

# Decomposition Strategy for the Global Optimization of Flexible Energy Polygeneration Systems

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*The optimal design and operation of flexible energy polygeneration systems using coal and biomass to coproduce power, liquid fuels, and chemicals are investigated. This problem is formulated as a multiperiod optimization problem, which is a potentially large-scale nonconvex mixed-integer nonlinear program (MINLP) and cannot be solved to global optimality by state-of-the-art global optimization solvers, such as BARON, within a reasonable time. A duality-based decomposition method, which can exploit the special structure of this problem, is applied. In this work, the decomposition method is enhanced by the introduction of additional dual information for faster convergence. The enhanced decomposition algorithm (EDA) guarantees to find an  $\epsilon$ -optimal solution in a finite time. The case study results show that the EDA achieves much faster convergence than both BARON and the original decomposition algorithm, and it solved the large-scale nonconvex MINLPs to  $\epsilon$ -optimality in practical times.*

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## Introduction

Coal and biomass are promising long-term energy sources due to their abundant reserves and wide distribution across the world.<sup>1–3</sup> In recent years, coal- and biomass-based polygeneration processes with multiple products such as electricity, liquid fuels, and chemicals have been proposed as an alternative to the current oil-based process.<sup>4–9</sup> Compared to several coal-based single-product processes with high-energy efficiency and low carbon dioxide (CO<sub>2</sub>) emissions, such as integrated gasification combined cycle and coal-to-liquids processes with carbon capture and sequestration,<sup>10–14</sup> polygeneration processes have some additional advantages, as economic risks can be reduced by diversification of product portfolios, and potentially higher profits can be achieved by optimization of the portfolios.<sup>8,9</sup> In addition, higher energy efficiency may also be attained in polygeneration processes through tight heat integration of the system.<sup>4</sup>

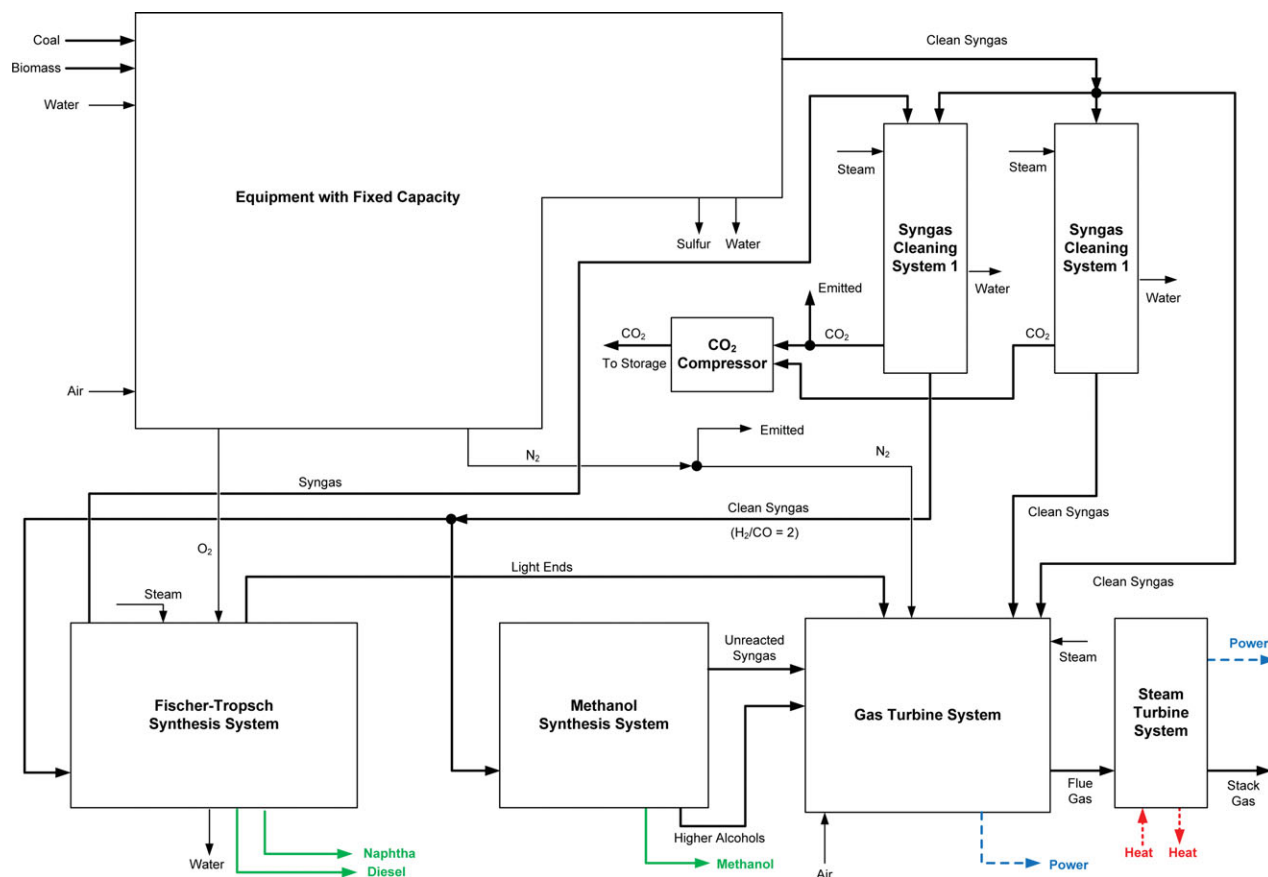
The concept of the flexible polygeneration system, which allows variable product mixes during the project lifetime according to market prices and demands, was proposed in previous work by the authors.<sup>9</sup> Unlike static plants that attempt

to maintain operations at their maximum capacities, a flexible polygeneration plant alters the production rates of individual products in response to changing market conditions by oversizing equipment. In other words, the flexible plant focuses on power generation during peak times when the power price is high and is switched to liquids production during off-peak times, when the power price drops significantly. It has been demonstrated that for coal- and biomass-based systems, flexible polygeneration plants generally achieve higher net present values (NPVS) than static, single-product or polygeneration plants, as the increased revenue provided by operational flexibility surpasses the cost of larger capital investments.<sup>9</sup>

In the design of flexible polygeneration systems, the optimal trade-off between operational flexibility and capital cost needs to be determined. In our previous work,<sup>9</sup> a multiperiod optimization problem, which is a potentially large-scale nonconvex mixed-integer nonlinear programming (MINLP) problem, was formulated to solve such a complicated design and operation problem, and a state-of-the-art global optimization solver, BARON,<sup>15</sup> was used to obtain the global optimum. However, BARON required a considerable amount of CPU time to solve the problem, and the solution time increases exponentially with the number of scenarios. Therefore, more efficient algorithms need to be developed to solve this multiperiod optimization problem for large numbers of scenarios.

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**Figure 2. Illustration of aggregate equipment.**

[Color figure can be viewed in the Online issue, which is available at [wileyonlinelibrary.com](http://wileyonlinelibrary.com).]

the CO<sub>2</sub> emission rate. For simplicity, a constant efficiency is assumed for all equipment during the whole project life time, which is considered as the best case analysis. In real applications, the efficiency of equipment may drop at their off-design modes. Addressing equipment efficiency correlations (which are typically highly nonlinear equations) in the model will be a topic of future work after more advanced optimization algorithms are developed. The mathematical model in this work is reformulated from the flexible poly-generation model in our prior work.<sup>9</sup> The major reformulations, including the application of aggregate equipment and discrete equipment capacities, were implemented in the capital cost calculations in the original model and will be discussed in the remaining part of this section.

### Aggregate equipment

The concept of “aggregate equipment” is introduced in this model to simplify the economic analysis and reduce the complexity of the model. Aggregate equipment is a set of equipment within the same subsystem that follow a similar scaling-up relationship. In capital cost calculations, aggregate equipment can be treated as a single unit with a scaling-up factor equal to the weighted average of all equipment in the group. Therefore, the number of units in the economic analysis is reduced from 30 to seven sets of aggregate equipment whose capacities need to be determined, including syngas cleaning system 1 (for the liquids production), syngas cleaning system 2 (for the power production), the CO<sub>2</sub> compressor, the Fischer–Tropsch synthesis system, the methanol synthesis system, the gas turbine system, and the steam turbine

system. These are illustrated in Figure 2, where each set of aggregate equipment is placed in the same position as Figure 1. Optimization of equipment capacities is, therefore, based on the seven sets of aggregate equipment instead of the 30 individual pieces of equipment.

In this work, the dry mass capacity of the gasifier is fixed to 1042 ton/h or 7.815 Mt/yr on the basis of industrial experience of BP engineers<sup>23</sup> (Mt = million tons). Therefore, the accessory equipment of the gasifier (including the radiant cooler and the convective cooler) and upstream and downstream equipment whose capacities are determined by the gasifier (such as the ASU, the carbonyl sulfide (COS) hydrolysis reactor, Selexol Unit 1, and the Claus plant) also have fixed capacities. All equipment with fixed capacities are grouped into one set of aggregate equipment (as shown in Figure 2 with the same position as in Figure 1), whose capacity is a specified parameter in the optimization model.

Note that the concept of aggregate equipment is only applied to the economic analysis, and all mass and energy balances are still based on individual equipment and are the same as those in our prior model.<sup>9</sup>

### Capital costs

The other major model reformulation is to change the equipment capacity variables in the optimization formulation from continuous variables to discrete variables. There are two reasons for this reformulation: (1) The current version of the decomposition method is developed for problems whose first stage decision variables (or design decision variables) contain only integer variables. Equipment capacities,

which are design decision variables, need to be discretized to fit the framework of the decomposition method. A direction for future research is to develop new versions of the decomposition method that can also handle continuous design decision variables. (2) In real applications, only a limited number of sizes are available in the market for many kinds of equipment, including gas turbines and steam turbines. It is, therefore, more reasonable to model these equipment capacities as discrete choices instead of continuous variables.

The capacity of a set of aggregate equipment  $w$  is now expressed as

$$E_w = \sum_{v=1}^d \bar{E}_{w,v} y_{w,v}, \quad \forall w \in \{1, \dots, e\} \quad (1)$$

where  $\bar{E}_{w,v}$  is the  $v$ th choice for the capacity of the set of equipment  $w$ , which is a specified parameter;  $y_{w,v}$  is a binary variable that determines whether the  $v$ th choice for the capacity of the set of equipment  $w$  is selected or not.  $d$  is the number of all choices for each set of equipment;  $e$  is the number of sets of aggregate equipment without fixed capacity, which is equal to 7. In this work, to obtain sufficiently accurate economic analysis results while keeping the optimization problem tractable for the DA,  $d$  is set to be 10.

Only one choice for capacity can be selected for each set of equipment; therefore, the following relationship holds

$$\sum_{v=1}^d y_{w,v} = 1, \quad \forall w \in \{1, \dots, e\} \quad (2)$$

The flow rate through each set of equipment is limited by its capacity, hence

$$F_{w,h} \leq E_w, \quad \forall w \in \{1, \dots, e\}, \quad \forall h \in \{1, \dots, s\} \quad (3)$$

where  $F_{w,h}$  is the input (or output) flow rate of the set of equipment  $w$  in scenario  $h$ .  $s$  is the number of scenarios, which is a given number.

The capital cost of a set of equipment  $w$  is given by

$$C_w = \sum_{v=1}^d \bar{C}_{w,v} y_{w,v}, \quad \forall w \in \{1, \dots, e\} \quad (4)$$

where  $\bar{C}_{w,v}$  is the  $v$ th choice for the capital cost of the set of equipment  $w$ , which is a specified parameter.

The total capital investment for the plant is given by

$$\text{Cap} = \sum_{w=1}^e C_w + \bar{C}_f \quad (5)$$

where  $\bar{C}_f$  is the total capital cost of equipment with fixed capacity, which is a specified parameter. In this work,  $\bar{C}_f = 2978$  million dollars.

The NPV is denoted by

$$\begin{aligned} \text{NPV} = & \text{Cap} \left[ -1 + \frac{R_{\text{tax}}}{t_{\text{dp}}} \frac{1}{r} \left( 1 - \frac{1}{(1+r)^{t_{\text{dp}}}} \right) \right] \\ & + \sum_{h=1}^s \text{Occu}_h \text{Pro}_{\text{net},h} \frac{1}{r} \left( 1 - \frac{1}{(1+r)^{t_{\text{lf}}}} \right) \end{aligned} \quad (6)$$

where  $\text{Pro}_{\text{net},h}$  is the annualized net profit in scenario  $h$ .  $\text{Occu}_h$  is the fraction of occurrence of scenario  $h$ ,  $R_{\text{tax}}$  is the tax rate (including both federal and state taxes),  $r$  is the annual discount rate,  $t_{\text{dp}}$  is the depreciation time of the project, and  $t_{\text{lf}}$  is the lifetime of the project, which are the specified parameters. In this study,  $R_{\text{tax}} = 40\%$ ,<sup>12,13</sup>  $r = 12\%$ ,<sup>12,13</sup>  $t_{\text{dp}} = 10$  yr,<sup>24</sup> and  $t_{\text{lf}} = 30$  yr.

For the ease of computation, the objective of this model is selected to be the scaled NPV, which is given as follows

$$\begin{aligned} \text{NPV}_{\text{scale}} &= \frac{\text{NPV}}{\frac{1}{r} \left( 1 - \frac{1}{(1+r)^{t_{\text{lf}}}} \right)} \\ &= \sum_{h=1}^s \text{Occu}_h \text{Pro}_{\text{net},h} + \text{Cap} \frac{-1 + \frac{R_{\text{tax}}}{t_{\text{dp}}} \frac{1}{r} \left( 1 - \frac{1}{(1+r)^{t_{\text{dp}}}} \right)}{\frac{1}{r} \left( 1 - \frac{1}{(1+r)^{t_{\text{lf}}}} \right)} \end{aligned} \quad (7)$$

The binary variables  $y_{w,v}$  ( $\forall w \in \{1, \dots, e\}, \forall v \in \{1, \dots, d\}$ ) are the only design decision variables in this model. All other design variables, including  $E_w$ ,  $C_w$ , and  $\text{Cap}$ , can be replaced by their expressions in terms of  $y_{w,v}$  (such as Eqs 1, 4 and 5).

Therefore, the only design constraints in this model are

$$F_{w,h} \leq \sum_{v=1}^d \bar{E}_{w,v} y_{w,v}, \quad \forall w \in \{1, \dots, e\}, \quad \forall h \in \{1, \dots, s\} \quad (8)$$

The objective function to be minimized is expressed as

$$\begin{aligned} -\text{NPV}_{\text{scale}} = & - \sum_{h=1}^s \text{Occu}_h \text{Pro}_{\text{net},h} \\ & - \left( \sum_{w=1}^e \sum_{v=1}^d \bar{C}_{w,v} y_{w,v} + \bar{C}_f \right) \frac{-1 + \frac{R_{\text{tax}}}{t_{\text{dp}}} \frac{1}{r} \left( 1 - \frac{1}{(1+r)^{t_{\text{dp}}}} \right)}{\frac{1}{r} \left( 1 - \frac{1}{(1+r)^{t_{\text{lf}}}} \right)} \end{aligned} \quad (9)$$

Estimation of equipment capacity and cost parameters, including  $\bar{E}_{w,v}$  and  $\bar{C}_{w,v}$  ( $\forall w \in \{1, \dots, e\}, \forall v \in \{1, \dots, d\}$ ), are provided in Appendix.

### Other reformulations

Topology constraints for aggregate equipment are added into the model to reduce the integer possibilities. The minimum capacity of equipment ( $\bar{E}_w^L$ ) (or the first choice for equipment capacity) is typically set to be zero (except for the gas turbine system and steam turbine system), which implies that the set of equipment is not included in the process. The following topology constraint indicates that if an upstream unit is not included, all downstream equipment should not be included either

$$y_{w_u,1} \leq y_{w_d,1} \quad (10)$$

where  $y_{w_u,1}$  and  $y_{w_d,1}$  are the first choice for capacity of a set of upper stream equipment  $w_u$  and a set of downstream equipment  $w_d$ , respectively.

The reformulation-linearization technique is used to generate redundant constraints for tighter convex relaxations. The resulting model is similar to the pq-formulation<sup>25</sup> for the pooling problem.



## Model summary

The optimization model for flexible polygeneration systems is a large-scale nonconvex MINLP, including 70 binary variables and 613  $s$  continuous variables ( $s$  is the number of scenarios). The nonconvexity originates from bilinear terms in mass balances. The overall model can be expressed in the following general form

$$\begin{aligned} \min_{\substack{y \in \{0,1\}^{n_y}, \dots, s, \\ q_1, \dots, q_s, u_1, \dots, u_s}} \quad & c_1^T y + \sum_{h=1}^s \left( c_{2,h}^T x_h + c_{3,h}^T q_h + c_{4,h}^T u_h \right) \\ \text{s.t.} \quad & u_{h,l,t} = x_{h,l} q_{h,t}, \quad \forall (l,t) \in \Omega, \forall h \in \{1, \dots, s\}, \\ & A_{1,h} y + A_{2,h} x_h + A_{3,h} q_h + A_{4,h} u_h \leq b_h, \quad \forall h \in \{1, \dots, s\}, \\ & (x_h, q_h, u_h) \in \Pi_h, \quad \forall h \in \{1, \dots, s\}, y \in Y, \end{aligned} \quad (\text{P})$$

where  $x_h$  represents flow rates and heat/power consumption rates in scenario  $h$ ,  $q_h$  represents split fractions in scenario  $h$ , and  $u_h$  represents intermediate variables introduced for bilinear terms in scenario  $h$ , which are all continuous variables;  $y$  represents the binary variables that determine equipment capacities (which is equivalent to  $y_{w,v}$ ); the objective function is the general form of Eq. 9; the first set of constraints represents the bilinear functions in mass balances, which are the only nonconvex functions in the model; the second set of constraints represents the design constraints (or equipment capacity constraints as shown in Eq. 8), which contain both the binary and the continuous variables. The set for the continuous variables is a nonempty, compact, and convex polyhedron

$$\Pi_h = \{ (x_h, q_h, u_h) \in \mathbb{R}^{n_x} \times \mathbb{R}^{n_q} \times \mathbb{R}^{n_u} : \tilde{A}_{2,h} x_h + \tilde{A}_{3,h} q_h + \tilde{A}_{4,h} u_h \leq \tilde{b}_h, x_h^L \leq x_h \leq x_h^U, q_h^L \leq q_h \leq q_h^U \}$$

where the inequality represents the linear operational constraints, including mass and energy balances, production and feedstock consumption rates, reactor feedstock specifications, and emission regulations;  $x_h^L$ ,  $x_h^U$ ,  $q_h^L$ , and  $q_h^U$  are the lower and upper bounds for  $x_h$  and  $q_h$ , respectively. The set for the binary variables is

$$Y = \{ y \in \{0,1\}^{n_y} : B y \leq a \}.$$

where the inequality represents Eqs. 2 and 10.

Note that the classical pooling problem formulations, including p-, q-, and pq-formulations,<sup>25</sup> can all be written in the form of Problem (P).

**REMARK 1.** Problem (P) has finite optimal objective values or is infeasible, because the set  $\Pi_h$  is compact.

## The Decomposition Method

### Overview of decomposition method

The decomposition method is an extension of Benders decomposition<sup>26</sup> and is developed based on the framework of concepts presented by Geoffrion for the design of large-scale mathematical programming techniques.<sup>22</sup> This framework includes two groups of concepts: problem manipulations and solution strategies. Problem manipulations, including convexification, projection, and dualization, are devices for restating a given problem in an alternative form more amenable to solution. The result is often what is referred to as a master problem. Solution strategies, including relaxation and restriction, reduce the master problem to a related sequence of simpler subproblems.

In the decomposition method, Problem (P) is reformulated into a lower bounding problem by convexification and underestimation of the bilinear functions. The lower bounding problem is potentially a large-scale mixed-integer linear program (MILP), which can be transformed into an equivalent master problem by the principle of projection and dualization.<sup>22</sup>

The master problem contains an infinite number of constraints and is usually difficult to solve directly. Instead, it is solved through solving a sequence of Primal bounding problems (PBPs), Feasibility problems (FPs), and Relaxed master problems (RMPs), which are much easier to solve.

The PBP is constructed by restricting the integer variables to specific values in the lower bounding problem, whose solution yields a valid upper bound on the optimal objective value of the lower bounding problem (and hence the master problem). When the PBP is infeasible for an integer realization, a corresponding FP is solved, which yields valid information for the algorithm to proceed. Both the PBPs and the FPs are potentially large-scale linear programs (LPs), but they can be further decomposed into LP subproblems for each scenario with much smaller sizes.

The RMP is constructed by relaxing the master problem with a finite subset of the constraints (or cuts). Canonical integer cuts are also added into the problem, so that no integer realizations will be visited twice by the algorithm. The solution of the relaxed master problem yields a valid lower bound on the optimal objective value of the master problem augmented with the integer cuts. The RMP is a MILP whose size is independent of the number of scenarios.

On the other hand, a restriction of Problem (P), which is called the primal problem (PP), is constructed by restricting the integer variables to specific values in Problem (P), whose optimal objective value yields an upper bound of that of Problem (P). The PP is potentially a large-scale nonconvex nonlinear program (NLP), but it can be further decomposed into NLP subproblems for each scenario with much smaller sizes.

The details of the aforementioned subproblems are shown in the next subsection.

### Subproblems in the decomposition method

**PBP.** The PBP is generated by fixing the integer variables in the lower bounding problem to  $y^{(k)}$ , which is the integer realization at the  $k$ th iteration. Problem (PBP) can be naturally decomposed into subproblems (PBP <sub>$h$</sub> ) for the  $s$  scenarios

$$\begin{aligned} \text{obj}_{\text{PBP}_h}(y^{(k)}) = \min_{x_h, q_h, u_h} \quad & c_{2,h}^T x_h + c_{3,h}^T q_h + c_{4,h}^T u_h \\ \text{s.t.} \quad & A_{1,h} y^{(k)} + A_{2,h} x_h + A_{3,h} q_h + A_{4,h} u_h \leq b_h, \\ & (x_h, q_h, u_h) \in \hat{\Pi}_h \end{aligned} \quad (\text{PBP}_h)$$

where

$$\begin{aligned} \hat{\Pi}_h = \{ (x_h, q_h, u_h) \in \Pi_h : u_{h,l,t} \geq x_{h,l}^L q_{h,t}^L + x_{h,l}^U q_{h,t}^U - x_{h,l}^L q_{h,t}^U, \\ u_{h,l,t} \leq x_{h,l}^U q_{h,t}^L + x_{h,l}^L q_{h,t}^U - x_{h,l}^L q_{h,t}^U, \\ u_{h,l,t} \leq x_{h,l}^U q_{h,t}^L + x_{h,l}^L q_{h,t}^U - x_{h,l}^L q_{h,t}^U, \\ u_{h,l,t} \leq x_{h,l}^L q_{h,t}^L + x_{h,l}^U q_{h,t}^U - x_{h,l}^L q_{h,t}^U, \\ \forall (l,t) \in \Omega \} \end{aligned}$$

$\text{obj}_{\text{PBP}_h}(y^{(k)})$  is the optimal objective value of Problem (PBP <sub>$h$</sub> ) for  $y = y^{(k)}$ ,  $h = 1, \dots, s$ . The objectives of Problems (PBP) and (PBP <sub>$h$</sub> ) satisfy the following relationship

$$\text{obj}_{\text{PBP}}(y^{(k)}) = c_1^T y^{(k)} + \sum_{h=1}^s \text{obj}_{\text{PBP}_h}(y^{(k)}) \quad (11)$$

where  $\text{obj}_{\text{PBP}}(y^{(k)})$  is the optimal objective value of Problem (PBP) for  $y = y^{(k)}$ .

**FP.** If Problem (PBP) is infeasible, the corresponding FP is solved. Problem (FP) can be naturally decomposed into subproblems ( $\text{FP}_h$ ) for the  $s$  scenarios

$$\begin{aligned} \min_{x_h, q_h, u_h, z_h} \quad & \sum_{i=1}^m z_{h,i} \\ \text{s.t.} \quad & A_{1,h}y^{(k)} + A_{2,h}x_h + A_{3,h}q_h + A_{4,h}u_h - b_h \leq z_h, \\ & (x_h, q_h, u_h) \in \hat{\Pi}_h, \quad z_h = (z_{h,1}, \dots, z_{h,m}) \in Z, \end{aligned} \quad (\text{FP}_h)$$

where  $Z = \{z \in \mathbb{R}^m : z \geq 0\}$ , and each non-negative variable  $z_{h,i}$  measures the violation of the corresponding constraint,  $h = 1, \dots, s$ .

**RMP.** After solving the primal bounding subproblems or feasibility subproblems for  $k$  integer realizations, a Problem ( $\text{RMP}^k$ ) is solved to generate a new integer realization

$$\begin{aligned} \min_{y, \eta} \quad & \eta \\ \text{s.t.} \quad & \eta \geq \alpha^{(j)}y + \beta^{(j)}, \quad \forall j \in T^k, \\ & \gamma^{(i)}y + \theta^{(i)} \leq 0, \quad \forall i \in S^k, \\ & \sum_{l \in \{l: y_l^{(i)} = 1\}} y_l - \sum_{l \in \{l: y_l^{(i)} = 0\}} y_l \leq |\{l : y^{(i)} = 1\}| - 1, \quad \forall t \in T^k \cup S^k, \\ & y \in Y, \quad \eta \in \mathbb{R} \end{aligned} \quad (\text{RMP}^k)$$

where

$$\begin{aligned} \alpha^{(j)} &= c_1^T + \sum_{h=1}^s (\lambda_h^{(j)})^T A_{1,h}, \\ \beta^{(j)} &= \sum_{h=1}^s \left[ c_{2,h}^T x_h^{(j)} + c_{3,h}^T q_h^{(j)} + c_{4,h}^T u_h^{(j)} \right] \\ &\quad + \sum_{h=1}^s \left[ (\lambda_h^{(j)})^T (A_{2,h}x_h^{(j)} + A_{3,h}q_h^{(j)} + A_{4,h}u_h^{(j)} - b_h) \right], \\ \gamma^{(i)} &= \sum_{h=1}^s (\mu_h^{(i)})^T A_{1,h}, \\ \theta^{(i)} &= \sum_{h=1}^s \left[ (\mu_h^{(i)})^T (A_{2,h}x_h^{(i)} + A_{3,h}q_h^{(i)} + A_{4,h}u_h^{(i)} - b_h) \right], \end{aligned}$$

and the index sets are

$$\begin{aligned} T^k &= \{j \in \{1, \dots, k\} : \text{Problem PBP}(y^{(j)}) \text{ is feasible}\} \\ S^k &= \{i \in \{1, \dots, k\} : \text{Problem PBP}(y^{(i)}) \text{ is infeasible}\} \end{aligned}$$

$\lambda_h^{(j)}$  denotes the Lagrange multipliers of Problem ( $\text{PBP}_h$ ) when  $y = y^{(j)}$  ( $\forall j \in T^k$ ), and  $\mu_h^{(i)}$  denotes the Lagrange multipliers of Problem ( $\text{FP}_h$ ) when  $y = y^{(i)}$  ( $\forall i \in S^k$ ).  $(x_h^{(j)}, q_h^{(j)}, u_h^{(j)})$  is a minimum of Problem ( $\text{PBP}_h$ ) ( $\forall h \in \{1, \dots, s\}$ ) when  $y = y^{(j)}$ , and  $(x_h^{(i)}, q_h^{(i)}, u_h^{(i)})$  is a minimum of Problem ( $\text{FP}_h$ ) ( $\forall h \in \{1, \dots, s\}$ ) when  $y = y^{(i)}$ . The last group of constraints represent a set of canonical integer cuts that prevent the previously examined

integer realizations from becoming a solution.<sup>27</sup> In this article, these integer cuts are called “Balas cuts.”

When no feasible integer realization for Problem (PBP) has been found (i.e.,  $T^k = \emptyset$ ), an alternative feasibility relaxed master problem ( $\text{RMFP}^k$ ), which yields a feasible solution for Problem ( $\text{RMP}^k$ ), is solved to allow the algorithm to proceed

$$\begin{aligned} \min_y \quad & \sum_{l=1}^{n_y} y_l \\ \text{s.t.} \quad & \gamma^{(i)}y + \theta^{(i)} \leq 0, \quad \forall i \in S^k, \\ & \sum_{l \in \{l: y_l^{(i)} = 1\}} y_l - \sum_{l \in \{l: y_l^{(i)} = 0\}} y_l \leq |\{l : y^{(i)} = 1\}| - 1, \quad \forall t \in S^k, \\ & y \in Y \end{aligned} \quad (\text{RMPF}^k)$$

**PP.** The Problem (PP) is generated by fixing the integer variables in the original Problem (P) to  $y^{(k)}$ , which is the integer realization at the  $k$ th iteration. Problem (PP) can be naturally decomposed into subproblems ( $\text{PP}_h$ ) for the  $s$  scenarios

$$\begin{aligned} \text{obj}_{\text{PP}_h}(y^{(k)}) &= \min_{x_h, q_h, u_h} c_{2,h}^T x_h + c_{3,h}^T q_h + c_{4,h}^T u_h \\ \text{s.t.} \quad & u_{h,l,t} = x_{h,l}q_{h,t}, \quad \forall (l, t) \in \Omega, \\ & A_{1,h}y^{(k)} + A_{2,h}x_h + A_{3,h}q_h + A_{4,h}u_h \leq b_h, \\ & (x_h, q_h, u_h) \in \Pi_h \end{aligned} \quad (\text{PP}_h)$$

where  $\text{obj}_{\text{PP}_h}(y^{(k)})$  is the optimal objective value of Problem ( $\text{PP}_h$ ) for  $y = y^{(k)}$ ,  $h = 1, \dots, s$ . The objectives of Problems (PP) and ( $\text{PP}_h$ ) satisfy the following relationship

$$\text{obj}_{\text{PP}}(y^{(k)}) = c_1^T y^{(k)} + \sum_{h=1}^s \text{obj}_{\text{PP}_h}(y^{(k)}) \quad (12)$$

where  $\text{obj}_{\text{PP}}(y^{(k)})$  is the optimal objective value of Problem (PP) for  $y = y^{(k)}$ .

**REMARK 2.** According to Ref. 20, the solution of Problem ( $\text{PP}_h$ ) can be accelerated with the inclusion of additional cuts.

**DA.** The DA and flowchart are described in Ref. 18 and 20. The proof of the finite convergence of the DA can be found in Ref. 20.

## Enhanced Decomposition Method with More Dual Information

### Relaxed dual of PP

To accelerate the convergence of the DA, tighter lower bounds need to be generated by the lower bounding problems. A possible way is the incorporation of dual information of the PP into the RMP. Such dual information can be obtained by solving the dual of Problem (PP), which is a quite difficult problem, as it is a bilevel program. Instead, a restriction of the dual of Problem (PP) [called Problem (DPP)], which is generated by fixing the multipliers in the dual of Problem (PP) to some specified values, is solved here. The optimal value of Problem (DPP) is a lower bound of that of the dual of Problem (PP). Problem (DPP) can be naturally decomposed into subproblems ( $\text{DPP}_h$ ) for the  $s$  scenarios

$$\begin{aligned} \min_{x_h, q_h, u_h} \quad & c_{2,h}^T x_h + c_{3,h}^T q_h + c_{4,h}^T u_h \\ & + \left( \kappa_h^{(k)} \right) \left( A_{1,h} y^{(k)} + A_{2,h} x_h + A_{3,h} q_h + A_{4,h} u_h - b_h \right) \\ \text{s.t.} \quad & u_{h,l,t} = x_{h,l} q_{h,t}, \quad \forall (l, t) \in \Omega, \\ & (x_h, q_h, u_h) \in \Pi_h \end{aligned} \quad (\text{DPP}_h)$$

where  $\kappa_h^{(k)}$  can be either  $\lambda_h^{(k)}$ , which denotes Karush–Kuhn–Tucker (KKT) multipliers of Problem (PBP<sub>h</sub>) when  $y = y^{(k)}$ , or  $\check{\lambda}_h^{(k)}$ , which denotes KKT multipliers of Problem (PP<sub>h</sub>) when  $y = y^{(k)}$ . Problem (DPP<sub>h</sub>) is solved for both values of the KKT multipliers in this article to obtain additional dual information from the PP.

**REMARK 3.** Problem (DPP<sub>h</sub>) is always feasible, and its optimal objective value is finite, because the set  $\Pi_h$  is compact. By weak duality,<sup>28</sup> it provides a lower bound on Problem (PP<sub>h</sub>).

**REMARK 4.** Problem (DPP<sub>h</sub>) is nonconvex, hence global optimization solvers, such as BARON, need to be used here to obtain  $\epsilon$ -optimal solutions. As discussed later, solving Problem (DPP<sub>h</sub>) is the most time-consuming step in the whole algorithm. To reduce the overall solution time, Problem (DPP<sub>h</sub>) is only solved for those integer realizations for which Problem (PP) is feasible and updates the current upper bound (UBD).

### Enhanced relaxed master problem

The optimal solutions of Problem (DPP<sub>h</sub>) together with the KKT multipliers of Problem (PBP<sub>h</sub>) and (PP<sub>h</sub>) provide additional cuts for the Problem (RMP<sup>k</sup>) to obtain tighter lower bounds for Problem (P). The updated RMP, which is called the enhanced relaxed master problem (ERMP<sup>k</sup>), is as follows

$$\begin{aligned} \min_{y, \eta} \quad & \eta \\ \text{s.t.} \quad & \eta \geq \tilde{\alpha}^{(r)} y + \tilde{\beta}^{(r)}, \quad \forall r \in V^k, \\ & \eta \geq \check{\alpha}^{(r)} y + \check{\beta}^{(r)}, \quad \forall r \in V^k, \\ & \eta \geq \alpha^{(j)} y + \beta^{(j)}, \quad \forall j \in T^k \setminus V^k, \\ & \gamma^{(i)} y + \theta^{(i)} \leq 0, \quad \forall i \in S^k, \\ & \sum_{l \in \{l: y_l^{(i)} = 1\}} y_l - \sum_{l \in \{l: y_l^{(i)} = 0\}} y_l \leq |\{l: y^{(i)} = 1\}| - 1, \quad \forall t \in T^k \cup S^k, \\ & y \in Y, \quad \eta \in \mathbb{R} \end{aligned} \quad (\text{ERMP}^k)$$

where

$$\begin{aligned} \tilde{\alpha}^{(r)} &= c_1^T + \sum_{h=1}^s \left( \lambda_h^{(r)} \right)^T A_{1,h}, \\ \tilde{\beta}^{(r)} &= \sum_{h=1}^s \left[ c_{2,h}^T \tilde{x}_h^{(r)} + c_{3,h}^T \tilde{q}_h^{(r)} + c_{4,h}^T \tilde{u}_h^{(r)} \right] \\ &\quad + \sum_{h=1}^s \left[ \left( \lambda_h^{(r)} \right)^T \left( A_{2,h} \tilde{x}_h^{(r)} + A_{3,h} \tilde{q}_h^{(r)} + A_{4,h} \tilde{u}_h^{(r)} - b_h \right) \right], \\ \check{\alpha}^{(r)} &= c_1^T + \sum_{h=1}^s \left( \check{\lambda}_h^{(r)} \right)^T A_{1,h}, \\ \check{\beta}^{(r)} &= \sum_{h=1}^s \left[ c_{2,h}^T \check{x}_h^{(r)} + c_{3,h}^T \check{q}_h^{(r)} + c_{4,h}^T \check{u}_h^{(r)} \right] \\ &\quad + \sum_{h=1}^s \left[ \left( \check{\lambda}_h^{(r)} \right)^T \left( A_{2,h} \check{x}_h^{(r)} + A_{3,h} \check{q}_h^{(r)} + A_{4,h} \check{u}_h^{(r)} - b_h \right) \right], \end{aligned}$$

$$\begin{aligned} V^k &= \{r \in \{1, \dots, k\} \\ &\quad : \text{Problem PP}(y^{(r)}) \text{ is feasible and updates UBD}\} \subset T^k. \end{aligned}$$

$(\tilde{x}_h^{(r)}, \tilde{q}_h^{(r)}, \tilde{u}_h^{(r)})$  is a minimum of Problem (DPP<sub>h</sub>) with the KKT multipliers of Problem (PBP<sub>h</sub>) ( $\forall h \in \{1, \dots, s\}$ ) when  $y = y^{(r)}$  and  $(\check{x}_h^{(r)}, \check{q}_h^{(r)}, \check{u}_h^{(r)})$  is a minimum of Problem (DPP<sub>h</sub>) with the KKT multipliers of Problem (PP<sub>h</sub>) ( $\forall h \in \{1, \dots, s\}$ ) when  $y = y^{(r)}$ . The first two sets of constraints are called primal dual cuts, because they are constructed according to the dual information of the PP.

**REMARK 5.** According to the separability in the integer and continuous variables, Problem (ERMP<sup>k</sup>) is equivalent to the following problem

$$\begin{aligned} \min_{y, \eta} \quad & \eta \\ \text{s.t.} \quad & \eta \geq F_P(y, \lambda_1^{(r)}, \dots, \lambda_s^{(r)}), \quad \forall r \in V^k, \\ & \eta \geq F_P(y, \check{\lambda}_1^{(r)}, \dots, \check{\lambda}_s^{(r)}), \quad \forall r \in V^k, \\ & \eta \geq F(y, \lambda_1^{(j)}, \dots, \lambda_s^{(j)}), \quad \forall j \in T^k \setminus V^k, \\ & G(y, \mu_1^{(i)}, \dots, \mu_s^{(i)}) \leq 0, \quad \forall i \in S^k, \\ & \sum_{l \in \{l: y_l^{(i)} = 1\}} y_l - \sum_{l \in \{l: y_l^{(i)} = 0\}} y_l \leq |\{l: y^{(i)} = 1\}| - 1, \\ & \forall t \in T^k \cup S^k, \\ & y \in Y, \quad \eta \in \mathbb{R} \end{aligned} \quad (\text{ERMP}^k)$$

where

$$\begin{aligned} F_P(y, \lambda_1^{(r)}, \dots, \lambda_s^{(r)}) &= \inf_{\substack{(x_h, q_h, u_h) \in \Pi_h, \\ \forall h \in \{1, \dots, s\}}} c_1^T y + \sum_{h=1}^s \left( c_{2,h}^T x_h + c_{3,h}^T q_h \right. \\ &\quad \left. + c_{4,h}^T u_h + \left( \lambda_h^{(r)} \right)^T (A_{1,h} y + A_{2,h} x_h + A_{3,h} q_h + A_{4,h} u_h - b_h) \right), \\ F_P(y, \check{\lambda}_1^{(r)}, \dots, \check{\lambda}_s^{(r)}) &= \inf_{\substack{(x_h, q_h, u_h) \in \Pi_h, \\ \forall h \in \{1, \dots, s\}}} c_1^T y + \sum_{h=1}^s \left( c_{2,h}^T x_h + c_{3,h}^T q_h \right. \\ &\quad \left. + c_{4,h}^T u_h + \left( \check{\lambda}_h^{(r)} \right)^T (A_{1,h} y + A_{2,h} x_h + A_{3,h} q_h + A_{4,h} u_h - b_h) \right), \\ F(y, \lambda_1^{(j)}, \dots, \lambda_s^{(j)}) &= \inf_{\substack{(x_h, q_h, u_h) \in \Pi_h, \\ \forall h \in \{1, \dots, s\}}} c_1^T y + \sum_{h=1}^s \left( c_{2,h}^T x_h + c_{3,h}^T q_h \right. \\ &\quad \left. + c_{4,h}^T u_h + \left( \lambda_h^{(j)} \right)^T (A_{1,h} y + A_{2,h} x_h + A_{3,h} q_h + A_{4,h} u_h - b_h) \right), \\ G(y, \mu_1^{(i)}, \dots, \mu_s^{(i)}) &= \inf_{\substack{(x_h, q_h, u_h) \in \Pi_h, \\ \forall h \in \{1, \dots, s\}}} \sum_{h=1}^s \left( \mu_h^{(i)} \right)^T \left( A_{1,h} y + A_{2,h} x_h \right. \\ &\quad \left. + A_{3,h} q_h + A_{4,h} u_h - b_h \right), \end{aligned}$$

and the set

$$\tilde{\Pi}_h = \{(x_h, q_h, u_h) \in \Pi_h : u_{h,l,t} = x_{h,l} q_{h,t}, \quad \forall (l, t) \in \Omega\}$$

**Proposition 1.** Any  $y$  that is feasible for Problem (P) augmented with the Balas cuts is also feasible for Problem (ERMP<sup>k</sup>), and the optimal objective of Problem (ERMP<sup>k</sup>) is a lower bound of that of Problem (P) augmented with the Balas cuts.

**Proof.** See Appendix. ■

**Proposition 2.** Problem (ERMP<sup>k</sup>) is a tighter (or equal) underestimate of Problem (P) augmented with the Balas cuts compared to Problem (RMP<sup>k</sup>).

**Proof.** See Appendix. ■

### ERMP with primal dual multicuts

Problem (ERMP<sup>k</sup>) can be further enhanced by replacing each single primal dual cut with  $s$  cuts for the  $s$  scenarios following the multicut strategy in Ref. 29. The new primal dual cuts are called primal dual multicuts in this article. The ERMP with primal dual multicuts, which is called multicut ERMP (MERMP<sup>k</sup>), is constructed as follows (in which the optimality and feasibility cuts are also replaced by multicuts)

$$\begin{aligned}
 \min_{\substack{y, \eta \\ \eta_1, \dots, \eta_s}} \quad & \eta \\
 \text{s.t.} \quad & \eta \geq c_1^T y + \sum_{h=1}^s \eta_h, \\
 & \eta_h \geq \tilde{\alpha}_h^{(r)} y + \tilde{\beta}_h^{(r)}, \quad \forall h \in \{1, \dots, s\}, \forall r \in V^k, \\
 & \eta_h \geq \check{\alpha}_h^{(r)} y + \check{\beta}_h^{(r)}, \quad \forall h \in \{1, \dots, s\}, \forall r \in V^k, \\
 & \eta_h \geq \alpha_h^{(j)} y + \beta_h^{(j)}, \quad \forall h \in \{1, \dots, s\}, \forall j \in T^k \setminus V^k, \\
 & \gamma_h^{(i)} y + \theta_h^{(i)} \leq 0, \quad \forall h \in \{1, \dots, s\}, \forall i \in S^k, \\
 & \sum_{l \in \{l: y_l^{(i)}=1\}} y_l - \sum_{l \in \{l: y_l^{(i)}=0\}} y_l \leq |\{l: y^{(i)}=1\}| - 1, \\
 & \forall t \in T^k \cup S^k, \\
 & y \in Y, \eta \in \mathbb{R}
 \end{aligned} \tag{MERMP<sup>k</sup>}$$

where

$$\begin{aligned}
 \tilde{\alpha}_h^{(r)} &= \left( \lambda_h^{(r)} \right)^T A_{1,h}, \\
 \tilde{\beta}_h^{(r)} &= c_{2,h}^T \tilde{x}_h^{(r)} + c_{3,h}^T \tilde{q}_h^{(r)} + c_{4,h}^T \tilde{u}_h^{(r)} \\
 &\quad + \left( \lambda_h^{(r)} \right)^T \left( A_{2,h} \tilde{x}_h^{(r)} + A_{3,h} \tilde{q}_h^{(r)} + A_{4,h} \tilde{u}_h^{(r)} - b_h \right), \\
 \check{\alpha}_h^{(r)} &= \left( \check{\lambda}_h^{(r)} \right)^T A_{1,h}, \\
 \check{\beta}_h^{(r)} &= c_{2,h}^T \check{x}_h^{(r)} + c_{3,h}^T \check{q}_h^{(r)} + c_{4,h}^T \check{u}_h^{(r)} \\
 &\quad + \left( \check{\lambda}_h^{(r)} \right)^T \left( A_{2,h} \check{x}_h^{(r)} + A_{3,h} \check{q}_h^{(r)} + A_{4,h} \check{u}_h^{(r)} - b_h \right), \\
 \alpha_h^{(j)} &= \left( \lambda_h^{(j)} \right)^T A_{1,h}, \\
 \beta_h^{(j)} &= c_{2,h}^T x_h^{(j)} + c_{3,h}^T q_h^{(j)} + c_{4,h}^T u_h^{(j)} \\
 &\quad + \left( \lambda_h^{(j)} \right)^T \left( A_{2,h} x_h^{(j)} + A_{3,h} q_h^{(j)} + A_{4,h} u_h^{(j)} - b_h \right), \\
 \gamma_h^{(i)} &= \left( \mu_h^{(i)} \right)^T A_{1,h}, \\
 \theta_h^{(i)} &= \left( \mu_h^{(i)} \right)^T \left( A_{2,h} x_h^{(i)} + A_{3,h} q_h^{(i)} + A_{4,h} u_h^{(i)} - b_h \right).
 \end{aligned}$$

**REMARK 6.** According to the separability in the integer and continuous variables, Problem (MERMP<sup>k</sup>) is equivalent to the following problem

$$\begin{aligned}
 \min_{\substack{y, \eta \\ \eta_1, \dots, \eta_s}} \quad & \eta \\
 \text{s.t.} \quad & \eta \geq c_1^T y + \sum_{h=1}^s \eta_h, \\
 & \eta_h \geq F_{P,h}(y, \lambda_h^{(r)}), \quad \forall h \in \{1, \dots, s\}, \forall r \in V^k, \\
 & \eta_h \geq F_{P,h}(y, \check{\lambda}_h^{(r)}), \quad \forall h \in \{1, \dots, s\}, \forall r \in V^k, \\
 & \eta_h \geq F_h(y, \lambda_h^{(j)}), \quad \forall h \in \{1, \dots, s\}, \forall j \in T^k \setminus V^k, \\
 & G_h(y, \mu_h^{(i)}) \leq 0, \quad \forall h \in \{1, \dots, s\}, \forall i \in S^k, \\
 & \sum_{l \in \{l: y_l^{(i)}=1\}} y_l - \sum_{l \in \{l: y_l^{(i)}=0\}} y_l \leq |\{l: y^{(i)}=1\}| - 1, \\
 & \forall t \in T^k \cup S^k, \\
 & y \in Y, \eta \in \mathbb{R}
 \end{aligned} \tag{MERMP1<sup>k</sup>}$$

where

$$\begin{aligned}
 F_{P,h}(y, \lambda_h^{(r)}) &= \inf_{(x_h, q_h, u_h) \in \tilde{\Pi}_h} c_{2,h}^T x_h + c_{3,h}^T q_h + c_{4,h}^T u_h \\
 &\quad + \left( \lambda_h^{(r)} \right)^T (A_{1,h} y + A_{2,h} x_h + A_{3,h} q_h + A_{4,h} u_h - b_h), \\
 F_{P,h}(y, \check{\lambda}_h^{(r)}) &= \inf_{(x_h, q_h, u_h) \in \tilde{\Pi}_h} c_{2,h}^T x_h + c_{3,h}^T q_h + c_{4,h}^T u_h \\
 &\quad + \left( \check{\lambda}_h^{(r)} \right)^T (A_{1,h} y + A_{2,h} x_h + A_{3,h} q_h + A_{4,h} u_h - b_h), \\
 F_h(y, \lambda_h^{(j)}) &= \inf_{(x_h, q_h, u_h) \in \tilde{\Pi}_h} c_{2,h}^T x_h + c_{3,h}^T q_h + c_{4,h}^T u_h \\
 &\quad + \left( \lambda_h^{(j)} \right)^T (A_{1,h} y + A_{2,h} x_h + A_{3,h} q_h + A_{4,h} u_h - b_h), \\
 G_h(y, \mu_h^{(i)}) &= \inf_{(x_h, q_h, u_h) \in \tilde{\Pi}_h} \left( \mu_h^{(i)} \right)^T \\
 &\quad \times (A_{1,h} y + A_{2,h} x_h + A_{3,h} q_h + A_{4,h} u_h - b_h).
 \end{aligned}$$

**Proposition 3.** Any  $y$  that is feasible for Problem (P) augmented with the Balas cuts is also feasible for Problem (MERMP<sup>k</sup>), and the optimal objective of Problem (MERMP<sup>k</sup>) is a lower bound of that of the original problem (P) augmented with the Balas cuts.

**Proof.** See Appendix. ■

**Proposition 4.** Problem (MERMP<sup>k</sup>) is a tighter (or equal) underestimate of Problem (P) augmented with the Balas cuts compared to Problem (ERMP<sup>k</sup>).

**Proof.** See Appendix. ■

**REMARK 7.** After incorporation of multicuts, the number of continuous variables in Problem (MERMP<sup>k</sup>) depends on the number of scenarios linearly while the number of binary variables, which dominates the solution time of MILPs, remains the same; on the other hand, the number of iterations (and hence the number of Problems (PP<sub>h</sub>) and (DPP<sub>h</sub>) to be solved) may be significantly reduced, as will be shown by the case study results.

### EDA

Either the ERMP or the MERMP can be used in the EDA. The following algorithm is stated with Problem (ERMP<sup>k</sup>):

Initialize:

1. Iteration counters  $k = 0$ ,  $l = 1$ , and the index sets  $T^0 = \emptyset$ ,  $S^0 = \emptyset$ ,  $U^0 = \emptyset$ ,  $V^0 = \emptyset$ .

2. Upper bound on the problem  $UBD = +\infty$ , upper bound on the lower bounding problem  $UBDPB = +\infty$ , lower bound on the lower bounding problem  $LB = -\infty$ .

3. Set tolerances  $\varepsilon_h$  and  $\varepsilon$  such that  $\sum_{h=1}^s \varepsilon_h \leq \varepsilon$ .

4. Integer realization  $y^{(1)}$  is given.



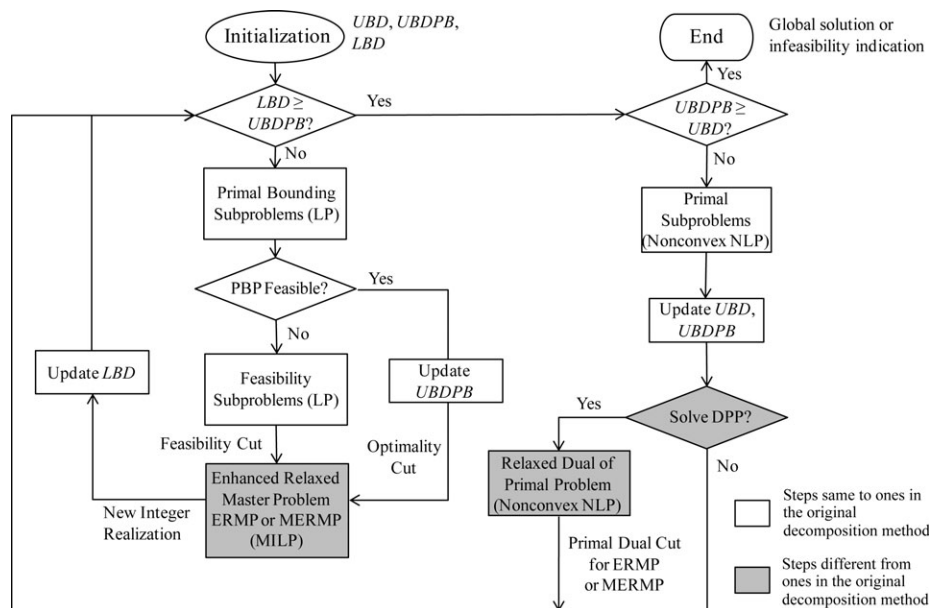


Figure 3. Flowchart for the EDA.

repeat

if  $k = 0$  or (Problem (ERMP<sup>k</sup>) is feasible and  $LBD < UBDPB$  and  $LBD < UBD - \varepsilon$ ) then

repeat

Set  $k = k + 1$

1. Solve the Problem (PBP<sub>h</sub>(y<sup>(k)</sup>)) for each scenario  $h = 1, \dots, s$  sequentially. If Problem (PBP<sub>h</sub>(y<sup>(k)</sup>)) is feasible for all the scenarios with KKT multipliers  $\lambda_h^{(k)}$ , add optimality cuts to the Problem (ERMP<sup>k</sup>) according to  $\lambda_1^{(k)}, \dots, \lambda_s^{(k)}$ , set  $T^k = T^{k-1} \cup \{k\}$ . If  $\text{obj}_{PBP}(y^{(k)}) = c_1^T y^{(k)} + \sum_{h=1}^s \text{obj}_{PBP_h}(y^{(k)}) < UBDPB$ , update  $UBDPB = \text{obj}_{PBP}(y^{(k)})$ ,  $y^* = y^{(k)}$ ,  $k^* = k$ .
2. If Problem (PBP<sub>h</sub>(y<sup>(k)</sup>)) is infeasible for one scenario, stop solving it for the remaining scenarios and set  $S^k = S^{k-1} \cup \{k\}$ . Then, solve the Problem (FP<sub>h</sub>(y<sup>(k)</sup>)) for  $h = 1, \dots, s$  and obtain the corresponding KKT multipliers  $\mu_h^{(k)}$ . Add feasibility cuts to Problem (ERMP<sup>k</sup>) according to these multipliers.
3. If  $T^k = \emptyset$ , solve the Problem (RMFP<sup>k</sup>); otherwise, solve Problem (ERMP<sup>k</sup>). In the latter case, if Problem (ERMP<sup>k</sup>) is feasible, set  $LBD$  to its optimal objective value and set  $y^{(k+1)}$  to the  $y$  value at its optimum.

until  $LBD \geq UBDPB$  or (Problem (ERMP<sup>k</sup>) or (RMFP<sup>k</sup>) is infeasible).

end if

if  $UBDPB < UBD - \varepsilon$  then

1. Solve the Problem (PP<sub>h</sub>(y\*)) to  $\varepsilon_h$ -optimality for each scenario  $h = 1, \dots, s$  sequentially. Set  $U^l = U^{l-1} \cup \{k^*\}$ . If Problem (PP<sub>h</sub>(y\*)) is feasible with optimum  $(x_{p,h}^*, q_{p,h}^*, u_{p,h}^*)$  for all the scenarios and  $\text{obj}_{PP}(y^*) = c_1^T y^* + \sum_{h=1}^s \text{obj}_{PP_h}(y^*) < UBD$ , obtain the corresponding KKT multipliers  $\lambda_h^{(k^*)}$ , update  $UBD = \text{obj}_{PP}(y^*)$  and  $y_p^* = y^*$ , set  $V^k = V^{k-1} \cup \{k^*\}$ .
2. If  $k^* \in V^k$ , solve the Problem (DPP<sub>h</sub>(y\*)) to  $\varepsilon_h$ -optimality for each scenario  $h = 1, \dots, s$  sequentially with KKT multipliers  $\lambda_h^{(k^*)}$  and  $\lambda_h^{(k^*)}$ . Add primal dual cuts to Problem (ERMP<sup>k</sup>) according to these multipliers and the optimal solutions of Problem (DPP<sub>h</sub>(y\*)).
3. If  $T^k \setminus U^l = \emptyset$ , set  $UBDPB = +\infty$ .
4. If  $T^k \setminus U^l \neq \emptyset$ , pick  $i \in T^k \setminus U^l$  such that  $\text{obj}_{PBP}(y^{(i)}) = \min_{j \in T^k \setminus U^l} \{\text{obj}_{PBP}(y^{(j)})\}$ . Update  $UBDPB = \text{obj}_{PBP}(y^{(i)})$ ,  $y^* = y^{(i)}$ ,  $k^* = i$ . Set  $l = l + 1$ .

end if

until  $UBDPB \geq UBD - \varepsilon$  and [(Problem (ERMP<sup>k</sup>) or (RMFP<sup>k</sup>) is infeasible) or  $LBD \geq UBD - \varepsilon$ ].

An  $\varepsilon$ -global optimum of the original problem (P) is given by

$$(y_p^*, x_{p,1}^*, \dots, x_{p,s}^*, q_{p,1}^*, \dots, q_{p,s}^*, u_{p,1}^*, \dots, u_{p,s}^*)$$

or (P) is infeasible.

If the Problem (MERMP<sup>k</sup>) is applied, replace Problem (ERMP<sup>k</sup>) in the aforementioned algorithm by Problem (MERMP<sup>k</sup>).

The algorithm flowchart is shown in Figure 3, in which differences between the EDA and the original DA are highlighted in gray. Compared to the flowchart of the original DA, two new steps, "Solve DPP?" and "Relaxed Dual of PP", are added in this flowchart, and the step "RMP" is replaced by "ERMP or MERMP." Note that the nested loops are designed to minimize the number of PP solved.<sup>20,30</sup>

**Table 1. Case Study Problems**

	Case 1	Case 2
Settings	Middle oil price Middle carbon tax 100% operational flexibility	Middle oil price Middle carbon tax 100% operational flexibility
Number of scenarios	8	24
Description of scenarios	Peak and off-peak times in four seasons	Peak and off-peak times in 12 months
Number of binary variables	70	70
Number of continuous variables	4904	14,712

As the EDA just uses a tighter RMP that does not exclude the global optimum of Problem (P) for the set of integer realizations not yet visited (Propositions 1, 2, 3, and 4), and no integer will be visited twice by the algorithm, the convergence property for the original DA still holds.

## Case Study

### Case study problems and implementation

Two case study problems are investigated in this work, which are modified from the case study problems in our prior work.<sup>9</sup> The description and problem sizes of the two cases are listed in Table 1.

The average feedstock prices, average product prices and carbon tax under the middle oil price and middle carbon tax are provided in our prior work,<sup>9</sup> and are listed in Table 2.

The peak time is defined to be 7 a.m. – 11 p.m. on working days, and the off-peak time is the rest of the time in the year, including 11 p.m. – 7 a.m. on weekdays and the whole day on weekends and holidays. The fraction of occurrence of all scenarios over the lifetime of the plant for Cases 1 and 2 are given in Appendix.

For simplicity, the feedstock prices and sulfur price are assumed to be constant in all scenarios, whose values are equal to their average prices. The prices of other products, including power, naphtha, diesel, and methanol, vary seasonally, and the power price also changes between peak and off-peak. The product prices (except for sulfur) in each scenario are given by the following relationship

$$Pr_{p,h} = Pr_p \text{Scf}_{p,h}, \quad \forall p \in N_{\text{pro}}, \forall h \in \{1, \dots, s\} \quad (13)$$

where  $Pr_{p,h}$  is the price of product  $p$  in scenario  $h$ ,  $Pr_p$  is the average price of product  $p$  whose value is given in Table 2, and  $\text{Scf}_{p,h}$  is the scale factor for the product  $p$  in scenario  $h$ .  $N_{\text{pro}} \equiv \{\text{electricity, naphtha, diesel, methanol}\}$  is the set of products

**Table 2. Parameters for Prices and Carbon Tax**

	Value	Unit
Feedstock price		
Coal	39.5	\$/ton
Biomass	59.2	\$/ton
Water	0.8	\$/ton
Product price		
Electricity	98.9	\$/MW h
Naphtha	1012.8	\$/ton
Diesel	1035.5	\$/ton
Methanol	449.8	\$/ton
Sulfur	100.0	\$/ton
Carbon tax	20.0	\$/ton of CO <sub>2</sub>

**Table 3. Optimal Equipment Designs for Cases 1 and 2**

Aggregate Equipment	Capacity Choice	Capacity	Capital Cost (million dollars)
Syngas cleaning system 1	1	0 Mmol/h	0
Syngas cleaning system 2	7	137 Mmol/h	102
CO <sub>2</sub> compressor	6	1389 ton/h	180
Fischer–Tropsch synthesis system	1	0 ton/h	0
Methanol synthesis system	10	840 ton/h	858
Gas turbine system	10	4750 MW	799
Steam turbine system	10	1800 MW	448

with variable prices in different scenarios. The scale factors represent the degree of fluctuation of product prices in different scenarios. Their values for Cases 1 and 2, which are estimated from historical market data,<sup>31–33</sup> are shown in Appendix.

The solver times of the following four methods are compared for the aforementioned two case study problems: (1) Branch-and-Reduce Method (realized by BARON 9.0.6<sup>15</sup>), (2) DA with the master problem (RMP<sup>k</sup>), (3) EDA with the master problem (ERMP<sup>k</sup>) (4) EDA with the master problem (MERMP<sup>k</sup>) (or Multicut Enhanced Decomposition Algorithm, MEDA).

BARON 9.0.6 uses CONOPT 3.14<sup>34</sup> for local NLP subproblems and CPLEX 12.2<sup>35</sup> for LP subproblems. DA, EDA, and MEDA use BARON 9.0.6 (with the same settings described above) for NLP subproblems and CPLEX 12.2 for LP and MILP subproblems.

Case study problems are solved on a computer allocated a single 2.66 GHz CPU and running Linux kernel. GAMS 23.5.2 is used to formulate the models, program the DA, EDA, and MEDA, and interface the various solvers for the subproblems. For all the methods, the absolute and relative termination criteria are  $10^{-2}$ , and the initial integer realization ( $y^{(1)}$ ) is 0. Only the solver time reported by GAMS is reported here.

**Table 4. Optimal Operations in Case 1**

	Value	Unit
Feedstock consumption rate		
Coal		
All seasons, peak and off-peak	1172	ton/h
Biomass		
All seasons, peak and off-peak	0	ton/h
Water		
All seasons, peak	205	ton/h
All seasons, off-peak	412	ton/h
Production rate		
Electricity		
All seasons, peak	3966	MW
All seasons, off-peak	72	MW
Naphtha		
All seasons, peak and off-peak	0	ton/h
Diesel		
All seasons, peak and off-peak	0	ton/h
Methanol		
All seasons, peak	0	ton/h
All seasons, off-peak	831	ton/h
Sulfur		
All seasons, peak and off-peak	29	ton/h
CO <sub>2</sub>		
Sequestration rate		
All seasons, peak	0	ton/h
All seasons, off-peak	1389	ton/h
Emission rate		
All seasons, peak	2684	ton/h
All seasons, off-peak	153	ton/h

**Table 5. Optimal Operations in Case 2**

	Value	Unit
Feedstock consumption rate		
Coal		
All months, peak and off-peak	1172	ton/h
Biomass		
All months, peak and off-peak	0	ton/h
Water		
All months except November, peak	205	ton/h
November, peak	87	ton/h
All months, off-peak	412	ton/h
Production rate		
Electricity		
All months except November, peak	3966	MW
November, peak	3630	MW
All months, off-peak	72	MW
Naphtha		
All months, peak and off-peak	0	ton/h
Diesel		
All months, peak and off-peak	0	ton/h
Methanol		
All months except November, peak	0	ton/h
November, peak	74	ton/h
All months, off-peak	831	ton/h
Sulfur		
All months, peak and off-peak	29	ton/h
CO <sub>2</sub>		
Sequestration rate		
All months except November, peak	0	ton/h
November, peak	131	ton/h
All months, off-peak	1389	ton/h
Emission rate		
All months except November, peak	2684	ton/h
November, peak	2450	ton/h
All months, off-peak	153	ton/h

### Optimization results

The optimal objective values (which are negative scaled NPVs) for Cases 1 and 2 are −1123.017 and −1124.385 million dollars, respectively. The optimal equipment selections for Cases 1 and 2 are the same, whose values are listed in Table 3. The optimal feedstock consumption rates, production rates, CO<sub>2</sub> sequestration rates, and CO<sub>2</sub> emission rates for Cases 1 and 2 are shown in Tables 4 and 5, respectively. Total capital investments, annual net profits, and NPVs of Cases 1 and 2 are compared in Table 6.

In both cases, power generation is preferred during peak times while methanol production is preferred during off-peak times because of the large variation of power prices between peak and off-peak. Liquid fuels, including naphtha and diesel, are not produced in any scenario due to their low prices when compared with other products. CO<sub>2</sub> emissions are relatively high in peak times, because all feedstocks are used for power generation and carbon sequestration is not implemented to save power for export. However, CO<sub>2</sub> emissions significantly drop in off-peak times, as most of carbon in feedstocks now flows into the methanol, and carbon sequestration becomes profitable to implement because of the low power price.

The fact that the equipment capacities are the same in Cases 1 and 2 (as shown in Table 3) implies that the operational flexibility of the polygeneration plant does not increase by

**Table 6. Economics of Cases 1 and 2**

	Case 1	Case 2	Unit
Capital investment	5363	5363	Million dollars
Annual net profit	1638	1640	Million dollars per year
NPV	9046	9057	Million dollars

**Table 7. Computational Performance of Different Solvers for Case 1**

	BARON	DA	EDA	MEDA
Total solver time (s)	—*	64316.5	7898.7	7426.4
Solver time for problem (PBP <sub>h</sub> ) (s)	n/a	17.3	8.9	1.8
Solver time for problem (FP <sub>h</sub> ) (s)	n/a	0.3	1.1	1.1
Solver time for the master problem <sup>†</sup> (s)	n/a	282.2	20.0	7.1
Solver time for problem (PP <sub>h</sub> ) (s)	n/a	64016.7	4750.8	2631.7
Solver time for problem (DPP <sub>h</sub> ) (s)	n/a	n/a	3118.0	4784.7
Integer realizations visited by problem (PBP <sub>h</sub> )	n/a	464	128	53
Integer realizations visited by problem (PP <sub>h</sub> )	n/a	396	73	15
Integer realizations visited by problem (DPP <sub>h</sub> )	n/a	n/a	5	3

\*No global solution was returned within 30 days.

<sup>†</sup>The master problem is Problem (RMP) or (ERMP) or (MERMP).

considering monthly price variations instead of seasonal ones. Discussions in our prior work<sup>9</sup> indicated the degree of price fluctuations between peak and off-peak times had significant impacts on the optimal design and operation while the seasonal price changes, which were much smaller than those between peak and off-peak, had little or no influence. Although, the monthly price changes are larger than the seasonal ones in this work, they are still not comparable with price differences between peak and off-peak. Therefore, monthly price fluctuations are not reflected in the optimal design and operation in both cases (except for the November peak times in Case 2), and the economic improvement of Case 2 compared to Case 1 is not significant (as shown in Table 6).

### Computational performance

The computational performance of the different methods for Cases 1 and 2 are compared in Tables 7 and 8, respectively. BARON did not return a global solution within 30 days for either problem, while DA, EDA, and MEDA all obtained a global solution within 18 h for Case 1 and within 60 h for Case 2. These results demonstrate that viability of the decomposition strategy for the global optimization of flexible polygeneration systems.

**Table 8. Computational Performance of Different Solvers for Case 2**

	BARON	DA	EDA	MEDA
Total solver time (s)	—*	215280.2	26390.0	15158.6
Solver time for Problem (PBP <sub>h</sub> ) (s)	n/a	202.2	39.7	1.2
Solver time for Problem (FP <sub>h</sub> ) (s)	n/a	6.6	2.4	0.8
Solver time for the master problem <sup>†</sup> (s)	n/a	612.5	26.3	10.3
Solver time for Problem (PP <sub>h</sub> ) (s)	n/a	214458.9	12454.7	4519.8
Solver time for Problem (DPP <sub>h</sub> ) (s)	n/a	n/a	13867.0	10626.5
Integer realizations visited by Problem (PBP <sub>h</sub> )	n/a	613	132	46
Integer realizations visited by Problem (PP <sub>h</sub> )	n/a	537	77	14
Integer realizations visited by Problem (DPP <sub>h</sub> )	n/a	n/a	6	3

\*No global solution was returned within 30 days.

<sup>†</sup>The master problem is Problem (RMP) or (ERMP) or (MERMP).

Note that the solution time for Problem (PP) dominates the total solution time within DA, because Problem (PP) is the only nonconvex NLP subproblem in DA, and the solution time for it is much longer than that for other subproblems. By introducing extra dual information from the PP to form a tighter master problem, EDA significantly reduced the number of iterations for convergence, and it solved much fewer Problem (PBP) and (more importantly) Problem (PP). The solution time with EDA was reduced by almost an order of magnitude compared to that with DA for both cases, although it spent a fairly large amount of time to solve Problem (DPP) to obtain extra dual information for a tighter relaxation. In addition, by adopting the multicut strategy for an even tighter relaxation, MEDA achieved faster convergence than EDA and further reduced the solution time for both cases.

Also, note that the number of scenarios in Case 2 is three times of that in Case 1, and the solution time for Case 2 was around two to four times of that for Case 1 for all of the three decomposition methods. This indicates the favorable scalability of the decomposition strategy with respect to the number of scenarios as also shown by the case studies in Ref. 18.

## Conclusions and Future Work

An enhanced decomposition method has been developed for the global optimal design and operation of a flexible energy polygeneration system. This method obtains tighter relaxations than the original decomposition method by exploiting more dual information, and it guarantees finite termination with an  $\varepsilon$ -optimal solution or infeasibility indication. The case study results demonstrate that the enhanced decomposition method achieves much faster convergence than the original decomposition method and the state-of-the-art global optimization solver, BARON. By introducing the primal dual multicuts, the performance of enhanced decomposition method is further improved. The global optimal solution of the polygeneration optimization problem can be obtained by the enhanced decomposition method in relatively short times.

Several interesting issues will be addressed in the future work. First, the dual information of the PP can be exploited in a more efficient and effective manner, so that the solution can be further accelerated. For example, a better heuristic may be developed to determine whether to solve Problem (DPP<sub>h</sub>) or not at each iteration, so that this difficult nonconvex NLP is only solved when it can provide strong primal dual cuts to accelerate the solution. Second, more sophisticated models, that is, (a) stochastic models with uncertainties in market prices and demands and (b) large-scale nonconvex mixed-integer nonlinear models with more technical choices, will be developed. Third, parallel computation will be considered for solving subproblems in different scenarios to accelerate computational speed.

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## Literature Cited

- BP Statistical Review of World Energy (June 2010). Available at <http://www.bp.com/productlanding.do?categoryId=6929&contentId=7044622> (accessed August 2010).
- Ansolahehere S, Beer J, Deutch J, Ellerman AD, Friedmann SJ, Herzog H, Jacoby HD, Joskow PL, Mcrae G, Lester R, Moniz EJ, Steinfeld E, Katzer J. *The future of coal: options for a carbon-constrained world*. Tech. rep. Cambridge, MA: Massachusetts Institute of Technology, 2007.
- Hamelinck CN, Faaij APC, Uil H, Boerrigter H. *Production of FT transportation fuels from biomass: technical options, process analysis and optimization, and development potential*. Tech. Rep. NWS-E-2003-08, The Netherlands: Universiteit Utrecht, Utrecht, 2003.
- Liu P, Gerogiorgis DI, Pistikopoulos EN. Modeling and optimization of polygeneration energy systems. *Catal Today*. 2007;127(1-4):347-359.
- Liu P, Pistikopoulos EN, Li Z. A mixed-integer optimization approach for polygeneration energy systems design. *Comput Chem Eng*. 2009;33(3):759-768.
- Liu P, Pistikopoulos EN, Li Z. A multi-objective optimization approach to polygeneration energy systems design. *AIChE J*. 2010;56(5):1218-1234.
- Liu P, Pistikopoulos EN, Li Z. Decomposition based stochastic programming approach for polygeneration energy systems design under uncertainty. *Ind Eng Chem Res*. 2010;49(7):3295-3305.
- Chen Y, Adams TA II, Barton PI. Optimal design and operation of static energy polygeneration systems. *Ind Eng Chem Res*. 2011;50(9):5099-5113.
- Chen Y, Adams TA II, Barton PI. Optimal design and operation of flexible energy polygeneration systems. *Ind Eng Chem Res*. 2011;50(8):4553-4566.
- Li F, Fan L. Clean coal conversion processes — progress and challenges. *Energy Environ Sci*. 2008;1(2):248-267.
- Woods MC, Capicotto PJ, Haslbeck JL, Kuehn NJ, Matuszewski M, Pinkerton LL, Rutkowski MD, Schoff RL, Vaysman V. *Cost and performance baseline for fossil energy plants. Volume 1: bituminous coal and natural gas to electricity*. Tech. Rep. DOE/NETL-2007/1281. Pittsburgh, PA: National Energy Technology Laboratory, 2007.
- van Bibber L, Shuster E, Haslbeck J, Rutkowski M, Olson S, Kramer S. Baseline technical and economic assessment of a commercial scale Fischer-Tropsch liquids facility. Tech. Rep. DOE/NETL-2007/1260. Pittsburgh, PA: National Energy Technology Laboratory, 2007.
- van Bibber L, Shuster E, Haslbeck J, Rutkowski M, Olson S, Kramer S. *Technical and economic assessment of small-scale Fischer-Tropsch liquids facilities*. Tech. Rep. DOE/NETL-2007/1253. Pittsburgh, PA: National Energy Technology Laboratory, 2007.
- Adams TA II, Barton PI. High-efficiency power production from coal with carbon capture. *AIChE J*. 2010;56(12):3120-3136.
- Tawarmalani M, Sahinidis NV. Global optimization of mixed-integer nonlinear programs: a theoretical and computational study. *Math Program*. 2004;99(3):563-591.
- Khajavirad A, Michalek JJ. A deterministic Lagrangian-based global optimization approach for quasiseparable nonconvex mixed-integer nonlinear programs. *J Mech Des*. 2009;131(5):051009.
- Karupiah R, Grossmann IE. A Lagrangean based branch-and-cut algorithm for global optimization of nonconvex mixed-integer nonlinear programs with decomposable structures. *J Glob Optim*. 2008;41(2):163-186.
- Li X, Armagan E, Tomasgard A, Barton PI. Stochastic pooling problem for natural gas production network design and operation under uncertainty. *AIChE J*. 2011;57(8):2120-2135.
- Li X, Tomasgard A, Barton PI. Decomposition strategy for natural gas production network design under uncertainty. *Proceedings of the 49th IEEE Conference on Decision and Control*. Atlanta, GA, 2010:188-193.
- Li X, Tomasgard A, Barton PI. Decomposition strategy for the stochastic pooling problem. *J Glob Optim*. 2011; DOI: 10.1007/s10898-011-9792-0.
- Li X, Tomasgard A, Barton PI. Nonconvex generalized Benders decomposition for stochastic separable mixed-integer nonlinear programs. *Optim Theory Appl*. 2011;151(3):425-454.
- Geoffrion AM. Generalized Benders decomposition. *J Optim Theory Appl*. 1972;10(4):237-260.
- Adams TA II, Barton PI. Combining coal gasification and natural gas reforming for efficient polygeneration. *Fuel Process Technol*. 2011;92(3):639-655.
- Seider WD, Seader JD, Lewin DR, Widagdo S. *Product and Process Design Principles: Synthesis, Analysis, and Evaluation*. Hoboken, NJ: Wiley, 2009.
- Tawarmalani M, Sahinidis N. *Convexification and Global Optimization in Continuous and Mixed-Integer Nonlinear Programming*. Dordrecht, The Netherlands: Kluwer Academic Publishers, 2002.
- Benders JF. Partitioning procedures for solving mixed-variables programming problems. *Numer Math*. 1962;4:238-252.



27. Balas E, Jeroslow R. Canonical cuts on the unit hypercube. *SIAM J Appl Math.* 1972;23(1):61–69.
28. Bertsekas DP. *Nonlinear Programming*. Cambridge, MA: Athena Scientific, 1999.
29. Birge JR, Louveaux FV. A multicut algorithm for two-stage stochastic linear programs. *Eur J Oper Res.* 1988;34(3):384–392.
30. Kesavan P, Allgor RJ, Gatzke EP, Barton PI. Outer approximation algorithms for separable nonconvex mixed-integer nonlinear programs. *Math Program.* 2004;100(3):517–535.
31. Intercontinental Exchange (ICE) Report Data. Available at <https://www.theice.com/marketdata/reports/ReportCenter.shtml> (accessed December 2010).
32. U.S. Energy Information Administration. Petroleum Navigator: Monthly Spot Prices. Available at [http://tonto.eia.doe.gov/dnav/pet/pet\\_pri\\_spt\\_s1\\_m.htm](http://tonto.eia.doe.gov/dnav/pet/pet_pri_spt_s1_m.htm) (accessed December 2010).
33. Methanex Monthly Average Regional Posted Contract Price History. Available at <http://www.methanex.com/products/methanolprice.html> (accessed December 2010).
34. Drud A. CONOPT. ARKI Consulting and Development A/S, Bagsvaerd, Denmark. Available at <http://www.gams.com/docs/document/conopt.pdf> (accessed January 2011).
35. CPLEX 12. Available at <http://www.gams.com/docs/document/cplex.pdf> (accessed January 2011).

## Appendix: Estimation of Equipment Capacity and Cost Parameters

The choices for the capacity of the set of equipment  $w$  ( $\bar{E}_{w,v}$ ) are assumed to be uniformly distributed and can be generated as follows

$$\bar{E}_{w,v} = \bar{E}_w^L + \frac{v-1}{d-1} (\bar{E}_w^U - \bar{E}_w^L), \quad \forall w \in \{1, \dots, e\} \quad (A1)$$

where  $\bar{E}_w^L$  and  $\bar{E}_w^U$  are the minimum and maximum possible capacity for the set of equipment  $w$  in the process, respectively, which are specified parameters.  $\bar{E}_w^L$  and  $\bar{E}_w^U$  can be estimated by the rough mass balance calculations given the aforementioned gasifier capacity, and their values are listed in Table A1.

The choices for the capital cost of the set of equipment  $w$  ( $\bar{C}_{w,v}$ ) are estimated by the following power law scaling relationship

$$\bar{C}_{w,v} = \bar{C}_{b,w} \left( \frac{\bar{E}_{w,v}}{\bar{E}_{b,w}} \right)^{\text{sf}_w}, \quad \forall w \in \{1, \dots, e\}, \quad \forall v \in \{1, \dots, d\} \quad (A2)$$

where  $\bar{E}_{b,w}$  is the capacity of the set of equipment  $w$  in the base case,  $\bar{C}_{b,w}$  is the capital cost of the set of equipment  $w$  in the corresponding base case, and  $\text{sf}_w$  is the sizing factor of the set of equipment  $w$ , which are specified parameters. The values of  $\bar{E}_{b,w}$ ,  $\bar{C}_{b,w}$ , and  $\text{sf}_w$  for aggregate equipment, which are estimated from those for individual equipment in our prior work,<sup>9</sup> are provided in Table A2.

**Table A1. Parameters for Equipment Capacities**

Aggregate Equipment $w$	$\bar{E}_w^L$	$\bar{E}_w^U$	Unit
Syngas cleaning system 1	0	150	Mmol/h
Syngas cleaning system 2	0	205	Mmol/h
CO <sub>2</sub> compressor	0	2500	ton/h
Fischer–Tropsch synthesis system	0	340	ton/h
Methanol synthesis system	0	840	ton/h
Gas turbine system	200	4750	MW
Steam turbine system	600	1800	MW

**Table A2. Parameters for Equipment Capital Costs**

Aggregate Equipment $w$	$\bar{E}_{b,w}$	$\bar{C}_{b,w}$ (million dollars)	$\text{sf}_w$
Syngas cleaning system 1	28.2 Mmol/h	34.0	0.69
Syngas cleaning system 2	28.2 Mmol/h	34.0	0.69
CO <sub>2</sub> compressor	469.0 ton/h	75.1	0.80
Fischer–Tropsch synthesis system	34.2 ton/h	183.4	0.70
Methanol synthesis system	110.4 ton/h	220.3	0.67
Gas turbine system	464.0 MW	136.4	0.76
Steam turbine system	274.7 MW	123.3	0.69

## Mathematical Proofs

### Proof of Proposition 1

**Proof.** According to the equivalency of Problems (ERMP<sup>k</sup>) and (ERMP1<sup>k</sup>), the following property is proved: any  $y$  that is feasible for Problem (P) augmented with the Balas cuts is also feasible for Problem (ERMP1<sup>k</sup>), and the optimal objective of Problem (ERMP1<sup>k</sup>) is a lower bound of that of Problem (P) augmented with the Balas cuts.

Define

$$\begin{aligned} \text{obj}_{\text{PP}}(y) = \min_{\substack{(x_h, q_h, u_h) \in \bar{\Pi}_h, \\ \forall h \in \{1, \dots, s\}}} & c_1^T y + \sum_{h=1}^s (c_{2,h}^T x_h + c_{3,h}^T q_h + c_{4,h}^T u_h) \\ \text{s.t.} & A_{1,h} y + A_{2,h} x_h + A_{3,h} q_h \\ & + A_{4,h} u_h \leq b_h, \quad \forall h \in \{1, \dots, s\} \end{aligned}$$

From weak duality,

$$F_P(y, \lambda_1^{(r)}, \dots, \lambda_s^{(r)}) \leq \text{obj}_{\text{PP}}(y), \quad \forall r \in V^k, \quad \forall y \in Y \quad (A3)$$

$$F_P(y, \check{\lambda}_1^{(r)}, \dots, \check{\lambda}_s^{(r)}) \leq \text{obj}_{\text{PP}}(y), \quad \forall r \in V^k, \quad \forall y \in Y \quad (A4)$$

For all  $\hat{y}$  that is feasible for Problem (P) augmented with the Balas cuts, pick  $\hat{\eta} = \text{obj}_{\text{PP}}(\hat{y})$ , then

$$\hat{\eta} \geq F_P(\hat{y}, \lambda_1^{(r)}, \dots, \lambda_s^{(r)}) \quad (A5)$$

and

$$\hat{\eta} \geq F_P(\hat{y}, \check{\lambda}_1^{(r)}, \dots, \check{\lambda}_s^{(r)}) \quad (A6)$$

Define

$$\begin{aligned} \text{obj}_{\text{PBP}}(y) = \min_{\substack{(x_h, q_h, u_h) \in \tilde{\Pi}_h, \\ \forall h \in \{1, \dots, s\}}} & c_1^T y + \sum_{h=1}^s (c_{2,h}^T x_h + c_{3,h}^T q_h + c_{4,h}^T u_h) \\ \text{s.t.} & A_{1,h} y + A_{2,h} x_h + A_{3,h} q_h + A_{4,h} u_h \leq b_h, \\ & \forall h \in \{1, \dots, s\} \end{aligned}$$

Due to their definitions, set  $\tilde{\Pi}_h$  is a convex relaxation of the set  $\bar{\Pi}_h$ , hence

$$\tilde{\Pi}_h \subset \bar{\Pi}_h, \quad \forall h \in \{1, \dots, s\} \quad (A7)$$

then

$$\text{obj}_{\text{PP}}(y) \geq \text{obj}_{\text{PBP}}(y), \quad \forall y \in Y \quad (A8)$$

From strong duality for linear programs<sup>28</sup>

$$F(y, \lambda_1^{(j)}, \dots, \lambda_s^{(j)}) = \text{obj}_{\text{PBP}}(y), \quad \forall j \in T^k \setminus V^k, \quad \forall y \in Y \quad (A9)$$

So

$$\hat{\eta} \geq F(\hat{y}, \lambda_1^{(j)}, \dots, \lambda_s^{(j)}) \quad (\text{A10})$$

holds from Eqs. A8 and A9.

According to the definition of Problem (RMP<sup>k</sup>), for all  $\hat{y}$  that is feasible for Problem (P) augmented with the Balas cuts is also feasible for Problem (RMP<sup>k</sup>).<sup>20</sup> So

$$G(\hat{y}, \mu_1^{(i)}, \dots, \mu_s^{(i)}) \leq 0 \quad (\text{A11})$$

holds.

Equations A5, A6, A10, and A11 imply that  $(\hat{y}, \hat{\eta})$  is feasible for Problem (ERMP1<sup>k</sup>), and

$$\text{obj}_{\text{ERMP1}^k} \leq \hat{\eta} = \text{obj}_{\text{PP}}(\hat{y}), \quad \forall \hat{y} \in \Phi \quad (\text{A12})$$

where  $\text{obj}_{\text{ERMP1}^k}$  is the optimal objective value of Problem (ERMP1<sup>k</sup>), and the set

$$\Phi \equiv \{y \in Y : A_{1,h}y + A_{2,h}x_h + A_{3,h}q_h + A_{4,h}u_h \leq b_h \\ \text{for some } (x_h, q_h, u_h) \in \tilde{\Pi}_h\}$$

Hence,

$$\text{obj}_{\text{ERMP1}^k} \leq \min_{\hat{y} \in \Phi} \text{obj}_{\text{PP}}(\hat{y}) = \text{obj}_{\text{P}} \quad (\text{A13})$$

where  $\text{obj}_{\text{P}}$  is the optimal objective of Problem (P). ■

### Proof of Proposition 2

**Proof.** Problem (RMP<sup>k</sup>) can be equivalently reformulated into the following problem<sup>20</sup>

$$\begin{aligned} \min_{y, \eta} \quad & \eta \\ \text{s.t.} \quad & \eta \geq F(y, \lambda_1^{(j)}, \dots, \lambda_s^{(j)}), \quad \forall j \in T^k, \\ & G(y, \mu_1^{(i)}, \dots, \mu_s^{(i)}) \leq 0, \quad \forall i \in S^k, \\ & \sum_{l \in \{l: y_l^{(i)} = 1\}} y_l - \sum_{l \in \{l: y_l^{(i)} = 0\}} y_l \leq |\{l : y^{(i)} = 1\}| - 1, \quad \forall t \in T^k \cup S^k, \\ & y \in Y, \quad \eta \in \mathbb{R} \end{aligned} \quad (\text{RMP1}^k)$$

According to the equivalency of Problems (RMP<sup>k</sup>) and (RMP1<sup>k</sup>) and the equivalency of Problems (ERMP<sup>k</sup>) and (ERMP1<sup>k</sup>), the following property is proved: problem (ERMP1<sup>k</sup>) is a tighter (or equal) underestimate of Problem (P) augmented with the Balas cuts compared to Problem (RMP1<sup>k</sup>).

For all  $(\hat{y}, \hat{\eta})$  feasible for Problem (ERMP1<sup>k</sup>),

$$\hat{\eta} \geq F(\hat{y}, \lambda_1^{(j)}, \dots, \lambda_s^{(j)}), \quad \forall j \in T^k \setminus V^k \quad (\text{A14})$$

$$G(\hat{y}, \mu_1^{(i)}, \dots, \mu_s^{(i)}) \leq 0, \quad \forall i \in S^k \quad (\text{A15})$$

and

$$\hat{\eta} \geq F_{\text{P}}(\hat{y}, \lambda_1^{(r)}, \dots, \lambda_s^{(r)}), \quad \forall r \in V^k \quad (\text{A16})$$

Based on Eq. A7, the following relationship holds

$$F_{\text{P}}(y, \lambda_1^{(r)}, \dots, \lambda_s^{(r)}) \geq F(y, \lambda_1^{(r)}, \dots, \lambda_s^{(r)}), \quad \forall r \in V^k, \quad \forall y \in Y \quad (\text{A17})$$

So  $\hat{\eta} \geq F(\hat{y}, \lambda_1^{(r)}, \dots, \lambda_s^{(r)})$  ( $\forall r \in V^k$ ). Hence,  $(\hat{y}, \hat{\eta})$  is also feasible for problem (RMP1<sup>k</sup>).

Therefore, Problem (ERMP1<sup>k</sup>) is a tighter (or equal) underestimate of Problem (P) augmented with the Balas cuts compared to Problem (RMP1<sup>k</sup>). ■

### Proof of Proposition 3

**Proof.** According to the idea in Ref. 22, Problem (P) can be equivalently transformed into the following form by projection from the space of both continuous and integer variables to the space of only the integer variables

$$\begin{aligned} \min_y \quad & c_1^T y + \sum_{h=1}^s v_h(y) \\ \text{s.t.} \quad & v_h(y) = \min_{x_h, q_h, u_h} \left\{ \begin{aligned} & c_{2,h}^T x_h + c_{3,h}^T q_h + c_{4,h}^T u_h \\ & \text{s.t. } A_{1,h}y + A_{2,h}x_h + A_{3,h}q_h + A_{4,h}u_h \leq b_h, \\ & (x_h, q_h, u_h) \in \tilde{\Pi}_h, \end{aligned} \right\} \\ & \forall h \in \{1, \dots, s\} \\ & y \in \Phi \end{aligned} \quad (\text{P1})$$

According to the equivalency of Problems (P) and (P1) and the equivalency of Problems (MERMP<sup>k</sup>) and (MERMP1<sup>k</sup>), the following property is proved: any  $y$  that is feasible for Problem (P1) augmented with the Balas cuts is also feasible for Problem (MERMP1<sup>k</sup>), and the optimal objective of Problem (MERMP1<sup>k</sup>) is a lower bound of that of Problem (P1) augmented with the Balas cuts.

Based on weak duality

$$F_{\text{P},h}(y, \lambda_h^{(r)}) \leq v_h(y), \quad \forall h \in \{1, \dots, s\}, \quad \forall r \in V^k, \quad \forall y \in \Phi \quad (\text{A18})$$

$$F_{\text{P},h}(y, \check{\lambda}_h^{(r)}) \leq v_h(y), \quad \forall h \in \{1, \dots, s\}, \quad \forall r \in V^k, \quad \forall y \in \Phi \quad (\text{A19})$$

For all  $\hat{y}$  feasible for Problem (P1) augmented with the Balas cuts, pick  $\hat{\eta}_h = v_h(\hat{y})$  and  $\hat{\eta} = c_1^T \hat{y} + \sum_{h=1}^s \hat{\eta}_h$ , then

$$\hat{\eta}_h \geq F_{\text{P},h}(\hat{y}, \lambda_h^{(r)}), \quad \forall h \in \{1, \dots, s\} \quad (\text{A20})$$

$$\hat{\eta}_h \geq F_{\text{P},h}(\hat{y}, \check{\lambda}_h^{(r)}), \quad \forall h \in \{1, \dots, s\} \quad (\text{A21})$$

**Table A3. Fractions of Occurrence of All Scenarios for Case 1**

Scenario	Occurrence (%)
Spring peak*	12.01
Spring off-peak	13.21
Summer peak†	11.82
Summer off-peak	13.39
Fall peak‡	11.32
Fall off-peak	13.61
Winter peak§	11.19
Winter off-peak	13.46

\*Spring  $\equiv$  {March, April, May}.

†Summer  $\equiv$  {June, July, August}.

‡Fall  $\equiv$  {September, October, November}.

§Winter  $\equiv$  {December, January, February}.

**Table A4. Fractions of Occurrence of All Scenarios for Case 2**

Scenario	Occurrence (%)
January peak	3.86
January off-peak	4.63
February peak	3.65
February off-peak	4.02
March peak	4.04
March off-peak	4.45
April peak	3.91
April off-peak	4.31
May peak	4.04
May off-peak	4.45
June peak	3.91
June off-peak	4.31
July peak	3.86
July off-peak	4.63
August peak	4.04
August off-peak	4.45
September peak	3.73
September off-peak	4.49
October peak	4.05
October off-peak	4.45
November peak	3.55
November off-peak	4.67
December peak	3.68
December off-peak	4.82

and

$$\hat{\eta} \geq c_1^T \hat{y} + \sum_{h=1}^s \hat{\eta}_h \quad (\text{A22})$$

Define

$$v_h^R(y) = \min_{(x_h, q_h, u_h) \in \tilde{\Pi}_h} c_{2,h}^T x_h + c_{3,h}^T q_h + c_{4,h}^T u_h$$

s.t.  $A_{1,h}y + A_{2,h}x_h + A_{3,h}q_h + A_{4,h}u_h \leq b_h$

Based on Eq. A7

$$v_h(y) \geq v_h^R(y), \quad \forall y \in \Phi \quad (\text{A23})$$

According to strong duality for linear programs

$$F_h(y, \lambda_h^{(j)}) = v_h^R(y), \quad \forall h \in \{1, \dots, s\}, \quad \forall j \in T^k \setminus V^k, \quad \forall y \in Y \quad (\text{A24})$$

Hence

$$\hat{\eta}_h \geq F_h(\hat{y}, \lambda_h^{(j)}), \quad \forall h \in \{1, \dots, s\} \quad (\text{A25})$$

from Eqs. A23 and A24.

In addition,  $\hat{y} \in \Phi$  implies  $\exists(x_h, q_h, u_h) \in \tilde{\Pi}_h \subset \hat{\Pi}_h$  (Eq. A7) such that

$$A_{1,h}\hat{y} + A_{2,h}x_h + A_{3,h}q_h + A_{4,h}u_h - b_h \leq 0, \quad \forall h \in \{1, \dots, s\} \quad (\text{A26})$$

As Lagrange multipliers

$$\mu_h^{(i)} \geq 0, \quad \forall h \in \{1, \dots, s\}, \quad \forall i \in S^k \quad (\text{A27})$$

So

$$G_h(\hat{y}, \mu_h^{(i)}) \leq 0, \quad \forall h \in \{1, \dots, s\} \quad (\text{A28})$$

Equations A20, A21, A25, and A27 imply  $(\hat{y}, \hat{\eta}, \hat{\eta}_1, \dots, \hat{\eta}_s)$  is feasible for Problem (MERMP1<sup>k</sup>), and

$$\text{obj}_{\text{MERMP1}^k} \leq \hat{\eta} = c_1^T \hat{y} + \sum_{h=1}^s \hat{\eta}_h = c_1^T \hat{y} + \sum_{h=1}^s v_h(\hat{y}), \quad \forall \hat{y} \in \Phi \quad (\text{A29})$$

where  $\text{obj}_{\text{MERMP1}^k}$  is the optimal objective value of Problem (MERMP1<sup>k</sup>). Hence,

$$\text{obj}_{\text{MERMP1}^k} \leq \min_{\hat{y} \in \Phi} c_1^T \hat{y} + \sum_{h=1}^s v_h(\hat{y}) = \text{obj}_{\text{P1}} \quad (\text{A30})$$

where  $\text{obj}_{\text{P1}}$  is the optimal objective value of Problem (P1). ■

#### Proof of Proposition 4

**Proof.** For all  $(\hat{y}, \hat{\eta}, \hat{\eta}_1, \dots, \hat{\eta}_s)$  feasible for Problem (MERMP1<sup>k</sup>),

$$\hat{\eta} \geq c_1^T \hat{y} + \sum_{h=1}^s \hat{\eta}_h \quad (\text{A31})$$

$$\hat{\eta}_h \geq \tilde{\alpha}_h^{(r)} \hat{y} + \tilde{\beta}_h^{(r)}, \quad \forall h \in \{1, \dots, s\}, \quad \forall r \in V^k \quad (\text{A32})$$

$$\hat{\eta}_h \geq \check{\alpha}_h^{(r)} \hat{y} + \check{\beta}_h^{(r)}, \quad \forall h \in \{1, \dots, s\}, \quad \forall r \in V^k \quad (\text{A33})$$

$$\hat{\eta}_h \geq \alpha_h^{(j)} \hat{y} + \beta_h^{(j)}, \quad \forall h \in \{1, \dots, s\}, \quad \forall j \in T^k \setminus V^k \quad (\text{A34})$$

$$\gamma_h^{(i)} \hat{y} + \theta_h^{(i)} \leq 0, \quad \forall h \in \{1, \dots, s\}, \quad \forall i \in S^k \quad (\text{A35})$$

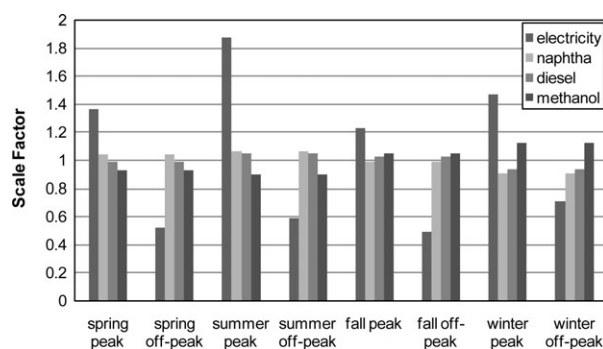
Sum Eq. A32 over all the scenarios, then

$$\hat{\eta} \geq \tilde{\alpha}^{(r)} \hat{y} + \tilde{\beta}^{(r)}, \quad \forall r \in V^k \quad (\text{A36})$$

Similarly, Eqs. A33–A35 imply

$$\hat{\eta} \geq \check{\alpha}^{(r)} \hat{y} + \check{\beta}^{(r)}, \quad \forall r \in V^k \quad (\text{A37})$$

$$\hat{\eta} \geq \alpha^{(j)} \hat{y} + \beta^{(j)}, \quad \forall j \in T^k \setminus V^k \quad (\text{A38})$$



**Figure A1. Scale factors of product prices in all scenarios for Case 1.**

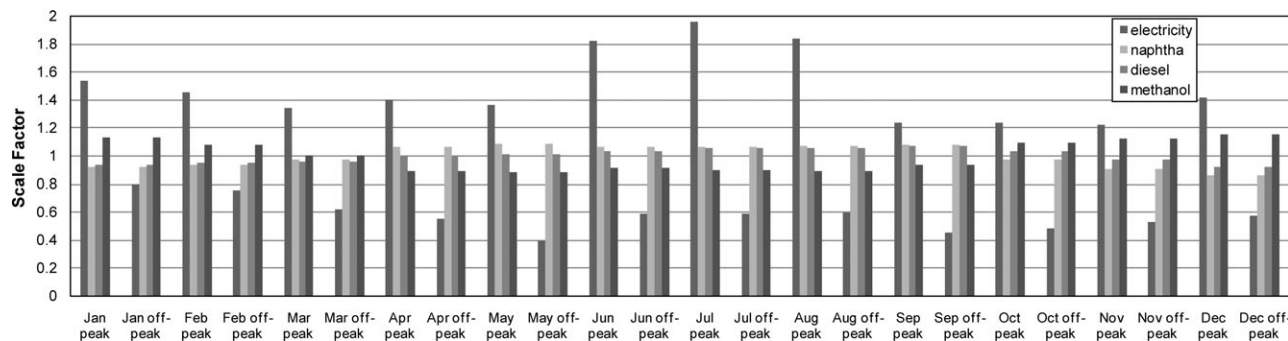


Figure A2. Scale factors of product prices in all scenarios for Case 2.

$$\gamma^{(i)}\hat{y} + \theta^{(i)} \leq 0, \quad \forall i \in S^k \quad (\text{A39})$$

Hence  $(\hat{y}, \hat{\eta})$  is also feasible for Problem (ERMP<sup>k</sup>).

Therefore, Problem (MERMP<sup>k</sup>) is a tighter (or equal) underestimate of Problem (P) augmented with the Balas cuts compared to Problem (ERMP<sup>k</sup>). ■

### Parameters for Scenarios

This part includes the fractions of occurrence of all scenarios for Cases 1 and 2 (as shown in Tables A3 and A4) and scale factors of product prices in all scenarios for Cases 1 and 2 (as shown in Figures A1 and A2).

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