# Optimal Design and Operation of Energy Systems under Uncertainty

Paul I. Barton<sup>\*</sup> Xiang Li<sup>\*\*</sup>

 \* Process Systems Engineering Laboratory, Department of Chemical Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139 USA (e-mail: pib@ mit.edu).
 \*\* Department of Chemical Engineering, Queen's University, 19 Division Street, Kingston, ON K7L3N6 Canada (e-mail: xiang.li@ chee.queensu.ca).

Abstract: This paper is concerned with integrated design and operation of energy systems that are subject to significant uncertainties. The problem is cast as a two-stage stochastic nonconvex mixed-integer nonlinear program, in which the first and second stages include design decisions and operational decisions, respectively. By exploiting the separable and decomposable structure of the problem, an efficient global optimization method, called nonconvex generalized Benders decomposition (NGBD), is developed based on convex relaxation and generalized Benders decomposition. The efficiency of NGBD can be further improved via the notion of piecewise convex relaxations. The advantages of the proposed formulation and solution method are demonstrated through case studies of two industrial energy systems, a natural gas production network and a polygeneration plant. The first example shows that the stochastic programming formulation can result in better expected economic performance than the deterministic formulation, and that the NGBD solution method is dramatically more efficient than a state-of-the-art global optimization solver, especially for large numbers of scenarios. The second example further shows that the integration of piecewise convex relaxations can improve the efficiency of NGBD by at least an order of magnitude.

*Keywords:* Keywords: Integrated design and operation; Energy systems; Uncertainty; Stochastic mixed-integer nonlinear program; Global optimization.

#### 1. INTRODUCTION

Global primary energy demand is projected to increase by over one third from 2012 to 2035 (International Energy Agency (2012)). This will result in increasing needs for developing new and expanding existing energy systems, especially clean and/or renewable energy systems (e.g. natural gas production systems, biofuel plants), due to concerns with energy and environmental sustainability. The energy system development problem can be viewed as an integrated design and operation problem, as both design and operational decisions have to be involved in finding an optimal solution. The design decisions are those to be determined before and implemented during the development of the system, such as the layout of the system and the capacities of the units involved. The operational decisions are those to be implemented *after* development of the system, such as the physical conditions under which the system is operated. In addition, uncertainty in the energy resources and fluctuations in market conditions need to be considered in the problem, as they usually have significant impact on the optimality and even feasibility of operating the system.

This paper focuses on the optimal design and operation of energy systems under uncertainty through mathematical programming. The mathematical programming formulation to be considered can be expressed in the following form:

$$\min_{\substack{x_1,...,x_s,y \\ s.t. \ g_h(x_h) + B_h y \le 0, \\ y \in X_h, \ \forall h \in \{1,...,s\}, \\ y \in Y, \end{aligned}} \begin{cases} \min_{\substack{x_1,...,x_s \\ s \in X_h, \\ y \in Y, \\ s = 1, \dots, s \\ h \in \{1,...,s\}, \\ h \in \{1,...,s\}, \\ h \in \{1,...,s\}, \end{cases}$$
(P)

where  $X_h = \{x_h \in \Pi_h \subset \mathbb{R}^{n_x} : p_h(x_h) \leq 0\}, Y = \{y \in \{0,1\}^{n_y} : Ay \leq d\}, \Pi_h \text{ is convex, functions } f_h : \Pi_h \to \mathbb{R}, g_h : \Pi_h \to \mathbb{R}^m \text{ and } p_h : \Pi_h \to \mathbb{R}^{m_p} \text{ are continuous, and it is assumed that at least one function is nonconvex. The binary variables <math>y$  represent design decisions such as whether to develop a unit or connection in the system. The discrete and/or continuous variables  $x_h$  represent operational decisions, such as the throughput of the system, for scenario h. A scenario may represent a possible realization of uncertain parameters whose outcome is known only after development of the system; in this case  $w_h > 0$  represents the probability of occurrence of the scenario. Or a scenario may be associated with a particular operating period in which values of some parameters are different from those in other operating periods; in this case  $w_h$  represents the frequency of occurrence of the operating period. In the

objective function of Problem (P),  $c_h^{\mathrm{T}}y$  represents the cost associated with the design decisions for scenario h and  $f_h(x_h)$  represents the cost associated with the operational decisions for scenario h. Note that any equality constraint in the problem can always be expressed as paired inequalities. Obviously, the size of Problem (P) depends on the number of scenarios addressed, s. As the uncertainty usually needs to be characterized with a large number of scenarios, Problem (P) is usually a large-scale nonconvex mixed-integer nonlinear program (MINLP).

Problem (P) needs to be solved to global optimality to achieve the highest profits (or lowest costs), but solution of this nonconvex MINLP is often computationally challenging. This is because the solution times of classical global optimization methods, such as branch-and-reduce (Tawarmalani and Sahinidis (2004)), SMIN- $\alpha$ BB and GMIN- $\alpha$ BB (Adjiman et al. (2000)), and nonconvex outer approximation (Kesavan et al. (2004)), increase dramatically with the the sizes of the problems to be solved. Recently, a decomposition-based global optimization method, called nonconvex generalized Benders decomposition (NGBD), has been developed based on dual decomposition and convex relaxation (Li et al. (2011b)). By exploitation of the decomposable structure of Problem (P), NGBD can solve Problem (P) to global optimality efficiently, and the solution time for NGBD does not grow dramatically with the number of scenarios involved in the problem. In addition, NGBD performs better with tighter convex relaxations that are used to bound the final solution. Therefore, the performance of NGBD can be further improved by integration of a piecewise convex relaxation framework, which is known to enable tighter convex relaxations.

This paper is organized as follows: Section 2 gives an introduction to NGBD, and Section 3 presents a piecewise relaxation framework for factorable functions and the integration of the framework in NGBD. The benefits of explicit consideration of uncertainty and NGBD method are demonstrated through two industrial case studies in Section 4 and the paper concludes in Section 5.

## 2. NONCONVEX GENERALIZED BENDERS DECOMPOSITION

## 2.1 Subproblems

NGBD solves Problem (P) by solving a sequence of subproblems, which generate a sequence of upper bounds and a sequence of lower bounds that converge to a global optimum of the problem. The subproblems are constructed via restriction, relaxation, projection and dualization of the original problem or the intermediate subproblems.

On the one hand, Problem (P) can be restricted through fixing  $y = y^{(l)}$  at the *l*th iteration, and the resulting subproblem is called the **Primal Problem (PP)**, whose optimal objective value  $obj_{PP}(y^{(l)})$  is an upper bound for Problem (P). The primal problem can naturally be decomposed into *s* subproblems in the following form:

$$obj_{\mathrm{PP}_h}(y^{(l)}) = \min_{x_h} w_h \left( c_h^{\mathrm{T}} y^{(l)} + f_h(x_h) \right)$$
  
s.t.  $g_h(x_h) + B_h y^{(l)} \leq 0, \qquad (\mathrm{PP}_h^l)$   
 $x_h \in X_h.$ 

Obviously,  $\sum_{h=1}^{s} obj_{\text{PP}_h}(y^{(l)}) = obj_{\text{PP}}(y^{(l)})$ . The size of this nonconvex nonlinear programming (NLP) or MINLP problem ( $\text{PP}_h^l$ ) is independent of the number of scenarios and the problem can be solved to  $\epsilon$ -optimality in finite time by state-of-the-art global optimization solvers, such as BARON (Tawarmalani and Sahinidis (2004)). The solution time can be significantly reduced by adding an additional cut derived from the solution of the previously solved subproblems (Li et al. (2011b)).

On the other hand, Problem (P) can be relaxed by convex relaxation of the nonconvex functions therein, and the resulting subproblem is called the lower bounding problem whose optimal objective value is an lower bound for Problem (P). The lower bounding problem can be expressed in the following form:

$$\min_{\substack{x_1,...,x_s,\\e_1,...,e_s,y}} \sum_{h=1}^s w_h \left( c_h^{\mathrm{T}} y + u_{f,h}(x_h, e_h) \right) \\
\text{s.t. } u_{g,h}(x_h, e_h) + B_h y \le 0, \quad \forall h \in \{1, ..., s\}, \quad (\text{LBP}) \\
(x_h, e_h) \in D_h, \quad \forall h \in \{1, ..., s\}, \\
y \in Y,$$

where  $D_h = \{(x_h, e_h) \in \Pi_h \times \Theta_h : u_{p,h}(x_h, e_h) \leq 0, u_{q,h}(x_h, e_h) \leq 0\}, \Theta_h$  is convex, and functions  $u_{f,h} : \Pi_h \times \Theta_h \to \mathbb{R}, u_{g,h} : \Pi_h \times \Theta_h \to \mathbb{R}^m, u_{p,h} : \Pi_h \times \Theta_h \to \mathbb{R}^{m_p}$ and  $u_{e,h} : \Pi_h \times \Theta_h \to \mathbb{R}^{m_e}$  are convex on  $\Pi_h \times \Theta_h$ . So Problem (LBP) is a convex MINLP or a mixed-integer linear program (MILP). This problem involves auxiliary variables  $e_h$  and constraints  $u_{e,h}(x_h, e_h) \leq 0$  that may be required to construct smooth relaxations. Detailed discussions on convex relaxations can be found in Gatzke et al. (2002).

It is well known that the lower bounding problem (LBP) can be solved efficiently using generalized Benders decomposition (GBD) (Geoffrion (1972)). Here a similar decomposition strategy is used to solve Problem (LBP) and also provide integer realizations  $y^{(l)}$  to construct the primal subproblems  $(PP_h^l)$ . Assume that Problem (LBP) satisfies a constraint qualification (which implies strong duality) for any  $y \in Y$  for which Problem (LBP) is feasible, then the problem can be transformed into an equivalent master problem via the principles of projection and dualization (Li et al. (2011b)). Both Problem (LBP) and the master problem are difficult to solve directly, so they are solved via solving a sequence of **Primal Bounding Prob**lems (PBP), Feasibility Problems (FP) and Relaxed Master Problems (RMP), which are much easier to solve. The primal bounding problem is constructed at each iteration k by restricting the binary variables to specific values, say  $y = y^{(k)}$ , in the lower bounding problem, whose solution yields a valid upper bound for the lower bounding problem (and hence the master problem). Furthermore, it can naturally be decomposed into s subproblems of the following form:

$$obj_{\text{PBP}_{h}}(y^{(k)}) = \min_{x_{h}, e_{h}} w_{h} \left( c_{h}^{\text{T}} y^{(k)} + u_{f,h}(x_{h}, e_{h}) \right)$$
  
s.t.  $u_{g,h}(x_{h}, e_{h}) + B_{h} y^{(k)} \leq 0,$   
 $(x_{h}, e_{h}) \in D_{h}.$   
(PBP<sup>k</sup><sub>h</sub>)

Obviously,  $\sum_{h=1}^{s} obj_{\text{PBP}_h}(y^{(k)}) = obj_{\text{PBP}}(y^{(k)})$  where  $obj_{\text{PBP}}(y^{(k)})$  is the optimal objective value of the primal

bounding problem for  $y = y^{(k)}$ . When the primal bounding problem is infeasible for  $y = y^{(k)}$ , a corresponding feasibility problem is solved, which can also be decomposed into *s* subproblems of the following form:

$$obj_{FP_{h}}(y^{(k)}) = \min_{\substack{x_{h}, e_{h}, z_{h}}} w_{h} ||z_{h}||$$
  
s.t.  $u_{g,h}(x_{h}, e_{h}) + B_{h}y^{(k)} \leq z_{h}, \quad (FP_{h}^{k})$   
 $(x_{h}, e_{h}) \in D_{h}, \quad z_{h} \in Z_{h},$ 

where  $\sum_{h=1}^{s} obj_{\text{FP}_h}(y^{(k)}) = obj_{\text{FP}}(y^{(k)})$  and  $obj_{\text{FP}}(y^{(k)})$  is the optimal objective value of the feasibility problem. The relaxed master problem is constructed at each iteration k by relaxing the master problem with a finite number of constraints that are derived according to the solution information of all the previously solved primal bounding and feasibility problems, as follows:

$$\begin{split} \min_{\eta,y} & \eta \\ \text{s.t. } \eta \geq obj_{\text{PBP}}(y^{(j)}) \\ & + \left(\sum_{h=1}^{s} \left(w_{h}c_{h}^{\text{T}} + \left(\lambda_{h}^{(j)}\right)^{\text{T}}B_{h}\right)\right) \left(y - y^{(j)}\right), \quad \forall j \in T^{k}, \\ & 0 \geq obj_{\text{FP}}(y^{(i)}) \\ & + \left(\sum_{h=1}^{s} \left(\mu_{h}^{(i)}\right)^{\text{T}}B_{h}\right) \left(y - y^{(i)}\right), \quad \forall i \in S^{k}, \\ & \sum_{r \in R_{1}^{(t)}} y_{r} - \sum_{r \in R_{0}^{(t)}} y_{r} \leq |R_{1}| - 1, \quad \forall t \in T^{k} \cup S^{k}, \\ & y \in Y, \ \eta \in \mathbb{R}, \end{split}$$
(RMP<sup>k</sup>)

where the index sets

$$\begin{split} T^k &= \{j \in \{1, ..., k\} : (\text{LBP}) \text{ is feasible for } y = y^{(j)}\},\\ S^k &= \{i \in \{1, ..., k\} : (\text{LBP}) \text{ is infeasible for } y = y^{(i)}\},\\ R_1^{(t)} &= \{r \in \{1, ..., n_y\} : y_r^{(t)} = 1\},\\ R_0^{(t)} &= \{r \in \{1, ..., n_y\} : y_r^{(t)} = 0\}. \end{split}$$

The first group of constraints are called optimality cuts and  $\lambda_h^{(j)}$  are the Lagrange multipliers for Problem (PBP<sup>j</sup><sub>h</sub>). The second group of constraints are called feasibility cuts and  $\mu_h^{(i)}$  are the Lagrange multipliers for Problem (FP<sup>i</sup><sub>h</sub>). The last group of constraints is a set of canonical integer cuts that prevent the previously examined integer realizations from becoming a solution (Balas and Jeroslow (1972)). The solution of Problem (RMP<sup>k</sup>) yields a lower bound for the master problem (and therefore Problem (P)) augmented with the integer cuts. The size of Problem (RMP<sup>k</sup>) is determined by the current iteration number instead of the number of scenarios. In case  $T^k = \emptyset$ , the relaxed master problem is unbounded, then a feasibility version of it is solved to allow the algorithm to proceed.

## 2.2 Algorithm

Figure 1 illustrates the NGBD algorithmic flowchart. The inner loop of the algorithm is a GBD-like procedure to solve the lower bounding problem (LBP) via solving primal bounding subproblems (PBP<sub>h</sub><sup>k</sup>) or feasibility subproblems (FP<sub>h</sub><sup>k</sup>) and relaxed master problems (RMP<sup>k</sup>) iteratively. In addition, the solution of (RMP<sup>k</sup>) yields a sequence of



Fig. 1. NGBD Algorithmic Flowchart

integer realizations that will be used to construct primal subproblems  $(\mathrm{PP}_h^l)$  in the outer loop of the algorithm. A sequence of lower bounds will be generated via the solution of relaxed master problems  $(\mathrm{RMP}^k)$  in the inner loop, and a sequence of upper bounds will be generated via the solution of primal subproblems  $(\mathrm{PP}_h^l)$  in the out loop. Note that the sizes of all subproblems to be solved are independent of the number of scenarios. The following theorem states the finite termination of the algorithm.

Theorem 1. If all the subproblems can be solved to  $\epsilon$ optimality in a finite number of steps, then the NGBD
algorithm terminates in a finite number of steps with an  $\epsilon$ -optimal solution of Problem (P) or an indication that
Problem (P) is infeasible.

**Proof.** Proof can be found in Li et al. (2011b).

## 3. PIECEWISE CONVEX RELAXATION OF FACTORABLE FUNCTIONS

In NGBD, the lower bounding problem constructed via convex relaxation serves as a surrogate for Problem (P) for the purpose of valid decomposition. The tightness of the convex relaxation determines the quality of the lower bounding problem and the convergence rate of NGBD. As it is well known that piecewise linear relaxation yields tighter relaxations of bilinear programs than linear relaxation does (e.g. Gounaris et al. (2009)), a piecewise convex relaxation framework is presented in this section for tighter relaxations of functions that are factorable.

# 3.1 Factorable Functions

A function  $f : S \subset \mathbb{R}^{n_x} \to \mathbb{R}$  is called factorable if there exist factors  $q_1, ..., q_L$  such that the function can be represented by a finite sequence of addition, multiplication and univariate functions in the following form:

- $\begin{array}{l} (1) \ q_l = x_l, \ l \in \{1, ..., n_x\}, \\ (2) \ q_l = q_i + q_j, \ \forall (l, i, j) \in \Omega_A, \\ (3) \ q_l = q_i q_j, \ \forall (l, i, j) \in \Omega_M, \end{array}$
- (4)  $q_l = U_l(q_i), \forall (l,i) \in \Omega_U,$

(5) 
$$f(x) = q_L(x)$$
.

Here  $\Omega_A$ ,  $\Omega_M$  and  $\Omega_U$  are index sets that contain indices of the factors associated with additions, multiplications and univariate functions, respectively. Note that most engineering problems can be modelled with factorable functions.

With the factorable representation and the bounds on the factors, a convex underestimator and a concave overestimator of function f can be generated by performing McCormick relaxation (McCormick (1976)) for each multiplication and non-affine univariate function. The next two subsections extend classical McCormick relaxation to piecewise McCormick relaxation for multiplications and univariate functions.

#### 3.2 Relaxation of Multiplications

Consider multiplication z = xy and the known upper and lower bounds on x and y, say,  $x^{\text{lo}}$ ,  $x^{\text{up}}$ ,  $y^{\text{lo}}$ ,  $y^{\text{up}}$ . Let's partition the x domain,  $[x^{\text{lo}}, x^{\text{up}}]$ , into K subdomains (pieces), i.e., picking K + 1 points  $x^1 < x^2 < \ldots < x^{K+1}$ such that  $x^1 = x^{\text{lo}}$ ,  $x^{K+1} = x^{\text{up}}$ . Then the piecewise McCormick relaxation can be expressed as:

$$z^{r} = \sum_{k=1}^{K} z_{k}^{r}, \quad x = \sum_{k=1}^{K} x_{k}, \quad y = \sum_{k=1}^{K} y_{k},$$

$$z_{k}^{r} \ge x^{k+1}y_{k} + x_{k}y^{up} - x^{k+1}y^{up}\delta_{k},$$

$$z_{k}^{r} \ge x^{k}y_{k} + x_{k}y^{lo} - x^{k}y^{lo}\delta_{k},$$

$$z_{k}^{r} \le x^{k}y_{k} + x_{k}y^{up} - x^{k+1}y^{lo}\delta_{k},$$

$$z_{k}^{r} \le x^{k}y_{k} + x_{k}y^{up} - x^{k}y^{up}\delta_{k},$$

$$(1)$$

$$\delta_{k}x^{k} \le x_{k} \le \delta_{k}x^{k+1},$$

$$\delta_{k}y^{lo} \le y_{k} \le \delta_{k}y^{up},$$

$$\sum_{k=1}^{K} \delta_{k} = 1,$$

$$k = 1, ..., K.$$

This piecewise relaxation involves classical McCormick relaxations for the K subdomains, and binary variable  $\delta_k$  is to indicate whether the McCormick relaxation on subdomain k is activated or not. Note that when K = 1(i.e., when the x domain is not partitioned), the piecewise McCormick relaxation reduces to the classical McCormick relaxation.

#### 3.3 Relaxation of Univariate Functions

Consider a (nonaffine) univariate function z = U(x) that is defined on  $[x^{lo}, x^{up}]$ . Again, partition the x domain into K subdomains, then the piecewise McCormick relaxation can be expressed as:

$$z^{\mathrm{r}} = \sum_{k=1}^{K} z_{k}^{\mathrm{r}}, \quad x = \sum_{k=1}^{K} x_{k},$$

$$z_{k}^{\mathrm{r}} \leq U^{\mathrm{conc},k}(x_{k},\delta_{k},x^{k},x^{k+1}),$$

$$z_{k}^{\mathrm{r}} \geq U^{\mathrm{conv},k}(x_{k},\delta_{k},x^{k},x^{k+1}),$$

$$\delta_{k}x^{k} \leq x_{k} \leq \delta_{k}x^{k+1},$$

$$\sum_{k=1}^{K} \delta_{k} = 1,$$

$$k = 1, ..., K.$$

$$(2)$$

The binary variables and the partitioning points are as defined in the preceding subsection.  $U^{\operatorname{conc},k}(x, 1, x^k, x^{k+1})$  and  $U^{\operatorname{conv},k}(x, 1, x^k, x^{k+1})$  denote a concave relaxation and a convex relaxation of U(x) on  $[x^k, x^{k+1}]$ , respectively, and the following condition,

$$U^{\text{conc},k}(0,0,x^{k},x^{k+1}) = 0,$$
  

$$U^{\text{conv},k}(0,0,x^{k},x^{k+1}) = 0,$$
  

$$k = 1, ..., K,$$
  
(3)

is enforced such that  $z_k^{\rm r} = 0$  if  $\delta_k = 0$  (i.e., the convex relaxation on subdomain k is deactivated). When K = 1, the piecewise McCormick relaxation reduces to the classical McCormick relaxation.

#### 3.4 NGBD With Piecewise Convex Relaxations

With the proposed piecewise McCormick relaxations, factorable functions in Problem (P) can be relaxed by piecewise relaxation of the multiplications and univariate functions in their factorable representations. Then a new lower bounding problem that is tighter than Problem (LBP) can be constructed in the following form:

$$\min_{\substack{x_1,\dots,x_s,\\ \tilde{e}_1,\dots,\tilde{e}_s,\\ \delta_1,\dots,\delta_s,y}} \sum_{h=1}^s w_h \left( c_h^{\mathrm{T}} y + u_{f,h}^{\mathrm{pw}}(x_h, \tilde{e}_h, \delta_h) \right)$$
s.t.  $u_{g,h}^{\mathrm{pw}}(x_h, \tilde{e}_h, \delta_h) + B_h y \leq 0, \quad \forall h \in \{1, \dots, s\},$   
 $(x_h, \tilde{e}_h, \delta_h) \in D_h^{\mathrm{pw}} \times \{0, 1\}^{n_\delta}, \quad \forall h \in \{1, \dots, s\},$   
 $y \in Y,$ 
(LBP-PCR)

where  $\delta_h$  denotes binary variables introduced for the piecewise McCormick relaxation. This new lower bounding problem (LBP-PCR) is a convex MINLP or a MILP, which cannot be decomposed via GBD in general. However, Problem (LBP-PCR) can be used to generate tighter optimality cuts for the relaxed master problem (RMP<sup>k</sup>) to yield tighter lower bounds for Problem (P). The details of enhancing the relaxed master problem with tighter optimality cuts are not given here due to the space limit of the paper, and interested readers can find them in Li et al. (2012).

#### 4. CASE STUDIES

### 4.1 Case Study 1

This case study is inspired by a real industrial system, the Sarawak Gas Production System (SGPS) (Selot et al. (2008)). The superstructure and parameters of the SGPS are illustrated in Figures 2(a) and 2(b). In this system, natural gas is acquired from a set of gas fields (denoted by circles in the figures) and transported to three liquefied natural gas (LNG) plants (denoted by squares in the figures) through a pipeline network. Several gas platforms (denoted by ellipses in the figures) are involved in the system, at which gas flows are mixed and split. The solid lines in the figures indicate the existing part of the system. To meet the increasing customer demands, the system needs to be expanded to produce more LNG, and the superstructure of the new part of the system is indicated by the dashed lines in the figures. More detailed description of the system can be found in Li et al. (2011a).

(D35)(BY)(SC)(E11)(F6)

(EIIP)

BYP



(a) Superstructure and economic information

(B11)

B11P

(M3)

МЗР

E11R-B

SC-2

LNG2

(M1)

E11R-C

SC-3

LNG3

MIP

(F23) SW (F23) (BN)

F23P

(E11R-A

SC-1

LNG1



(c) Network design with the deterministic formulation

(d) Network design with the stochastic formulation

LNG1

LNG2

LNG3

Fig. 2. Case Study 1 superstructure, parameters, and design results

The objective of the system expansion problem is to choose from the superstructure the gas fields, platforms, pipelines, and LNG plants to be developed, such that the expected net present value of the expansion is maximized while the specifications on gas qualities at the LNG plants are satisfied. The uncertainty in the system may come from the qualities of the gas fields and demands at the different LNG plants. The problem can be cast as a MINLP problem in form of Problem (P). We call the MINLP formulation a *deterministic formulation* if no uncertainty is explicitly considered (i.e., Problem (P) only involves one scenario), and a stochastic formulation if several realizations of uncertainty parameters are considered in the problem (i.e., Problem (P) involves more than one scenario). Details of the deterministic and the stochastic formulations can be found in Li et al. (2011a).

The MINLP problems are solved with BARON 8.1.5 and the NGBD method on GAMS 22.8.1. The computer used has a 2.83 GHz CPU and runs a Linux system. The NGBD method employs BARON 8.1.5 for solving nonconvex NLP subproblems and CPLEX 11.1.1 for solving LP and MILP subproblems. The relative termination tolerance for global optimization is  $10^{-2}$ .

The advantage of using the stochastic formulation is demonstrated via a simple case in which the uncertainty only comes from the quality of gas field M1 (i.e.,  $CO_2$ mole percentage of gas from the field). Specifically, The  $CO_2$  mole percentage obeys a normal distribution with a mean of 3.34 and a standard deviation of 0.6. five sampled realizations of the uncertain  $CO_2$  mole percentage are considered in the stochastic formulation. Figures 2(c) and 2(d)show the SGPS network designed with the deterministic and the stochastic formulations, respectively. The deterministic formulation suggests a design involving fewer gas fields, which requires an infrastructure investment costs of 21.1 billion dollars and can achieve an expected net present value of 29.0 billion dollars. The drawback of this design is that the quality of M1 may be so bad that M1 cannot supply as much gas as expected by the deterministic formulation. When considering the uncertainty with the stochastic formulation, more gas fields are to be developed to make sure that the SGPS can consistently supply onspecification gas flows in spite of the quality of gas field M1. The resulting design requires a higher infrastructure investment cost of 21.6 billion dollars but can also achieve a higher expected net present value of 32.2 billion dollars.

The computational advantage of the NGBD method is demonstrated here with another case in which the uncertainty comes from the CO<sub>2</sub> mole percentages of gas from fields M1, JN and the maximum demands at LNG plants 2 and 3. The four uncertain parameters independently obey normal distributions with means 5.04, 2.63, 1736 Mmol/day and 2275 Mmol/day, and standard deviations 1, 0.4, 144 Mmol/day and 239 Mmol/day, respectively. 1, 2, 3, 4 and 5 realizations are generated for each uncertain parameter, leading to problems involving 1, 16, 81, 256 and 625 scenarios. The computational results are summarized in Table 1. Although NGBD is slower than BARON when the number of scenarios is 1, it is much faster when more scenarios are addressed, and the solver time with the decomposition method increases moderately with the

Table 1. Case Study 1 Computational Results

Num. of Scenarios	1	16	81	256	625
Num. of binary var.	38	38	38	38	38
Num. of cont. var.	59	929	4699	14849	36251
BARON Time (s)	1.6	3894.1	_ *	-	_
NGBD Time (s)	4.4	19.5	98.4	376.4	792.6

\* No solution is returned within  $10^5$  seconds.

Table 2. Case Study 2 Computational Results

	BARON	NGBD	NGBD-PCR
Time for 8 scenarios $(s)$	- *	65915	6104
Time for $24$ scenarios (s)	_ **	217855	23525

\* No global solution is returned within  $10^6$  seconds.

\*\* No global solution is returned within 30 days.

number of scenarios. In addition, BARON cannot obtain a solution for the problem within  $10^5$  seconds when 81 or more scenarios are involved in the problem.

## 4.2 Case Study 2

This problem is the synthesis of a flexible energy polygeneration plant co-producing power, liquid fuels (naphtha and diesel) and chemicals (methanol) from coal and biomass as feedstocks. The goal of the optimization is to determine the equipment capacities in the plant to achieve the best net present value over the plant lifetime while satisfying the design and operational constraints. This problem can be cast as a MINLP in the form of Problem (P). Two problem instances are considered here. One involves 8 scenarios, 70 binary variables and 4904 continuous variables, and the other involves 24 scenarios, 70 binary variables and 14712 continuous variables. Details of the MINLP models can be found in Chen et al. (2011).

The case study compares the performance of BARON 9.0.6, NGBD, and NGBD-PCR (i.e., the NGBD with piecewise relaxations). The problems are solved on GAMS 23.5.2 with a computer allocated a 2.66 GHz CPU and running a Linux system. The NGBD methods employs BARON 9.0.6 for solving nonconvex NLP subproblems and CPLEX 12.2.2 for solving LP and MILP subproblems. The NGBD-PCR method partitions the domain of each variable uniformly into 15 subdomains. The relative termination tolerance for global optimization is  $10^{-2}$ .

Tables 2 summarizes the computational results. It can be seen that BARON cannot return an  $\epsilon$ -optimal solution within 10<sup>6</sup> seconds and 30 days for the two problem instances, respectively, while NGBD can within 10<sup>5</sup> seconds and 3 days, respectively. This indicates that NGBD can reduce the solution time (with BARON) by at least an order of magnitude for both problem instances. It can also be seen that NGBD-PCR can further reduce the solution time by about another order of magnitude for both problem instances.

# 5. CONCLUSION

A MINLP problem (P) is considered for the integrated design and operation of energy systems under uncertainty. This MINLP problem is usually computationally challenging due to the large number of scenarios required to characterize the uncertainty. By exploitation of the decomposable structure of the problem, a NGBD method can solve Problem (P) to global optimality efficiently. Case study results show that NGBD is faster than a stateof-art global optimization solver by at least an order of magnitude, and with the integration of a piecewise convex relaxation framework, the NGBD solution procedure can be expedited by another order of magnitude.

## REFERENCES

- Adjiman, C.S., Androulakis, I.P., and Floudas, C.A. (2000). Global optimization of mixed-integer nonlinear problems. AIChE Journal, 46(9), 1769–1797.
- Balas, E. and Jeroslow, R. (1972). Canonical cuts on the unit hypercube. SIAM Journal on Applied Mathematics, 23(1), 61–69.
- Chen, Y., Li, X., Adams II, T.A., and Barton, P.I. (2011). Decomposition strategy for the global optimization of flexible energy polygeneration system. *AIChE Journal*, 58(10), 3080–3095.
- Gatzke, E.P., Tolsma, J.E., and Barton, P.I. (2002). Construction of convex relaxations using automated code generation technique. *Optimization and Engineering*, 3, 305–326.
- Geoffrion, A.M. (1972). Generalized Benders decomposition. Journal of Optimization Theory and Applications, 10(4), 237–260.
- Gounaris, C.E., Misener, R., and Floudas, C. (2009). Computational comparison of piecewise-linear relaxations for pooling problems. *Industrial and Engineering Chemistry Research*, 48, 5742–5766.
- International Energy Agency (2012). World energy outlook 2012.
- Kesavan, P., Allgor, R.J., Gatzke, E.P., and Barton, P.I. (2004). Outer approximation algorithms for separable nonconvex mixed-integer nonlinear programs. *Mathematical Programming, Series A*, 100, 517–535.
- Li, X., Armagan, E., Tomasgard, A., and Barton, P.I. (2011a). Stochastic pooling problem for natural gas production network design and operation under uncertainty. *AIChE Journal*, 57, 2120–2135.
- Li, X., Chen, Y., and Barton, P.I. (2012). Nonconvex generalized Benders decomposition with piecewise convex relaxation for global optimization of integrated process design and operation problems. *Industrial and Engineering Chemistry Research*, 51, 7287–7299.
- Li, X., Tomasgard, A., and Barton, P.I. (2011b). Nonconvex generalized Benders decomposition for stochastic separable mixed-integer nonlinear programs. *Journal of Optimization Theory and Applications*, 151, 425–454.
- McCormick, G.P. (1976). Computability of global solutions to factorable nonconvex programs: Part I - Convex underestimating problems. *Mathematical Programming*, 10, 147–175.
- Selot, A., Kuok, L.K., Robinson, M., Mason, T.L., and Barton, P.I. (2008). A short-term operational planning model for natural gas production systems. *AIChE Journal*, 54(2), 495–515.
- Tawarmalani, M. and Sahinidis, N.V. (2004). Global optimization of mixed-integer nonlinear programs: A theoretical and computational study. *Mathematical Programming*, 99, 563–591.