINLP model to design and operate a multi-energy microgrid by addressing carbon emission regulatory policies uncertainty. *Comput Chem Eng*. 2025;203:109351. doi:10.1016/j.compchemeng.2025.109351
22. Teichgraeber H, Brandt AR. Optimal design of an electricity-intensive industrial facility subject to electricity price uncertainty: Stochastic optimization and scenario reduction. *Chem Eng Res Des*. 2020;163:204-216. doi:10.1016/j.cherd.2020.08.022
23. Mucci S, Bongartz D. Feature-based scenario clustering and selective degrees of freedom reduction for two-stage stochastic optimization of power-to-methanol. *Chem Eng Res Des*. 2025;223:311-330. doi:10.1016/j.cherd.2025.09.046
24. Yunt M, Chachuat B, Mitsos A, Barton PI. Designing man-portable power generation systems for varying power demand. *AIChE J*. 2008;54(5):1254-1269. doi:10.1002/aic.11442
25. Birge JR, Louveaux F. *Introduction to Stochastic Optimization*. Springer; 2011. doi:10.1007/978-1-4614-0237-4
26. Conejo AJ, Carrión M, Morales JM. Stochastic programming fundamentals. *International Series in Operations Research and Management Science*. Vol 153. Springer; 2010:27-62. doi:10.1007/978-1-4419-7421-1˙2
27. Li C, Grossmann IE. A review of stochastic programming methods for optimization of process systems under uncertainty. *Front Chem Eng*. 2021;2:1. doi:10.3389/fceng.2020.622241
28. Mitsos A, Asprion N, Floudas CA, et al. Challenges in process optimization for new feedstocks and energy sources. *Comput Chem Eng*. 2018;113:209-221. doi:10.1016/j.compchemeng.2018.03.013
29. Roald LA, Pozo D, Papavasiliou A, Molzahn DK, Kazempour J, Conejo A. Power systems optimization under uncertainty: A review of methods and applications. *Electr Power Syst Res*. 2023;214:108725. doi:10.1016/j.epsr.2022.108725
30. Li C, Bernal DE, Furman KC, Duran MA, Grossmann IE. Sample average approximation for stochastic nonconvex mixed integer nonlinear programming via outer-approximation. *Optim Eng*. 2021;22:1245-1273. doi:10.1007/s11081-020-09563-2
31. Torres JJ, Li C, Apap RM, Grossmann IE. A review on the performance of linear and mixed integer two-stage stochastic programming software. *Algorithms*. 2022;15:103. doi:10.3390/a15040103
32. Li X, Tomasgard A, Barton PI. Nonconvex generalized benders decomposition for stochastic separable mixed-integer nonlinear programs. *J Optim Theory Appl*. 2011;151:425-454. doi:10.1007/s10957-011-9888-1
33. Rahmaniani R, Crainic TG, Gendreau M, Rei W. Accelerating the benders decomposition method: Application to stochastic network design problems. *SIAM J Optim*. 2018;28(1):875-903. doi:10.1137/17M1128204
34. García-Muñoz F, Dávila S, Quezada F. A benders decomposition approach for solving a two-stage local energy market problem under uncertainty. *Appl Energy*. 2023;329:120226. doi:10.1016/j.apenergy.2022.120226
35. Langiu M, Dahmen M, Bongartz D, Mitsos A. MUSE-BB: A decomposition algorithm for nonconvex two-stage problems using strong multisection branching. *J Glob Optim*. 2025;92:837-888. doi:10.1007/s10898-025-01489-2
36. Zhang H, Grossmann IE, Tomasgard A. Decomposition methods for multi-horizon stochastic programming. *Comput Manag Sci*. 2024;21:1-24. doi:10.1007/s10287-024-00509-y
37. Liu P, Pistikopoulos EN, Li Z. Decomposition based stochastic programming approach for polygeneration energy systems design under uncertainty. *Ind Eng Chem Res*. 2010;49:3295-3305. doi:10.1021/ie901490g
38. Heo T, Mallapragada DS, Macdonald R. A decomposition algorithm using multiple linear approximations to solve integrated design and scheduling optimization frameworks – case study of nuclear based co-production of electricity and hydrogen. *Computers Chem Eng*. 2025;202:109213. doi:10.1016/j.compchemeng.2025.109213
39. Baumgärtner N, Temme F, Hennen M, Bahl B, Hollermann D, Bardow A. RiSES^4 rigorous synthesis of energy supply systems with seasonal storage by relaxation and time-series aggregation to typical periods. *Proceedings of ECOS 2019 32nd International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems*. Silesian University of Technology; 2019:263-274.
40. Wang Y, Volkme M, Hagedorn DF, Reinert C, von der Assen N. RiNSES^4: Rigorous nonlinear synthesis of energy systems for seasonal energy supply and storage. Proceedings of the 10th International Conference on Foundations of Computer-Aided Process Design FOCAPD 2024. Vol 3; 2024:604-611. doi:10.69997/sct.105466
41. Hoffmann M, Kotzur L, Stolten D, Robinius M. A review on time series aggregation methods for energy system models. *Energies*. 2020;13:641. doi:10.3390/en13030641
42. Bahl B, Söhler T, Hennen M, Bardow A. Typical periods for two-stage synthesis by time-series aggregation with bounded error in objective function. *Front Energy Res*. 2018;5:35. doi:10.3389/fenrg.2017.00035
43. Kotzur L, Markewitz P, Robinius M, Stolten D. Impact of different time series aggregation methods on optimal energy system design. *Renew Energy*. 2018;117:474-487. doi:10.1016/j.renene.2017.10.017
44. Schäfer P, Schweidtmann AM, Lenz PH, Markgraf HM, Mitsos A. Wavelet-based grid-adaptation for nonlinear scheduling subject to time-variable electricity prices. *Comput Chem Eng*. 2020;132:106598. doi:10.1016/j.compchemeng.2019.106598
45. Zebian H, Mitsos A. Pressurized oxy-coal combustion: Ideally flexible to uncertainties. *Energy*. 2013;57:513-526. doi:10.1016/j.energy.2013.05.026
46. Baumgärtner N, Bahl B, Hennen M, Bardow A. RiSES^3: Rigorous synthesis of energy supply and storage systems via time-series relaxation and aggregation. *Comput Chem Eng*. 2019;127:127-139. doi:10.1016/j.compchemeng.2019.02.006
47. Merrick JH. On representation of temporal variability in electricity capacity planning models. *Energy Econ*. 2016;59:261-274. doi:10.1016/j.eneco.2016.08.001
48. Deng X, Kang L, Lin CD. Design of experiments for emulations: A selective review from a modeling perspective arXiv. 2025. doi:10.48550/arXiv.2505.09596
49. Liu S. Distance Correlation Function [Online]. Accessed September 24, 2025. https://www.mathworks.com/matlabcentral/fileexchange/39905-distance-correlation
50. Khajavirad A, Sahinidis NV. A hybrid LP/NLP paradigm for global optimization relaxations. *Math Program Comput*. 2018;10:383-421. doi:10.1007/s12532-018-0138-5
51. Mbatha S, Cui X, Panah PG, et al. Comparative evaluation of the power-to-methanol process configurations and assessment of process flexibility. *Energy Advances*. 2024;3:2245-2270. doi:10.1039/d4ya00433g
52. da Silva JL, Santana HS, Hodapp MJ. Numerical evaluation of methanol synthesis in catalytic wall-coated microreactors: Scale-up and performance analysis of planar and monolithic designs. *Frontiers in Chemical Engineering*. 2024;6:8. doi:10.3389/fceng.2024.1440657
53. Vaquerizo L, Kiss AA. Thermally self-sufficient process for cleaner production of e-methanol by CO2 hydrogenation. *J Clean Prod*. 2023;433:139845. doi:10.1016/j.jclepro.2023.139845
54. Kopp M, Coleman D, Stiller C, Scheffer K, Aichinger J, Scheppat B. Energiepark Mainz: Technical and economic analysis of the worldwide

largest power-to-gas plant with PEM electrolysis. *Int J Hydrogen Energy*. 2017;42:13311-13320. doi:10.1016/j.ijhydene.2016.12.145

55. BSE Engineering. Power-to-Methanol at Small-Scale: FlexMethanol 10&20 MW Module [Online]. Accessed August 08, 2025. http://www.wfbe.de/BSE-Flyer-BASF-DB_web.pdf
56. ENTSO-E Transparency Platform. Electricity Price Profiles [Online]. Accessed September 30, 2024. 2024 https://transparency.entsoe.eu/dashboard/show
57. Neumann F, Brown T. The near-optimal feasible space of a renewable power system model. *Electr Power Syst Res*. 2021;190:106690. doi:10.1016/j.epsr.2020.106690

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