Global optimization of an industrial natural
gas production network

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Abstract: A new stochastic programming model is proposed for integrated design and operation of natural gas production networks under uncertainty. The model not only addresses the uncertainties explicitly, but also considers the gas compositions and pressure-flow relationships for the whole production network. Due to the many nonconvex constraints, the new model leads to a very difficult large-scale nonconvex mixed-integer nonlinear programming (MINLP) problem. A modified nonconvex generalized Benders decomposition (NGBD) method is developed to efficiently solve this problem. This method integrates in NGBD several bound contraction strategies, which render tighter convex relaxations for constructing tighter lower bounding problems and accelerating the solution of nonconvex subproblems. Case study of an industrial natural gas production system shows the benefits of the proposed stochastic model and the bound contraction integrated NGBD method.

Keywords: Natural gas; Integrated design and operation; Uncertainty, Global optimization; Benders decomposition; Bound contraction; MINLP; Network optimization.

1. INTRODUCTION

As natural gas is becoming a more important source of energy, the application of mathematical programming to optimal design and operation of natural gas production networks (NGPN) has attracted more attention from both industry and academia. In the literature, the mathematical models developed for gas networks include at least one of the following three physical features. One is the relationship between pressures and gas flow rates at the wells, compressors and pipelines (e.g., Ríos-Mercado et al. (2006); Goel and Grossmann (2004)), the second is the compositions of gas flows in different parts of the network, such as the mole percentages of CO₂, H₂S (e.g., Selot et al. (2008); Li et al. (2011a)), and the third is the uncertainties in the systems (e.g., Levary and Dean (1980); Goel and Grossmann (2004)).

In order to address uncertainties in the integrated design and operation problem explicitly, the following scenario-based two-stage stochastic programming can be formulated (Birge and Louveaux (2011)):

\[
\begin{align*}
\min & \quad \sum_{w=1}^{s} p_w (c_w^T x_0 + f_w(x_w)) \\
\text{s.t.} & \quad B_w x_0 + g_w(x_w) \leq 0, \quad w = 1, \ldots, s, \\
& \quad x_w \in X_w, \quad w = 1, \ldots, s, \\
& \quad x_0 \in X_0,
\end{align*}
\]

which includes a finite number of uncertainty realizations (called scenarios) to characterize the uncertainties, \( p_w \) represents the probability for specific scenario \( w \), \( X_0 = \{x_0 \in \{0,1\}^n : Ax_0 \leq b\} \) is nonempty and compact, \( X_w \subseteq \mathbb{R}^{n_w} \) is nonempty and compact for \( w = 1, \ldots, s \). For NGPN, \( x_0 \) are first-stage binary variables which decide if specific facilities are to be developed or not, \( x_w \) are second-stage binary or/and continuous variables which determine the operating conditions for scenario \( w \). When gas pressure and flow relationship or compositions of gas flows are addressed in the model, Problem (P) becomes a large-scale nonconvex mixed-integer nonlinear programming (MINLP) problem, which is usually very difficult to solve. However, this problem has a special structure; when the first-stage variables are fixed, it can be decomposed into \( s \) subproblems. This special structure can be exploited for efficient global optimization via an extension of Benders decomposition (Benders (1962)) called nonconvex generalized Benders decomposition (NGBD, Li et al. (2011b)), which was developed based on convex relaxations and strong duality held by convex subproblems.

Recently, the authors have developed a stochastic programming model for integrated design and operation of NGPNs, which include all the three aforementioned physical features of the system (Li and Li (2015)). However, this model leads to a very difficult nonconvex MINLP that cannot be solved by the standard NGBD method efficiently. This is because the problem is highly nonconvex and the convex relaxations constructed in the standard NGBD are not tight enough. Therefore, we propose in this paper to construct tighter convex relaxations through bound contraction, which has been proven to be effective...
in branch-and-bound based global optimization (Zamora and Grossmann (1999)). The remaining part of the paper is organized as follows. In section 2, the new stochastic programming model for integrated design and operation of NGPN is introduced. In section 3, the NGBD framework is briefly described and the bound contraction problems to be solved within this framework are explained. Section 4 demonstrates the advantage of the new model as well as the updated NGBD method. The paper ends with conclusions in section 5.

2. THE STOCHASTIC NGPN MODEL

Here we briefly introduce a new stochastic NGPN model for an industrial NGPN called Sarawak Gas Production System (SGPS) (Selot et al. (2008)). This model is developed based on our recent work (Li and Li (2015)). The gas production network is formulated as a directed graph, in which vertices represent wells, pipeline connections, terminals and edges represent gas pipelines. The model consists of three major parts. The first part is a stochastic pooling model (Li et al. (2011a)) that captures the topological structure of the network and the material balances on different gas components in the system. The second part is a pressure-flow relationship model that describes how the gas flows are dependent on the pressures in pipelines. The third part is a compressor model that relates the energy consumption to the pressure rise provided by compression. With the stochastic symbols described in Table 1, the three parts are explained below.

The stochastic pooling model

Due to the space limit, the equations for the stochastic pooling model are not listed here. Readers are referred to the previous paper (Li et al. (2011a)) for the equations.

The stochastic pipeline pressure-flow model

\[ y_{i,j}((P_{i,w}^{\text{out}})^2 - (P_{j,w}^{\text{in}})^2) \geq \kappa_{i,j} Q_{i,j,w}^2, \quad \forall (i,j) \in E^L, \quad \forall w \in \Phi \] (1)

\[ y_{i,j}(P_{j,w}^{\text{in}} - P_{i,w}^{\text{out}}) \leq 0, \quad \forall (i,j) \in E, \quad \forall w \in \Phi \] (2)

\[ P_{i,w}^{\text{in}} \geq P_{i,w}^{\text{out}}, \quad \forall i \in V \setminus V^C, \quad \forall w \in \Phi \] (3)

\[ \vartheta_{i,w} Q_{i,j,w}^2 \leq y_{j,i}(\pi_{i,w}^2 - \lambda_{i,w}(P_{i,w}^{\text{out}})^2), \quad \forall (i,j) \in E^W, \quad \forall w \in \Phi \] (4)

\[ P_{i,w}^{\text{out}} \leq \pi_{i,w}, \quad \forall i \in V^W, \quad \forall w \in \Phi \] (5)

\[ y_{i,w}^{\text{GMB,UB}} \leq P_{i,w}^{\text{out}} \leq y_{i,w}^{\text{GMB,LB}}, \quad \forall i \in V, \quad \forall w \in \Phi \] (6)

\[ y_{i,w}^{\text{GMB,UB}} \leq P_{i,w}^{\text{out}} \leq y_{i,w}^{\text{GMB,LB}}, \quad \forall i \in V, \quad \forall w \in \Phi \] (7)

Eq. (1) describes how the gas flow rates in regular long pipelines are dependent on the pressures at both ends of the pipelines. Eq. (2) means that, if the pipeline represented by edge (i,j) is to be developed, the pressure at the entrance of the pipeline (i.e., $P_{i,w}^{\text{out}}$, which is also the pressure at the exit of vertex i) has to be greater than or equal to the pressure at the exit of the pipeline (i.e., $P_{j,w}^{\text{in}}$, which is also the pressure at the entrance of vertex j). Eq. (3) represents the relationship of inlet and outlet pressures at a vertex which does not involve a compressor. Eq. (4-5) provide the pressure-flow relationship in gas wells. Eq. (6-7) enforce bounds for all pressures. Note that Eq.(1),(2) and (4) involve multiplications of binary variables and continuous variables, and these bilinear terms can be linearized exactly using big-M method (Bemporad and Morari (1990)). Due to the space limit, we do not provide details on the reformulation here.

The stochastic compression model

\[ W_{j,w} - \sum_{i \in E} \left( f_{i,j,w} \left( \frac{P_{i,w}^{\text{out}}}{P_{i,w}^{\text{in}}} \right)^{\nu} - 1 \right) = 0, \quad \forall j \in V^C, \quad \forall w \in \Phi \] (8)

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| Symbol | Type       | Descriptions                   |
|--------|------------|--------------------------------|
| V      | set        | vertices in the directed flow graph |
| E      | set        | edges in the directed flow graph |
| Ω      | set        | index set for components in flow |
| Φ      | set        | index set for scenarios         |
| V_W    | subset of V| vertices representing wells     |
| V_T    | subset of V| vertices representing terminals  |
| V_C    | subset of V| vertices with compressors onsite |
| E_L    | subset of E| edges representing long pipelines |
| E_W    | subset of E| edges connecting wells to sources |

The stochastic pipeline pressure-flow model

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The stochastic compression model

\[ W_{j,w} - \sum_{i \in E} \left( f_{i,j,w} \left( \frac{P_{i,w}^{\text{out}}}{P_{i,w}^{\text{in}}} \right)^{\nu} - 1 \right) = 0, \quad \forall j \in V^C, \quad \forall w \in \Phi \] (8)
Eq. (8) relates the power consumption \( W_{i,w} \) to the gas flow rate and the acquired pressure rise for all compressors, where \( \omega_i \) is a constant obtained with ideal gas assumption.

Eq. (9) enforces bounds on the power of the compressor if the compressor is to be used to increase the pressure, where \( \delta_{i,w} \) is a binary variable determining whether compressor \( i \) is to be operated for scenario \( w \). Eq. (10) means that compressor at vertex \( i \) can be used to raise the pressure only when that vertex \( i \) is developed. Eq. (11), together with Eq. (8) ensure that a pressure rise is obtained when the compressor is under operation while it is zero when the compressor is not under operation.

Some other constraints are also needed for the stochastic programming model. The following Eq. (12-13) link the molar flow rates and the volumetric flow rates with ideal gas assumption:

\[
\begin{align*}
    f_{i,j,q,w} &= \phi U_{i,q,w} Q_{i,j,w}, \quad \forall (i,j) \in E^W, \forall w \in \Phi \\
    \sum_{q \in \Omega} f_{i,j,q,w} &= \phi Q_{i,j,w}, \quad \forall (i,j) \in E, \forall w \in \Phi
\end{align*}
\]

In order to maximize the expected net present value (NPV) for the integrated design and operation, the following equations are included:

\[
C^{(NPV)} = -C^{(CC)} - \sum_{t=1}^{L} \sum_{w} p_w C^{(OP)}_{w} (1 + \alpha)^t
\]

\[
C^{(CC)} = \sum_{i \in V} y_{i}^{p} c^{(CC)}_{i} + \sum_{i,j \in E} y_{i,j} c^{(CC)}_{i,j}
\]

\[
C^{(OP)}_{w} = -\sum_{k \in V^T} \left( \sum_{i \in \Omega} \sum_{j \in \{(j),(j)\} \in E} f_{i,j,q,w} C^{(OP)}_{k,w} \right) + \sum_{i \in V^W} \left( \sum_{j \in \{(j),(j)\} \in E} f_{i,j,q,w} C^{(OP)}_{i,w} \right) + \sum_{j \in V^C} \omega U_{j,w}
\]

The overall stochastic programming model can be expressed as:

\[
\max C^{(NPV)}
\]

\[
\text{s.t.} \quad \text{The stochastic pooling model (Li et al. (2011a)), Eq.}(1 - 16).
\]

\[
\text{(SNGPN)}
\]

Apparently, this problem can be written in form of (P).

3. THE GLOBAL OPTIMIZATION METHOD

This section introduces the bound contraction integrated NGBD framework for solving problems in form of (P). First, the standard NGBD method is briefly introduced. Then the bound contraction problems to be solved within NGBD are proposed. Finally, the integration of bound contraction in NGBD is discussed.
convergence. Therefore, it is not surprising that NGBD has been shown to be very efficient for the stochastic pooling model (Li et al. (2011a)) but it is still very inefficient for solving Problem (SNGPN), which includes more non-convex constraints (due to the inclusion of pressure-flow relationships).

3.2 Bound Contraction Problems

One way to improve the performance of NGBD is to obtain tighter convex relations via estimating tighter bounds for variables in Problem (P). Here we are to use the notion of bound contraction, which has been developed to improve branch-and-bound based global optimization algorithms (Zamora and Grossmann (1999)). Bound contraction was motivated by the fact that the bounds explicitly imposed on the variables in an optimization problem are usually much wider than the true range the variable can vary within. By solving extra bound contraction problems, better estimates of the true ranges of the variables can be obtained. Therefore, we can progressively improve the bounds used for convex relaxations by solving a sequence of bound contraction problems in the NGBD procedure.

Specifically, we solve two types of bound contraction problems in the NGBD procedure. Assume that the bounds of variable \( x_{i,w} \) are to be estimated, then the first type of bound contraction problems can be written as

\[
\max_{x_{i,w}, x_{0,i,w}} \min_{x_0,x_1,\ldots,x_s} \quad \text{s.t. } \\
B_h x_0 + \hat{g}_h(x_h) \leq 0, \quad h = 1, \ldots, s, \\
x_h \in \hat{X}_h, \quad h = 1, \ldots, s, \\
x_0 \in X_0, \\
\sum_{h=1}^{s} p_h(c^T_h x_0 + \hat{f}_h(x_h)) \leq UB,
\]

(\text{BC}_{i,w})

where \( \hat{f}_w, \hat{g}_w \) denote convex relaxations of functions \( f_w \) and \( g_w \), respectively, and \( \hat{X}_w \) denotes a convex relaxation of set \( X_w \). It can be seen that the feasible set of Problem (BC\(_{i,w}\)) is a convex relaxation of that of Problem (P), so the optimal value of the problem represents an underestimate of the lower bound of \( x_{i,w} \) (when it is a minimization problem) or an overestimate of the upper bound of \( x_{i,w} \) (when it is a maximization problem). When \( UB = +\infty \) (which means that no feasible solution of Problem (P) has been found), the last constraint is not included in the problem.

Note that the size of Problem (BC\(_{i,w}\)) grows linearly with the number of scenarios. When nonlinear convex relaxations are used and the number of scenarios is large, Problem (BC\(_{i,w}\)) is a large-scale convex MINLP, which can cost a lot of solution time. In order to reduce the time for bound contraction, we can modify Problem (BC\(_{i,w}\)) in two ways. One is to outer linearize the nonlinear convex relaxations in the problem, then Problem (BC\(_{i,w}\)) will become a MILP that can be much easier to solve. In this paper, we outer linearize nonlinear convex relaxations using the approach explained in Li et al. (2012). The other is to relax Problem (BC\(_{i,w}\)). Note that in Problem (BC\(_{i,w}\)), variables in scenarios other than scenario \( w \) affect the optimal value only through the last constraint. So if we can relax the last constraint into one that only involve variables for scenario \( w \), we can remove other variables from the problem. For the relaxation, we first rewrite the last constraint into the following form:

\[
p_w(c^T_w x_0 + \hat{f}_w(x_w)) \leq UB - \left( \sum_{h \neq w} p_h(c^T_h x_0 + \hat{f}_h(x_h)) \right).
\]

(17)

When \( \hat{f}_h \) is a linear relaxation of \( f_h \), it can be written as \( C^T_{f,h} x_h \), then the constraint can be transformed into:

\[
p_w(c^T_w x_0 + \hat{f}_w(x_w)) \leq UB - \left( \sum_{h \neq w} p_h(c^T_h x_0 + C^T_{f,h} x_h) \right) \\
\leq UB - \left( \sum_{h \neq w} p_h(c^T_h x^*_h + \hat{f}_h(x^*_h)) \right), \\
= UBR_w,
\]

(18)

where \( x^*_h \) or \( \hat{f}_h \) denotes the current upper or lower bounds of \( x_0 \) or \( f_h \). If the relevant coefficient in \( C^T_{f,h} \) or \( C^T_{f,h} \) is positive, then the lower bound is used; otherwise, the upper bound is used. Apparently, constraint (18) is a relaxation of constraint (17). So the following bound contraction problem is a relaxation of Problem (BC\(_{i,w}\))

\[
\max_{x_{i,w}} \min_{x_0,x_{0,w}} \quad \text{s.t. } \\
B_w x_0 + \hat{g}_w(x_w) \leq 0, \quad x_w \in \hat{X}_w, \\
x_0 \in X_0, \\
p_w(c^T_w x_0 + \hat{f}_w(x_w)) \leq UBR_w.
\]

(BCR\(_{i,w}\))

Problem (BCR\(_{i,w}\)) is a relaxation of Problem (BC\(_{i,w}\)), so the bounds estimated from (BCR\(_{i,w}\)) are usually not so good as those from (BC\(_{i,w}\)). However, Problem (BCR\(_{i,w}\)) contains much fewer variables and constraints and is a lot easier to solve. When all the nonlinear convex relaxations are outer linearized, Problem (BCR\(_{i,w}\)) is a mixed-integer linear programming (MILP) problem whose size is independent of the number of scenarios. In addition, Problem (BCR\(_{i,w}\)) becomes tighter as the algorithm proceeds, because the bounds used to calculate UBR\(_w\) become tighter.

The second type is to reduce variable bounds for the upper bounding subproblem (PP\(_w(x^*_0)\)), in which \( x_0 \) is fixed at a constant \( x^*_0 \):

\[
\max_{x_{i,w}} \min_{x_{w,0,w}} \quad \text{s.t. } \\
B_w x_0 + \hat{g}_w(x_w) \leq 0, \quad x_w \in \hat{X}_w, \\
p_w(c^T_w x_0^* + \hat{f}_w(x_w)) \leq UBD_w
\]

(BCPP\(_{i,w}(x^*_0)\))

where UBD\(_w\) denotes the upper bound on Problem (PP\(_w(x^*_0)\)), which can be obtained from UB and previously solved NGBD subproblems. Readers are referred to Li et al. (2011b) for how to calculate UBD\(_w\).

Since the tightness of convex relaxations is only influenced by variables that are involved in nonconvex functions in \( f_w \) and \( g_w \), we only need to solve bound contraction problems for these variables. For convenience of discussion, we call these variables nonconvex variables in the paper.
3.3 The NGBD integrated with bound contraction

Figure 1 illustrates the bound contraction integrated NGBD framework. Problem \((BC_{i,w}(x_0^*)\)) or \((BCR_{i,w}(x_0^*)\)) is solved at the beginning of the algorithm and every time when the solution of an upper bounding problem improves the current upper bound \(UB\). Before the solution of each nonconvex subproblem \((PP_{w}(x_0^*))\), Problem \((BC_{i,w}(x_0^*)\)) is solved to render reduced bounds for speeding up the solution of \((PP_{w}(x_0^*))\). However, the reduced bounds are only valid for \(x_0 = x_0^*\), so we have to recover the previous bounds after solving Problem \((PP_{w}(x_0^*))\).

A bound contraction problem can be solved for a group of variables multiple times, as the updated bounds for a variable can be used to tighten the feasible set of bound contraction problems for other variables. In this case study, we solve a bound contraction problem for a variable multiple times until the estimated bounds do not improve or the problem has been solved for 3 times.

The integration of bound contraction strategies does not hurt the finite convergence of NGBD, as these strategies do not alter the facts that are needed to ensure the finite convergence (Li et al., 2011b). First, these strategies tighten the lower bounds but they do not exclude global optima. Second, they do not allow to generate the same first-stage integer realizations twice before the convergence.

4. CASE STUDY

In this section, a case study based on the SGPS system is conducted to demonstrate the benefits of the proposed stochastic programming model and the bound-contraction based NGBD method. This an integrated design and operation problem initially formulated by Li et al. (2011a).

In this problem, the SGPS system is to be expanded to provide more gas products, and the superstructure of the part of the network to be expanded is known (shown in Figure 2). The goal of the optimization is to find the best subnetwork for the expansion to achieve the best expected NPV over the next 25 years.

In this case study, the uncertainties in the system are assumed to come from percentage of \(CO_2\) in the gas from gas field \(M1\), and the maximum demand at a off-shore liquefied natural gas (LNG) plant \(LN2\). The two uncertain parameters are assumed to be independent and follow normal distributions \(N(3.34, 0.6^2)\) and \(N(1355, 101^2)\), respectively. 9 scenarios are sampled for scenario-based stochastic programming, following a simple rule used in Li et al. (2011a).

The case study was conducted on a Linux platform with one 3.40GHz CPU and 8GB RAM. GAMS 24.2 was used to model the optimization problems. CPLEX 12.6 was used to solve MILP subproblems, CONOPT 3.15 to solve convex NLP subproblems and BARON 12.7 solve nonconvex MINLP subproblems in NGBD. The absolute and relative tolerances used for NGBD are \(10^{-2}\).

Figure 2 gives the SGPS network designed using the stochastic pooling model (that does not address the influence of pressures on gas flow rates) and the one designed using the new stochastic programming model. As the stochastic pooling model does not consider that the pressures in the pipelines can limit the rate of gas produced from the gas fields, it fails to choose enough gas fields to achieve the best possible expected NPV. The new model considers the pressure-flow relationships and it chooses to develop the gas field (JN) instead of (M1) such that the whole production system can produce gas as much as can be sold for different scenarios. As a result, the expected NPV can be achieved by the design obtained via the new model is larger than the one obtained via the stochastic pooling model, by about 5%.

Table 2 summarizes the computational results. Three NGBD methods are compared for solving the proposed stochastic programming model. NGBD1 denotes the standard NGBD method, NGBD2 denotes the NGBD method integrating bound contraction problems \((BC_{i,w}(x_0^*)\)) and \((BC_{PP, i,w}(x_0^*)\)), and NGBD3 denotes the NGBD method integrating \((BCR_{i,w}(x_0^*)\)) and \((BC_{PP, i,w}(x_0^*)\)). In addition, computational results of NGBD1 for the stochastic pooling problem are also shown. It can be seen that the stochastic pooling model is much easier to solve compared to the proposed model (although it leads to a worse expected NPV), because it involves much fewer variables and nonconvex constraints. For solving the proposed stochastic model, NGBD2 is much better than NGBD1. This is because by solving the bound contraction problems in NGBD2, the lower bounding problem becomes tighter and therefore fewer number of iterations (reflected by the number of \(PP_{w}\) solved) are needed before the convergence. In addition, due to the narrowed bounds, the solution time for each difficult nonconvex \(PP_{w}\) is significantly reduced. NGBD3 further improves the computational efficiency (by almost an order of magnitude in comparison to NGBD2). This is because the relaxing bound contraction problem \((BCR_{i,w}(x_0^*)\)) is a lot easier to solve compared to \((BC_{i,w}(x_0^*)\)) and the total bound contraction time is reduced by more than an order of magnitude; at the same time, the estimated bounds are still tight enough to accelerate the NGBD convergence and the solution of \(PP_{w}\).

Figure 3 provides more details about to what extent the variables bounds are reduced in NGBD3. The figure shows the scaled bounds of 180 nonconvex variables for the 5th scenario at the 3rd NGBD outer loop iteration. The initial lower and upper bounds of these variables are all scaled to 0 and 1, respectively, which are shown as the center and the perimeter of the circle. The reduced ranges of the variables are indicated by the gray radial lines that form the gray areas in the circle. The smaller the total gray area is, the more the bounds are reduced. Note that ranges of some variables are reduced to points, forcing these variables to be constants in the problem. This greatly simplifies the subproblems to be solved and reduces the solution time.
5. CONCLUSIONS

With the consideration of pressure-flow relationships, the proposed stochastic programming model leads to a better design for the SGPS problem than the stochastic pooling model does. By integrating bound contraction strategies in the NGBD framework, the solution time for the new model is reduced by more than an order of magnitude, indicating a promising direction to improve the NGBD method in the future.

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