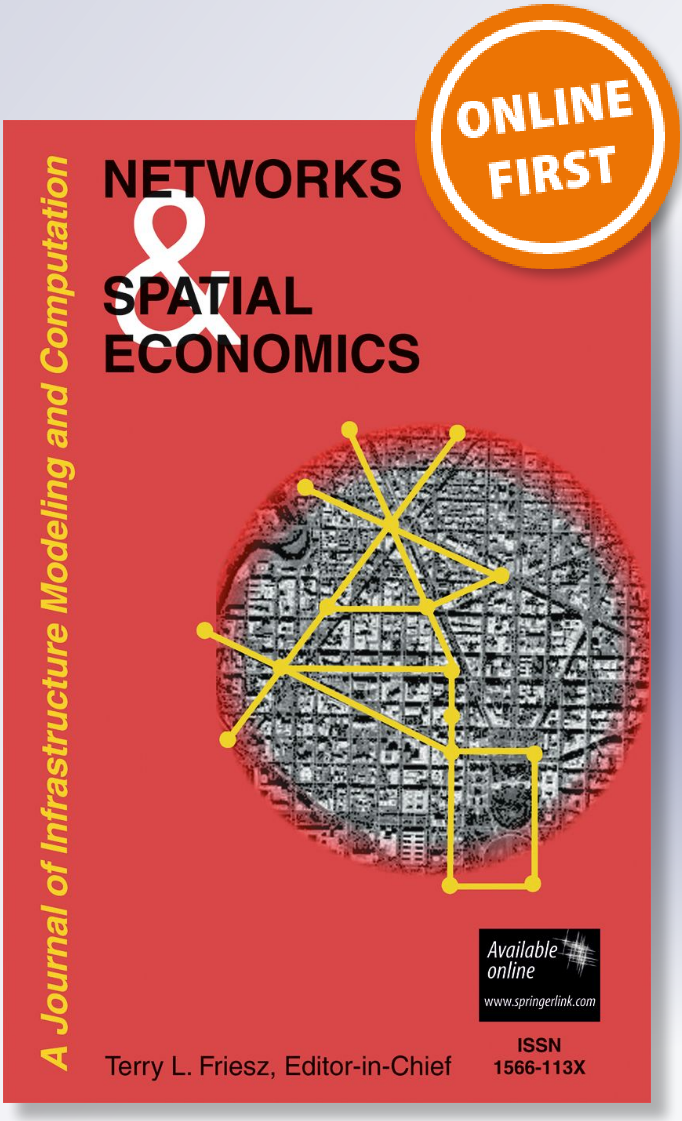
An SOS1-Based Approach for Solving MPECs with a Natural Gas Market Application

S. Siddiqui & S. A. Gabriel

Networks and Spatial Economics
A Journal of Infrastructure Modeling and Computation

ISSN 1566-113X

Netw Spat Econ
DOI 10.1007/s11067-012-9178-y



Springer

Netw Spat Econ
DOI 10.1007/s11067-012-9178-y

An SOS1-Based Approach for Solving MPECs with a Natural Gas Market Application

S. Siddiqui · S. A. Gabriel

Abstract This paper presents a new method for solving mathematical programs with equilibrium constraints. The approach uses a transformation of the original problem via Schur's decomposition coupled with two separate formulations for modeling related absolute value functions. The first formulation, based on SOS1 variables, when solved to optimality will provide a global solution to the MPEC. The second, penalty-based formulation is used to heuristically obtain local solutions to large-scale MPECs. The advantage of these methods over disjunctive constraints for solving MPECs is that computational time is much lower, which is corroborated by numerical examples. Finally, an application of the method to an MPEC representing the United States natural gas market is given.

Keywords Equilibrium problems · MPEC · EPEC · Shale · Natural gas · SOS type 1 · Schur's decomposition

1 Introduction

Finding solutions to mathematical programs with equilibrium constraints (MPECs) involves solving a two-level optimization problem where the lower level is an equilibrium problem. Typically, this equilibrium is defined as solving one or more optimization problems or more generally a complementarity problem (Cottle et al.

S. Siddiqui (✉)
Department of Civil Engineering, Johns Hopkins University, 3400 N Charles Street,
Baltimore, MD 21218, USA
e-mail: Siddiqui@jhu.edu

S. A. Gabriel
Department of Civil and Environmental Engineering, Applied Mathematics & Statistics, and Scientific Computation, University of Maryland, College Park, MD 20742, USA
e-mail: sgabriel@umd.edu

Published online: 21 July 2012

2009) and therefore includes non-convex, bilinear terms representing the product of two expressions equal to zero.

Many techniques exist to solve MPECs (Luo et al. 1996) including a disjunctive-constraints technique (Fortuny-Amat and McCarl 1981) as well as commercially available solvers (e.g., NLPEC). However, the two biggest drawbacks of disjunctive constraints are that the method is computationally expensive for large models (Luo et al. 1996) and that selecting a particular constant in the method is often troublesome (Hu et al. 2007; Gabriel and Leuthold 2010). A solution can be extremely sensitive to the selection of this constant, and be far from the true answer if not selected correctly. Nevertheless, this approach is relatively easy to set up in spite of its potential computational drawbacks.

The difficulty of solving general MPECs has given rise to many methods as of late. Some recent examples include works by Fletcher and Leyffer (2004); Fletcher et al. 2006); Leyffer et al. (2006), and Anitescu et al. (2007) that search for stationary points of these problems. These methods have been shown to obtain local solutions to moderately sized MPECs. However, given the non-convexity of MPECs, what works for smaller problems does not necessarily also work for large-scale ones. As an example, consider the reasonably large-scale MPEC described in (Chen et al. 2006) that was solved to global optimality via a two-stage process. General algorithms that provide global solutions (Gumus and Floudas 2001; Hu et al. 2007; Mitsos 2010) to MPECs were proposed in the literature as well. Other methods (Steffensen and Ulbrich 2010) and (Uderzo 2010) also exist but have not been shown to work for large-scale models.

This paper presents a new method for solving MPECs, based on transforming the bilinear, non-convex terms stemming from the lower-level problem using Schur's Decomposition and SOS Type 1 variables (Gabriel et al. 2006), along with techniques to reformulate the absolute value terms that arise. To clearly illustrate this method, it is applied to a small Stackelberg game with the number of players allowed to vary. Then, to further validate the usefulness of the method, it is applied to a large-scale MPEC for the U.S. natural gas market. In fact, the latter model was partial motivation for developing this method. Our algorithm is shown to solve this particular problem, where other algorithms we tried failed. Comparisons with other methods are presented to show that the method of this paper computationally outperforms other methods.

The MPEC model under consideration concerns the U.S. natural gas market which has recently been changing due to the abundance of unconventional gas.[1] This source of gas is plentiful in the U.S. (and other parts of the world) and has greatly increased due to engineering advances such as hydraulic fracturing and horizontal drilling (NPC 2007). The projected role of shale gas in particular, especially in the United States but also elsewhere (Skagen 2010) has lately been a major force in the increasing prominence of unconventional gas. Shale gas in the U.S. is characterized using the World Gas Model (WGM) (Gabriel et al. 2012), a large-scale complementarity model of global gas markets. The large-scale MPEC version of this model we

[1] Unconventional gas is defined as gas from tight sands, coalbed methane, and shale gas, and covers more low-permeability reservoirs that produce mostly natural gas (no associated hydrocarbon liquids) (NPC 2007).

created restricted the WGM to just the North American nodes and involved transforming it into a Stackelberg game. For the United States, the forecasts presented in the *Annual Energy Outlook* (April 2009 ARRA version) were used for the current MPEC study. For the rest of North America, the *World Energy Outlook* (International Energy Agency 2008) was used. The WGM was then extensively calibrated to match these multiple sources for all countries/aggregated countries and years considered (2005, 2010, 2015, 2020, 2025, and 2030).[2]

The most interesting change due to the presence of shale gas occurs in census region 7 (WGM node US_7) where the Haynesville and Barnett geological plays are present. This node is used as a test example for the new MPEC solution technique. The formulation proposed is that the producer of shale gas at node 7 is the first mover in the Stackelberg game (Gibbons 1996). The entire lower level is the rest of the World Gas Model restricted to North American nodes (conventional, unconventional and shale gas production modeled separately).

This paper is organized as follows. Section 2 outlines the general problem formulation and definition as well as the entire modeling and algorithm framework for MPECs including several theoretical results. Next, Section 3 provides a simple example of an MPEC, which is used to compare the proposed method to disjunctive constraints. Then, Section 4 explains how the World Gas Model was modified to include shale gas. This forms the basis of a larger MPEC example in Section 5: a shale firm as a top-level Stackelberg player in the U.S. natural gas market that validate the proposed approach.

2 Definition and formulation

In general, a mathematical program with equilibrium constraints is given by[3]

$$\begin{aligned} &\min f(x,y) \\ &\text{s.t.}(x,y) \in \Omega \\ &y \in S(x), \end{aligned} \tag{1}$$

where the continuous variables $x \in \Re^{n_x}, y \in \Re^{n_y}$ are, respectively, the vector of upper-level and lower-level variables. $f(x, y)$ is the upper-level, single-objective function, Ω is the joint feasible region between these sets of variables and $S(x)$ is the solution set of the lower-level problem that can be an optimization problem, a nonlinear complementarity problem (NCP), or variational inequality problem (Luo et al. 1996).

This main focus of this paper is when $S(x)$ corresponds to the solution set of a complementarity problem which includes the Karush-Kuhn-Tucker optimality conditions of nonlinear programs and many other problems in economics and

[2] See Gabriel et al. (2012) for details on the countries and regions included as well as other relevant geographic or nodal information.

[3] Without loss of generality, we assume that the variables x and y are nonnegative, which is incorporated in the decision space Ω.

engineering (Cottle et al. 2009). Given a function $h : \Re^n \to \Re^n$, this problem is to find a vector $z \in \Re^n$ such that:

$$\begin{aligned} & z \geq 0 \\ & h(z) \geq 0 \\ & z^T h(z) = 0. \end{aligned} \tag{2}$$

If $S(x)$ is the solution set of an NCP, (1) can be rewritten as

$$\begin{aligned} & \min f(x, y) \\ & \text{s.t.}(x, y) \in \Omega \\ & y \geq 0 \\ & g(x, y) \geq 0 \\ & y^T g(x, y) = 0, \end{aligned} \tag{3}$$

where $g(x, y) : \Re^{n_x} \times \Re^{n_y} \to \Re^{n_y}$ is a vector-valued function. The set of solutions to

$$y^T g(x, y) = 0 \tag{4}$$

is non-convex and can be computationally challenging to find even if $g(x, y)$ is linear. In particular, the presence of (4) in optimization problem (3) violates the Mangasarian-Fromovitz constraint qualification at any feasible point (Ye and Zhu 1995). It has been noted (Scheel and Scholtes 2000) that different constraint qualifications in fact result in solvers converging to different local solutions. One easily stated but potentially computationally challenging way to transform the complementarity constraints (4) is to use disjunctive constraints (Fortuny-Amat and McCarl 1981). In this approach, a large constant K is introduced, which can be difficult in general to select and cause computational issues (Gabriel and Leuthold 2010) but may in certain applications be easier to identify. Additionally a vector of binary variables r is introduced. Then, the original MPEC (3) is rewritten as

$$\begin{aligned} & \min f(x, y) \\ & \text{s.t.}(x, y) \in \Omega \\ & 0 \leq y \leq K(1 - r) \\ & 0 \leq g(x, y) \leq Kr \\ & \textit{where} \\ & r \in \{0, 1\}^{n_y} \text{ is a vector of binary values} \\ & K \in \Re_{++} \text{ is a large constant.} \end{aligned} \tag{5}$$

For large enough K, the solution set to (5) is equivalent to that of (3) if the feasible region is bounded. The binary vectors and large K force componentwise, at least one of y or g to be 0. However, choosing K too small can cause errors in problem formulation (Gabriel and Leuthold 2010) while choosing K too large can cause the condition number of the optimization problem (Renegar 1994, 1995) to be high and result in numerical errors. One of the main aims of this paper is to get around this problem by using decomposition and approximation techniques.

If g is linear, approximating the left-hand side of (4) often involves specialized techniques, one of which happens to be Schur's decomposition followed with an approximation by linear functions (Gabriel et al. 2006). However, results in this paper show that this can be extended to a vector-valued linear function g if linear constraints are included. First, using Schur's decomposition, vectors u and v (dependent on x and y) are used to rewrite problem (3) as

$$\begin{array}{l} \min f(x,y) \\ \text{s.t.} (x,y) \in \Omega \\ y \geq 0 \\ g(x,y) \geq 0 \\ u^T u - v^T v = 0 \\ u = \frac{y+g(x,y)}{2} \\ v = \frac{y-g(x,y)}{2}. \end{array} \tag{6}$$

Now, the optimization problem does not contain any bilinear terms. In fact

$$u^T u - v^T v = 0 \tag{7}$$

can be readily approximated using SOS type 2 (Beale 1975) variables[4] to create a piecewise-linear function. However, realizing that the complementarity conditions force $y \geq 0$ and $g(x,y) \geq 0$, shows that only the positive square root of u^2 will give a feasible solution to the problem. Hence, (6) can be reformulated as (8) below

$$\begin{array}{l} \min f(x,y) \\ \text{s.t.} (x,y) \in \Omega \\ y \geq 0 \\ g(x,y) \geq 0 \\ u - |v| = 0 \\ u = \frac{y+g(x,y)}{2} \\ v = \frac{y-g(x,y)}{2}. \end{array} \tag{8}$$

Note that the absolute value of v here is to be taken component-wise. The next theorem shows that the solution sets to (3), (5), and (8) are the same.

Theorem 1 Let the solution set to formulation (3) be given by S_3', the solution set to formulation (5) be given by S_5' and the solution set to formulation (8) be given by S_8'. Then, given a large enough value[5] of K, $S_3'=S_5'=S_8'$.

Proof Realize that all three formulations (3), (5), and (8) have the same objective function. Hence, it is sufficient to show that all three formulations have the same feasible region. Hence, assume that S_3, S_5, S_8 represent the feasible regions of formulation (3), (5), and (8), respectively. We will show these feasible regions are equivalent by showing $S_3 \subseteq S_5 \subseteq S_8 \subseteq S_3$. The subscript i will denote vector element computation.

Pick a point $(x^3, y^3) \in S_3$. We want to show that there exists a value of r such that $(x^3, y^3) \in S_5$. Then, for all i, either $y_i^3 = 0$, or $g_i(x^3, y^3) = 0$ or both. Suppose $y_i^3 = 0$. Then, in formulation (5), let r_i=1, which implies $y_i^3 = 0$ in formulation (5) as well. If $g_i(x^3, y^3) = 0$, then choose r_i=0, which implies $g_i(x^3, y^3) = 0$ in

[4] Special ordered sets of type 2 (SOS type 2) variables are defined as a set of positive variables of which at most two can be non-zero, and if two are non-zero then they need to be next to each other.
[5] So that the Disjunctive Constraints approach provides the same solution set as (3).

formulation (5) as well. If both are zero, choose r_i=1 (or r_i=0), which will ensure that $y_i^3 = 0$ and that $g_i(x^3, y^3) = 0$ is within the feasible region of (5). Since K is chosen to be large enough, these arguments imply that the solution set to (3) is contained in the solution set to (5), i.e., $S_3 \subseteq S_5$.

Next, pick $(x^5, y^5, r^5) \in S_5 \times \{0, 1\}^{n_y}$ which is a solution to (5). Consider any vector element i. Suppose that $r_i^5 = 0$. This implies $g_i(x^5, y^5) = 0$, which implies $u_i^5 = \frac{y_i^5}{2}$ and $v_i^5 = \frac{y_i^5}{2}$. Hence, this implies $u_i^5 - v_i^5 = 0$, and in particular $u_i^5 - |v_i^5| = 0$. On the other hand, $r_i^5 = 1$ implies $y_i^5 = 0$, $u_i^5 = \frac{g_i(x^5, y^5)}{2}$, and $v_i^5 = -\frac{g_i(x^5, y^5)}{2}$. Hence, this case also implies that $u_i^5 - |v_i^5| = 0$. Therefore, $(x^5, y^5) \in S_8$ and $S_5 \subseteq S_8$.

Now pick any solution $(x^8, y^8) \in S_8$. For this solution $u_i^8 - |v_i^8| = 0$ for each i. Hence, this implies $(u_i^8)^2 - (|v_i^8|)^2 = 0$ and, in particular $({u_i}^8)^2 - ({v_i}^8)^2 = 0$. Then, the following argument shows that $S_8 \subseteq S_3$.

$$\begin{aligned}({u_i}^8)^2 - ({v_i}^8)^2 = 0 \Leftrightarrow & \frac{({y_i}^8)^2 + 2 \cdot ({y_i}^8) \cdot g_i(x^8, y^8) + (g_i(x^8, y^8))^2}{4} - \frac{({y_i}^8)^2 - 2 \cdot ({y_i}^8) \cdot g_i(x^8, y^8) + (g_i(x^8, y^8))^2}{4} \\ & = 0 \Leftrightarrow {y_i}^8 \cdot g_i(x^8, y^8) = 0.\end{aligned}$$

Hence, S_3, S_5, and S_8 are subsets of each other so they are equivalent.■

From this theorem and the fact that an absolute value of a number can be written as the sum of its positive and negative parts leads to the use of special ordered sets of type 1 (SOS1) variables (Beale and Tomlin 1970) where at most one of a pair of variables can be non-zero. Note that formulation (9) if solved to optimality will provide a global solution to the original MPEC (3) but a transformation of the absolute value term is needed to simplify things, hence the use of SOS1 variables.

$$\begin{aligned}& \min f(x, y) \\ & s.t. (x, y) \in \Omega \\ & y \geq 0 \\ & g(x, y) \geq 0 \\ & u - (v^+ + v^-) = 0 \\ & u = \frac{y + g(x,y)}{2} \\ & (v^+ - v^-) = \frac{y - g(x,y)}{2} \\ & \text{where } v^+, v^- \text{are SOS 1 variables.}\end{aligned} \tag{9}$$

The following lemma then equates the solutions sets of formulations (8) and (9).

Lemma 1 The solution sets to formulation (9) and formulation (8), S_9' and S_8' respectively, are equivalent. That is, S_9'=S_8'.

Proof Again, since the objective functions for both formulations are the same, it is sufficient to show that both formulations have the same feasible region. Hence, assume that S_9 and S_8 represent the feasible regions of formulation (9) and (8), respectively. Set $v^+ - v^- = v$. Then, for all i, either $(v^+)_i$= 0 , or $(v^-)_i$= 0 or both because $(v^+)_i, (v^-)_i$ is a set of SOS1 variables where at most one can be nonzero. This implies that $v^+ + v^- = |v|$ (componentwise absolute value). Hence, we can substitute v in for $v^+ - v^-$ in formulation (9) and $|v|$ for $v^+ + v^-$ in formulation (9) to get formulation (8). The substitution the other way works as well, hence $S_9 = S_8$. ■

Several other alternatives were explored to reformulate or approximate the absolute value function that appears in (8), for example the smooth function approximation from (Steffensen and Ulbrich 2010). However, this latter methodology did not work when applied to the large-scale example of the gas market that we present in Section 5. Specifically, the method of Steffensen and Ulbrich (2010) terminated at an infeasible solution. In an attempt to increase the accuracy of the smoothing function, the solver kept terminating stating that there was no feasible solution available. An alternative way to reformulate the absolute value function is the penalty method (Bazaraa et al. 1993) but applied to the positive and negative parts of each component of v as shown in (10) where L_i is a positive penalty parameter.

$$\begin{aligned}
&\min f(x,y) + \sum_{i=1}^{n_y} L_i({v_i}^+ + {v_i}^-)\\
&s.t.(x,y) \in \Omega\\
&y \geq 0\\
&g(x,y) \geq 0\\
&u - (v^+ + v^-) = 0\\
&u = \tfrac{y+g(x,y)}{2}\\
&(v^+ - v^-) = \tfrac{y-g(x,y)}{2}\\
&\text{where } \mathrm{v}^+, \mathrm{v}^- \text{ are non} - \text{negative variables.}
\end{aligned} \tag{10}$$

Theorem 2 provides insight on how correctly selecting L_i can help obtain a feasible solution to the original MPEC. Note that from this point onward the proceeding framework applies to only convex MPECs with linear complementary constraints, still a fairly broad class of problems.

Theorem 2 Assume that the Karush-Kuhn-Tucker conditions are both necessary and sufficient for the optimization problem (10). If formulation (9) has a solution, then for any $L_i > 0$ and for each i, at most one of $(v^+)_i$ and $(v^-)_i$ is nonzero in formulation (10).

Proof We will show this by contradiction. Suppose that there exists a $L_i > 0$ such that a solution to (10) gives an index i where both $(v^+)_i > 0$ and $(v^-)_i > 0$. Let the following be the slightly altered form of (10) considered where the Lagrange multipliers are included in parentheses and $\{(x,y) \text{s.t. } C(x,y) \leq 0\}$ are the set of constraints that define Ω.

$$\begin{aligned}
&\min f(x,y) + \sum_{i=1}^{n_y} L_i({v_i}^+ + {v_i}^-) &&\\
&C(x,y) \leq 0 && (\lambda_1)\\
&-y \leq 0 && (\lambda_2)\\
&-g(x,y) \leq 0 && (\lambda_3)\\
&(v^+ + v^-) - \tfrac{y+g(x,y)}{2} = 0 && (\lambda_4)\\
&(v^+ - v^-) - \tfrac{y-g(x,y)}{2} = 0 && (\lambda_5)\\
&\text{where } v^+, v^- \text{ are non} - \text{negative variables.} &&
\end{aligned} \tag{11}$$

Then, taking the first-order Karush-Kuhn-Tucker conditions (Bazaraa et al. 1993), respectively, for $(v^+)_i$ and $(v^-)_i$ gives $L_i + (\lambda_4)_i + (\lambda_5)_i = 0$ and $L_i + (\lambda_4)_i - (\lambda_5)_i = 0$ since both $(v^+)_i > 0$ and $(v^-)_i > 0$. Together these two conditions imply $(\lambda_5)_i = 0$ and $L_i = -(\lambda_4)_i$. This implies that the Lagrangian (Λ) can equivalently be expressed as

$$\Lambda = f(x,y) + \sum_{j=1, j\neq i}^{n_y} L_j(v_j^+ + v_j^-) - (\lambda_4)_i(v_i^+ + v_i^-) + (\lambda_1)^T C(x,y) + (\lambda_2)^T(-y) + (\lambda_3)^T(-g(x,y))$$
$$+ (\lambda_4)^T\left((v^+ + v^-) - \frac{y + g(x,y)}{2}\right) + (\lambda_5)^T\left((v^+ - v^-) - \frac{y - g(x,y)}{2}\right).$$

Realizing that λ_4 now appears in two terms, we can factor this out and realize that the following optimization problem will give the same solution as formulation (11) above.

$$\begin{array}{ll}
\min f(x,y) + \sum_{j=1, j\neq i}^{n_y} L_j(v_j^+ + v_j^-) & \\
C(x,y) \leq 0 & (\lambda_1) \\
-y \leq 0 & (\lambda_2) \\
-g(x,y) \leq 0 & (\lambda_3) \\
(v_{j\neq i}^+ + v_{j\neq i}^-) - \frac{y_{j\neq i} + g_{j\neq i}(x,y)}{2} = 0 & (\lambda_4)_{j\neq i} \\
-\frac{y_i + g_i(x,y)}{2} = 0 & (\lambda_4)_i \\
(v^+ - v^-) - \frac{y - g(x,y)}{2} = 0 & (\lambda_5) \\
\text{where } v^+, v^- \text{ are non} - \text{negative variables.} &
\end{array} \quad (12)$$

But since $L_i > 0$, this implies $(\lambda_4)_i < 0$ and since the above formulation satisfies necessary and sufficient[6] conditions for the Karush-Kuhn-Tucker conditions, formulation (12) indicates that $\frac{y_i + g_i(x,y)}{2} = 0$. Since both y and g are constrained to be nonzero, this implies that $(v^+)_i = (v^-)_i = 0$ for the index i in (11). This is a contradiction. Hence, for all $L_i > 0$, the formulation (10) gives a solution where for each i, at most one of $(v^+)_i$ and $(v^-)_i$ is nonzero.■

From this point on, for simplicity, $L = \max\{L_i\}$ will be the constant in (10). The value of the constant L should be chosen to be small enough so it does not interfere with the solution (usually, the size of the chosen tolerance for the solver). Since for all positive L it is possible to get a solution that is a feasible point of (10) (given that a feasible point to the original MPEC exists), L can be chosen to be machine epsilon. Numerical results validate that as L approaches zero, the optimal objective function value of (10) approaches the optimal objective function value of (3). Moreover, Theorem 3 shows that under certain reasonable conditions, there exists a finite penalty parameter L that will produce a solution to the original MPEC (assuming one exists).

[6] Necessary conditions are needed to go from formulation (11) to the Karush-Kuhn-Tucker conditions and sufficient conditions to go from Karush-Kuhn-Tucker conditions of (11) to optimization formulation (12). Also, it can be argued that the constraint associated with $(\lambda_4)_i$ need not be an equality constraint. Hence, we include the fact that $(\lambda_4)_i < 0$ to ensure that we get equality for the associated constraint.

From a practical perspective, it is important to note that at times, solvers can fail to solve the MPEC in question by terminating at an infeasible solution for (3) where there exists an i, for which both of $(v^+)_i$ and $(v^-)_i$ are nonzero in (10). The point is feasible for (10) but not for (3). By Theorem 2, such a point is not optimal for (10), so the solver will have converged to a suboptimal solution to (10). An alternative to this is provided by the following (heuristic) Algorithm 1. Note that there is only numerical evidence that Algorithm 1 converges to an optimal solution for a given L, as it is based on the penalty method.

Algorithm 1 (Solving MPECs Using a Combination of (9) and (10))

Step 0: Pick a tolerance t.
Step 1: Solve the problem using the penalty method formulation (10) with $L=t$.
Step 2: Check for any pairs of variables v^+ and v^- that are both non-zero. If yes, go to Step 3. If not, skip to Step 6.
Step 3: Reformulate those particular variables as SOS1 variables as in formulation (9).
Step 4: Solve the problem again using the solution from Step 1 as an initial starting point. This will be a mixed-integer program due to the introduction of the SOS1 variables.
Step 5: Go to Step 2.
Step 6: Check solution by changing value of L in formulation. Decrease L until value for objective function stays the same. Then stop.

The next theorem shows that there exists a finite $L > 0$ so that a solution to the penalty formulation (10) is also a solution to the original problem (9) (or (8)). First we make the following assumption necessary for this result.

Assumption 1

Let $S = \{(x,y)|(x,y) \in \Omega, g(x,y) \geq 0, y \geq 0\}$, and $T = \{(x,y,u,v^+,v^-)|u-(v^+ + v^-) = 0, u = \frac{y+g(x,y)}{2}, (v^+ - v^-) = \frac{y-g(x,y)}{2}, v^+, v^- \geq 0\}$. The following problem has a finite optimal objective function value $\kappa > 0$:

$$\begin{aligned} &\max \sum_{i=1}^{n_y} (v_i^+ + v_i^-) \\ &\text{s.t.} (x,y) \in S \\ &(x,y,u,v^+,v^-) \in T. \end{aligned} \tag{13}$$

Remarks:

1. If the feasible region to the problem in Assumption 1 is both nonempty and compact, by the Weierstrass Theorem (Bazaraa et al. 1993), then this assumption is valid.
2. In engineering and economic examples, the primal variables x might relate to physical quantities which would then have realistic upper bounds. Via an appropriate inverse demand function (or other mechanism), the dual variables y could also be bounded as discussed in (Gabriel and Leuthold 2010).
3. Given the form of the problem in Assumption 1, to ensure compactness of the feasible region of given that all functions involved are assumed to be continuous,

it would suffice to have the set S be closed. This restriction is guaranteed when the set S is composed of polyhedral constraints.

Theorem 3 Suppose Assumption 1 is in force. Then, there exists an $L > 0$ so that for all positive $\widehat{L} \leq L$, a solution to (10) using the penalty $\widehat{L}$ will also solve (9).

Proof First note that by Theorem 2, for any positive values of L, a solution $z^* = \left(x^*, y^*, u^*, (v^+)^*, (v^-)^*\right)$ of (10) will satisfy the SOS1 property for each pair of components $(v^+)_i^*, (v^-)_i^*$. Given that the feasible regions to (9) and (10) are identical except for the SOS1 property, this means that $\alpha^* \leq \alpha^*(L)$ where α^* and $\alpha^*(L)$ are, respectively, the optimal objective function values to (9) and (10). The above inequality follows since a solution to (10), via Theorem 2 is feasible but not necessarily optimal to (9).

From Assumption 1, we know that the term $\sum_{i=1}^{n_y} (v_i^+ + v_i^-)$ is bounded above by $\kappa > 0$ over the set $S \cap T$. We see that $\alpha^*(L) \leq \beta^*(L)$ where $\beta^*(L)$ is the optimal objective function value to the problem

$$\begin{aligned} &\min f(x, y) + \kappa L \\ &\text{s.t.}(x, y) \in S \\ &(x, y, u, v^+, v^-) \in T. \end{aligned} \tag{14}$$

This inequality follows from Assumption 1 by replacing the term $\sum_{i=1}^{n_y} (v_i^+ + v_i^-)$ by its upper bound of κ on $S \cap T$. Note that since κL is a constant to the problem above, the solution set of this problem exactly matches that of

$$\begin{aligned} &\min f(x, y) \\ &\text{s.t.}(x, y) \in S \\ &(x, y, u, v^+, v^-) \in T, \end{aligned} \tag{15}$$

whose feasible region is a relaxation of (9) and whose optimal objective function value is designated as γ^*. Thus, we have the following equality:

$$\beta^*(L) = \gamma^* + \kappa L \leq \alpha^* + \kappa L \tag{16}$$

in light of the fact that adding in the SOS1 restrictions to the feasible region of (9) makes it smaller so that $\gamma^* \leq \alpha^*$. Thus, we see that

$$\alpha^* \leq \alpha^*(L) \leq \alpha^* + \kappa L. \tag{17}$$

Now assume for sake of contradiction that there does not exist an $L > 0$ small enough so that a solution to (10) solves (9) for all smaller positive penalties $\widehat{L} \leq L$. This means that for each $L > 0$ that the corresponding values for $(v^+)_i^*, (v^-)_i^*$ only correspond to a feasible but not optimal solution to (9). Except for the degenerate case where for all i, $v_i^+ = v_i^- = 0$, there are 2^{n_y} combinations of SOS1 variables in which

$(v^+)_i^* = 0$ or $(v^-)_i^* = 0$. Thus, correspondingly there exists a finite, minimum distance $\delta > 0$ such that $\left[\alpha^*(L) - \alpha^*\right] \geq \delta$ for all values of $L > 0$. But this last inequality involving δ is thus a contradiction to $\alpha^* \leq \alpha^*(L) \leq \alpha^* + \kappa L$ since we can choose $L < \frac{\delta}{\kappa}$ which shows that

$\left[\alpha^*(L) - \alpha^*\right] < \delta$, a contradiction.■

Note that the above theorem is only true for positive L since at a value of zero, the inequalties will in general not hold.

3 Numerical examples

To motivate the proposed method, consider the following sample MPEC where three firms compete to sell natural gas in the market. The firm leader, "Shale Firm," has market power and gets to move first while the other two firms are followers. Furthermore, we assume a linear demand and a quadratic cost function. The resulting MPEC is thus an instance of a Stackelberg game (Gibbons 1996), where the firms choose quantities to produce. Table 1 provides the definition of terms for the following example.

Shale Firm solves a constrained maximization problem where it maximizes its own profits. This is the upper-level problem:

$$\max_{Q \geq 0} \{(a - b(q_1 + q_2 + Q))Q - CQ\}. \tag{18}$$

Firm i=1,2 solves the following lower-level problem where it takes the upper-level quantity Q as fixed and tries to maximize profits while in Nash-Cournot competition with the other Stackelberg follower firm j.

$$\max_{q_i \geq 0} \left\{ \left(a - b\left(q_i + q_j + Q\right)\right) q_i - c_i q_i \right\}. \tag{19}$$

Table 1 Definition of terms for simple example

Parameters	Shale Firm	Firm 1	Firm 2
Intercept and Slope of Linear Demand	a,b	a,b	a,b
Marginal cost	C	c_1	c_2
Positive Constants Used to Replace Complementarities by Disjunctive Constraints	.	K_1	K_2
Variables	Shale Firm	Firm 1	Firm 2
Quantity Natural Gas Sold[a]	Q	q_1	q_2
Binary Variables Used to Replace Complementarities by Disjunctive Constraints	.	r_1	r_2
Outputs	Shale Firm	Firm 1	Firm 2
Market Price[b]	P	P	P
Profits	ProfitShale	Profit1	Profit2

[a] These quantities are constrained to be nonnegative

[b] We assume a linear demand with $P = a - b(q_1 + q_2 + Q)$

This lower-level Nash-Cournot game can be expressed as the following linear complementarity problem:

$$\begin{array}{l} 0 \leq -a + c_1 + 2bq_1 + bq_2 + bQ \perp q_1 \geq 0 \\ 0 \leq -a + c_2 + 2bq_2 + bq_1 + bQ \perp q_2 \geq 0\,. \end{array} \tag{20}$$

To solve the problem using disjunctive constraints, the KKT conditions (Bazaraa et al. 1993) are added to the constraint set in (18) to form one overall problem. By having sufficiently large positive constants K_1 and K_2, the complementarity problem (20) is reformulated as follows:

$$\begin{array}{l} 0 \leq -a + c_1 + 2bq_1 + bq_2 + bQ \ \leq K_1 r_1 \\ 0 \leq q_1 \ \leq K_1(1 - r_1) \\ 0 \leq -a + c_2 + 2bq_2 + bq_1 + bQ \ \leq K_2 r_2 \\ 0 \leq q_2 \ \leq K_2(1 - r_2). \end{array} \tag{21}$$

where r_1 are r_2 are binary variables. Let K_1=K_2 be the maximum of the x-intercept, y-intercept of the demand function, and the capacity restrictions, i.e., K_1=K_2=max $\{a/b, a\}$ following (Gabriel and Leuthold 2010).

Finally, replacing the original complementarity problem with the disjunctive constraints and combining with the upper-level problem, the following mixed-integer nonlinear program formulation is expressed in disjunctive form:

$$\begin{array}{l} \max\limits_{Q,q_1,q_2} \ \{(a - b(q_1 + q_2 + Q))Q - CQ\} \\ 0 \leq -a + c_1 + 2bq_1 + bq_2 + bQ \ \leq K_1 r_1 \\ 0 \leq q_1 \ \leq K_1(1 - r_1) \\ 0 \leq -a + c_2 + 2bq_2 + bq_1 + bQ \ \leq K_2 r_2 \\ 0 \leq q_2 \ \leq K_2(1 - r_2) \\ r_1, r_2 \in \{0, 1\}. \end{array} \tag{22}$$

The goal is to use (22) as a benchmark for comparison to the proposed method. Using (18) to (20), the MPEC under consideration is reformulated to demonstrate the SOS1 and penalty methods with some slight reorganization as shown below.

$$\begin{array}{l} z_1 = -a + c_1 + 2bq_1 + bq_2 + bQ \\ z_2 = -a + c_2 + 2bq_2 + bq_1 + bQ \\ z_1 \geq 0 \\ z_2 \geq 0 \\ z_1 q_1 = 0 \\ z_2 q_2 = 0. \end{array} \tag{23}$$

Now, for i=1, 2, $z_i q_i = u_i - |v_i|$ where $u_i = \frac{q_i+z_i}{2}$ and $v_i = \frac{q_i-z_i}{2}$ by Schur's decomposition. So the eventual formulation using SOS type 1 variables is:

$$\begin{aligned}
&\max_{Q,q_1,q_2} \{(a - b(q_1 + q_2 + Q))Q - CQ\}\\
&z_1 = -a + c_1 + 2bq_1 + bq_2 + bQ\\
&z_2 = -a + c_2 + 2bq_2 + bq_1 + bQ\\
&z_1 \geq 0\\
&z_2 \geq 0\\
&u_1 = \tfrac{q_1+z_1}{2}\\
&v_1^+ - v_1^- = \tfrac{q_1-z_1}{2}\\
&u_2 = \tfrac{q_2+z_2}{2}\\
&v_2^+ - v_2^- = \tfrac{q_2-z_2}{2}\\
&u_1 - (v_1^+ + v_1^-) = 0\\
&u_2 - (v_2^+ + v_2^-) = 0\\
&\text{where } v_i^+, v_i^- \text{ are SOS type1 variables}
\end{aligned} \tag{24}$$

Similarly, the formulation for the penalty method is given by

$$\begin{aligned}
&\max_{Q,q_1,q_2} \left\{(a - b(q_1 + q_2 + Q))Q - CQ - L(\sum_{i=1}^{2} v_i^+ + v_i^-)\right\}\\
&z_1 = -a + c_1 + 2bq_1 + bq_2 + bQ\\
&z_2 = -a + c_2 + 2bq_2 + bq_1 + bQ\\
&z_1 \geq 0\\
&z_2 \geq 0\\
&u_1 = \tfrac{q_1+z_1}{2}\\
&v_1^+ - v_1^- = \tfrac{q_1-z_1}{2}\\
&u_2 = \tfrac{q_2+z_2}{2}\\
&v_2^+ - v_2^- = \tfrac{q_2-z_2}{2}\\
&u_1 - (v_1^+ + v_1^-) = 0\\
&u_2 - (v_2^+ + v_2^-) = 0\\
&\text{where } v_i^+, v_i^- \text{ are non} - \text{negative variables}
\end{aligned} \quad . \tag{25}$$

The computational objective was to compare the results for the methods of disjunctive constraints (22), SOS1 variables (24) and the penalty method (25). This was accomplished using GAMS (GAMS 2009) with CONOPT being used as the nonlinear solver and SBB the mixed integer nonlinear solver.

The capacity constraints for production quantities are omitted for this first example, i.e., maximum production is only limited by rising costs. The following Table 2 shows the datasets used:

Table 2 Different Datasets to Compare (22), (24), and (25)

Dataset Parameters	Dataset 1	Dataset 2	Dataset 3
a	13	13	13
b	1	0.1	0.1
c_1=c_2=C	1	1	2

Table 3 Different Cases to Compare Solutions to (25)

	Case 1	Case 2
Value of L	0.0001	1

For the disjunctive constraints formulation (25), $K_1 = K_2 = \max\{b/a, a\} = 13$ consistent with (Gabriel and Leuthold 2010) for all the datasets while for the penalty method approximation (25), two different values of L were chosen to show how a lower value of L gives a better answer. Table 3 shows the different values of L for the two cases.

The following Tables 4, 5 and 6 report the results. The unique true answer[7] can be easily verified algebraically and is shown in the third column of the tables. Note that the disjunctive constraints approach obtained the correct answer for Dataset 1, implying that a correct value of K was chosen.

If the methodology to choose K as outlined in the literature (Gabriel and Leuthold 2010) is used, disjunctive constraints do not provide correct solutions in Datasets 2 and 3.[8] These results point out a big weakness with disjunctive constraints, namely that a computed solution can be very far from a true answer and the given solution can be extremely sensitive to the value of K if appropriate problem-specific values are not selected.

Two further methods were used to attempt to solve the above MPEC examples. First, the solver NLPEC (GAMS 2009), which is a commercial solver for MPECs was used. Second, since (3) is a nonlinear program, the solver CONOPT (GAMS 2009) was also used. Note that both solvers converged to the true answer for all the above numerical examples.

In a second set of numerical tests for this small MPEC, we compared the disjunctive constraints method with the penalty approach. Solving the formulation (22) with a large enough value of K can result in a solution. Likewise, choosing a small enough value for the penalty parameter L in (25) can produce a solution. The next set of numerical results were done with Dataset 3 using $K = 10000$ and $L = 10^{-16}$ (machine epsilon) where these values were reached after numerical and algebraic experimentation with the test problem. The test problem was changed so that now instead of two players at the lower level, there were M players with similar costs and parameters. The number of players was increased to test the computational time taken for the NLPEC solver for the disjunctive constraints formulation (22), the SOS1 formulation (24), and the penalty method formulation (25). The nonlinear solver CONOPT was unable to converge to a feasible point when the number of players was over 200, so has not been included in this analysis. The results are shown in Fig. 1. All methods were able to obtain the correct solutions.

Clearly, the disjunctive constraints approach becomes extremely computationally expensive when the number of players is increased. Note that the graphs for the penalty and SOS1 methods are overlapping, and greatly outperform the NLPEC solver for this example.

[7] It is simple algebra to show that this is the unique solution since there are no constraints and all objective functions are quadratic.

[8] The method in (Gabriel and Leuthold 2010) gives a correct value of K whenever maximum production (capacity constraints for production) is included in the problem formulation. Our goal was to give a very simple counterexample where the disjunctive constraints approach didn't work.

Table 4 Results for Dataset 1

Results	Disj Cons	True Answer	SOS	Case1	Case 2
$q_1=q_2$	2.000	2.000	2.000	2.000	1.833
Q	6.000	6.000	6.000	6.000	6.500
Price	3.000	3.000	3.000	3.000	2.833
Profit shale	12.000	12.000	12.000	12.000	11.917
Profit 1=2	4.000	4.000	4.000	4.000	3.361

4 Addition of shale gas to the world gas model

In this section we analyze our proposed methodology on a larger-scale MPEC for the U.S. natural gas market focusing on shale gas. In this problem, the shale gas data came from the U.S. Department of Energy's *Annual Energy Outlook* (2010) with shale gas production and Lower 48 onshore natural gas production datasets. [9] As compared to the version of the model from (Gabriel et al. 2012), the World Gas Model was modified to contain three production nodes for each census region of the United States: conventional gas, shale gas, and non-shale unconventional gas.

A "Golombek" production cost function (Golombek and Gjelsvik 1995)) was used:

$$C(q) = (\alpha - \gamma)q + \frac{1}{2}\beta q^2 + \gamma(Q - q)\ln\left(\frac{Q - q}{Q}\right), \tag{26}$$

for which the marginal supply cost curve is:

$$C'(\mathrm{q}) = \alpha + \beta \mathrm{q} + \gamma \ln\left(\frac{\mathrm{Q} - \mathrm{q}}{\mathrm{Q}}\right). \tag{27}$$

Here, Q is the production capacity, $\alpha > 0$ is the minimum per unit cost, $\beta>0$ is the per unit linearly increasing cost term, and $\gamma \leq 0$ is a term that induces high marginal costs when production is close to full capacity.

Skagen (2010) indicates that recent research has led to predicting a lower value of α for the cost function of shale gas when compared to conventional gas. Figure 2 shows that shale gas is now understood to have a lower price of extraction in the beginning phases.

Alternatively, others believe that initial positive results from shale gas extraction wells might not be sustainable in the long run (Cohen 2009). In particular, the geologist Art Berman claims that decline rates will be much higher than expected, and while shale appears to be a good resource right now, steep decline rates mean that higher extraction will lead to higher costs quickly (Cohen 2009).

In the modification of the WGM, the shale gas cost curve has α (the y-intercept of the marginal cost curve) lower and β (the slope of the marginal cost curve) higher than for conventional gas. While the lower initial cost of extraction is consistent with Skagen's observation, a higher marginal cost increase and higher marginal costs

[9] For a table relating the WGM nodes to the shale plays in the US, please refer to the Appendix.

Table 5 Results for Dataset 2

Results	Disj Cons	True Answer	SOS	Case1	Case 2
$q_1=q_2$	13.000	20.000	20.000	20.000	18.333
Q	81.000	60.000	60.000	60.000	65.000
Price	2.300	3.000	3.000	3.000	2.833
Profit shale	105.300	120.000	120.000	120.000	119.167
Profit 1=2	16.900	40.000	40.000	40.000	33.611

at higher quantities is consistent with Berman's claim that decline rates of shale wells will be higher. Hence, shale gas has a lower initial cost of extraction than conventional gas but a higher rate of increase for marginal cost and so the current debate about shale gas has been incorporated into our numerical tests.

The other initial condition imposed is that total production costs should be the same between shale and conventional gas. This leads to the integral of the marginal cost curve being the same for both functions (conventional and shale gas). This ensures a positive production of both types of gas, which can be calibrated to real data. Furthermore, a comparison is provided with two other cases with higher total costs for shale production. Another reason why the total costs should be equal in the reference case is that producers drilling in the same region would encounter similar terrain, similar taxes, similar hurdles etc. Hence, α was reduced by 20 % of the value of conventional gas based on Skagen (2010) and β was increased by an amount so that the integral of the marginal cost curve remains the same. An explanation of this is shown in Fig. 3 below. Note that the values of γ are kept the same for shale and conventional gas, so Fig. 3 only shows the linear portion of the marginal cost curve. The production cost data for conventional and unconventional (non-shale) gas was obtained as described in (Gabriel et al. 2012).

5 Application: using the world gas model to study the impact of a shale producer having market power

This section describes numerical results of solving the MPEC version of the World Gas Model described earlier. The point is to demonstrate that even on large MPECs, this new technique works well. Five different cases were run, which are described

Table 6 Results for Dataset 3

Results	Disj Cons	True Answer	SOS	Case1	Case 2
$q_1=q_2$	13.000	18.333	18.333	18.333	16.667
Q	71.000	55.000	55.000	55.000	60.000
Price	3.300	3.833	3.833	3.833	3.667
Profit shale	92.300	100.833	100.833	100.833	100.00
Profit 1=2	16.900	33.611	33.611	33.611	27.778

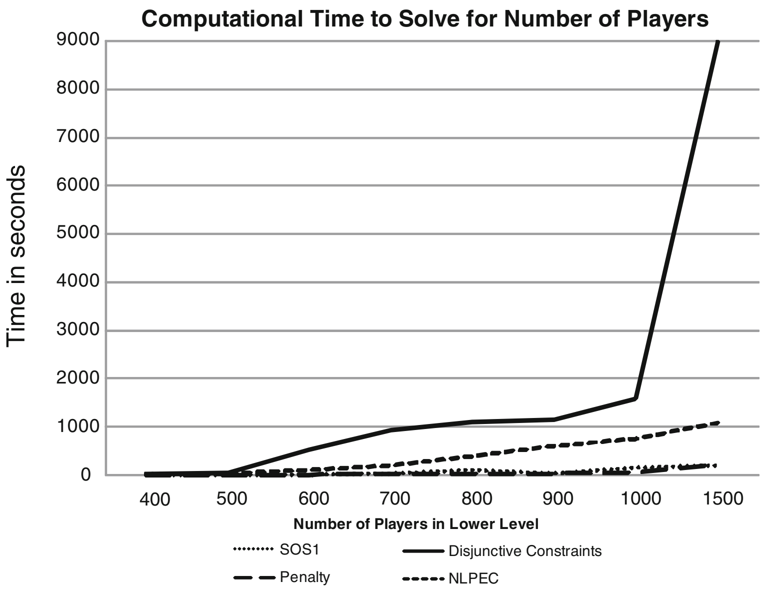


Fig. 1 Computational Time for Solving Problem

below. The results from these cases are consistent with economic theory, and are presented graphically in Figs. 4, 5, 6 and 7.

A solution exists for the lower-level complementarity problem, which means that a feasible solution for the MPEC exists as well. The method of disjunctive constraints did not provide a feasible solution for this problem with the solvers SBB and CONOPT (GAMS 2009). The solvers NLPEC for the MPEC formulation and CONOPT for the nonlinear formulation (3) terminated at an infeasible point. But a single iteration of Algorithm 1 provided a solution, further validating our approach.

The complementarity form of the WGM restricted to the North American nodes has 30 producers, of which seven are for shale gas and seven for unconventional, non-shale gas production in the United States. The rest produce conventional gas. There are a total of 15 production nodes, of which nine correspond to the census regions for the lower-48 states. There are also three traders (one each for the United States, Canada, and Mexico, the three countries in the model), along with eight periods from 2005–2040 (the last two five-year periods are not reported to avoid end-of-horizon bias), and two seasons (high and low demand) in each period. The

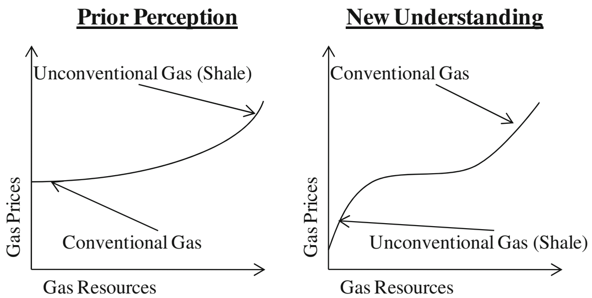
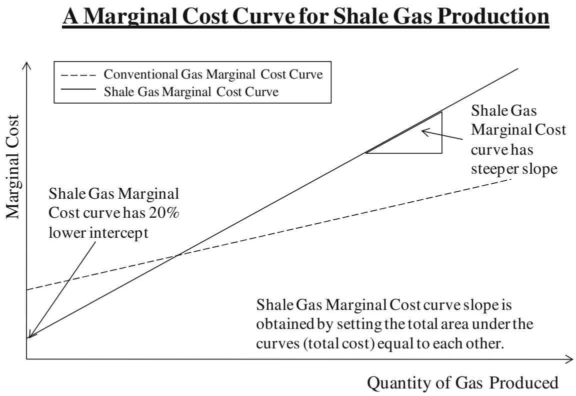


Fig. 2 A Marginal Cost Structure for Shale Gas (Skagen 2010)

Fig. 3 A Marginal Cost Structure for Shale Gas



decision variables are operating levels (production, storage injection, etc.) as well as investment levels (pipeline, liquefaction capacity, etc.). Consequently, the complementarity model has 9456 variables and takes 243.2 seconds to solve on a 2.0 GHz processor with 2 GB memory.

Additionally, it is important to note that the MPEC version of the WGM was formulated with the shale gas producer in census region 7 as the top-level player. Census region 7 contains both the Barnett and Haynesville shale plays, two of the most important ones in the United States. [10] The MPEC version was solved using Algorithm 1. The algorithm solved the problem in approximately 3 hours on the same computer described above, though the time was different for each case.

The following five cases were considered, with the Base Case modeled as a complementarity problem and the rest as MPECs for purposes of comparison:

1) **Base**: The Base Case for the WGM restricted to North America formulated as a complementarity problem and calibrated according to the *Annual Energy Outlook* (April 2009 ARRA version) and the *World Energy Outlook* (International Energy Agency 2008).
2) **MPEC**: The MPEC version of the Base Case. The shale producer in census region 7 was placed at the upper level and all other players at the lower level.
3) **MoreShale**: A higher production of shale gas was considered by increasing the daily capacity available, with a 10 % increase for 2015, 2020; a 15 % increase for 2025, 2030; and a 20 % increase for 2035, 2040. These numbers are approximations of increases given by the *Annual Energy Outlook* between the 2008 and 2009 reports' predictions. While the 2010 reports did not show such an increase, for our purposes this case was developed to show what might happen if a similar increase took place after 2015. This case is modeled as an MPEC.
4) **ShaleTax**: All shale-producing firms are taxed \$0.39/mcf (39 cents for every thousand cubic feet of natural gas produced) from 2015 to 2040. This is in line with the tax proposed for Pennsylvania shale production in the Marcellus shale play, which was later overturned (Barnes 2010). No other value for a shale tax has so far been found from any legislature. This case is modeled as an MPEC.

[10] Refer to www.eia.gov for more information.

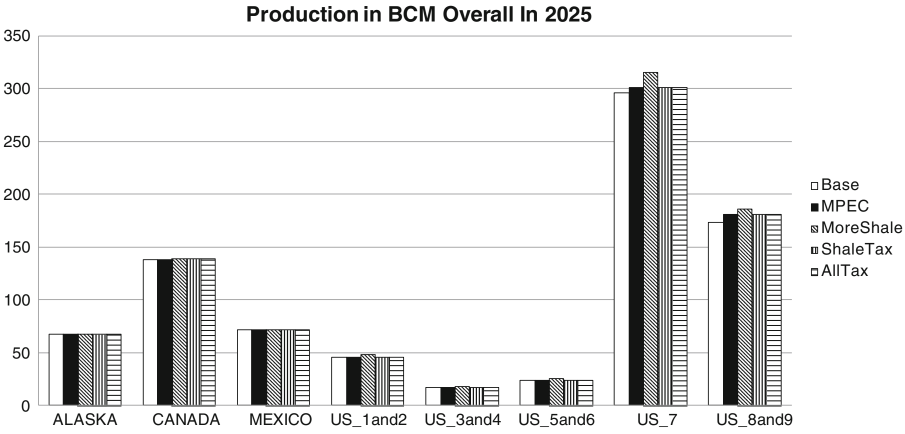


Fig. 4 Overall Production in 2025. US_1and2, for example, gives data for US census regions 1 and 2 combined

5) **AllTax**: All natural gas is taxed at \$0.39/mcf from 2015 to 2040. This case will help see if the shale players, especially the one in census region 7, have any comparative advantage when everyone is taxed. This case is modeled as an MPEC.

The results of solving each of these cases are presented below and are consistent with economic theory, in that the MPEC Case (number 2) produces lower average prices (e.g., \$6.74/MMBtu vs. \$6.94/MMBtu in 2025) and higher total production (e.g., 844.2 BCM vs. 830.2 BCM in 2025) and consumption (Gibbons 1996) when compared to the Base Case for all years. Moreover, as expected, the MoreShale Case showed an overall increase in shale production when compared to the Base Case (e.g., 111.5 BCM vs. 89.4 BCM in 2025) and for the shale producer in census region 7, proved to be the most profitable. The profits at node 7 increase by more than three times in 2025 when compared to the Base Case. This shows the advantage of being

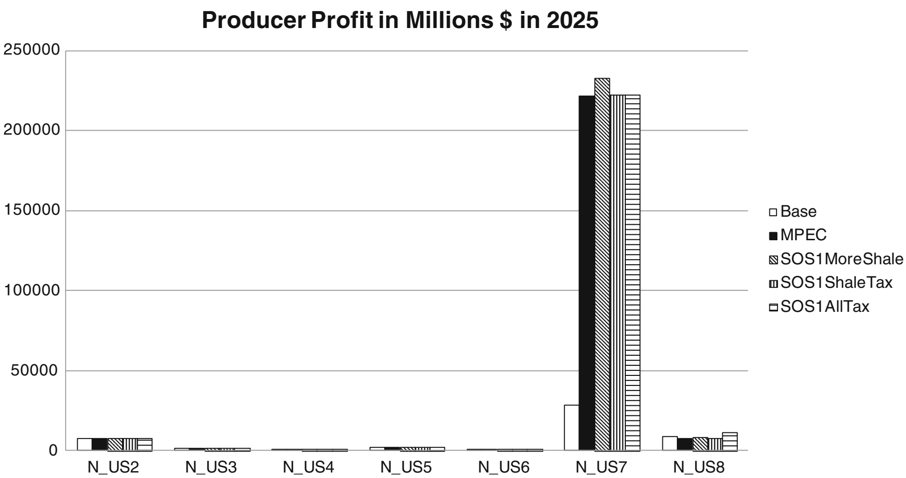


Fig. 5 Producer Profit in 2025. N_US3, for example, gives profit at the node for US census region 3

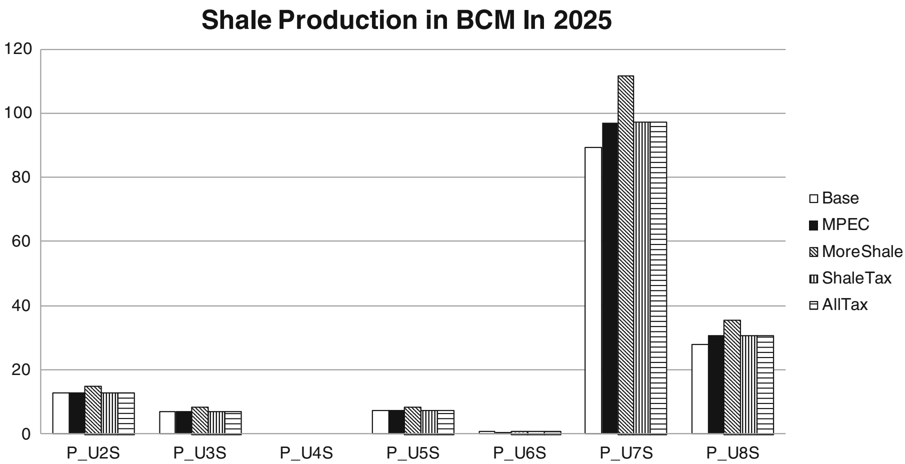


Fig. 6 Shale Producers in 2025. P_U5S, for example, gives the production at US node 5 for shale gas

the Stackelberg leader and allowing collection of more profits and also serves as a cautionary numerical result for market regulators and other interested parties.

Additionally, the MoreShale Case shows that it will be advantageous for producers as well as consumers (with prices dropping in nodes with large amounts of shale). However, the fact that total production doesn't change much with the invoking of the tax (shale or otherwise) shows that it will not be detrimental to the producers. This is corroborated by looking at producer profits as well, where the imposition of a tax barely changes total profit. Since Node 8 has a relatively abundant supply of conventional, unconventional, and shale gas, it can change production around depending on the demands. Hence, nodes 8 and 9 remain relatively unchanged with the imposition of a tax in both cases 4 and 5. Moreover, the production for shale producers is as expected, and the imposition of a tax does less to harm any production,

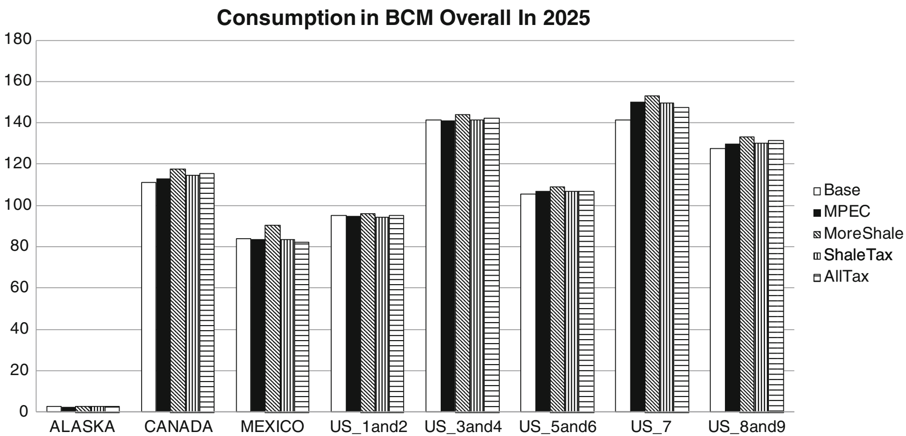


Fig. 7 Consumption in 2025

and overall profits remain relatively stable. Also, this might be a policy argument for saying that the tax will barely harm producers, but produce revenue for the state.

Data for consumption and prices (Fig. 7 and Table 7, respectively), however, show that the producers will pass most of the tax on to the consumers. This also shows the strength of the World Gas Model, by predicting which areas will show a change in prices. Nodes 5, and 6, will take on the burden of the tax with prices going slightly up ($7.14 $/MMBtu vs. $7.07/MMBtu) and consumption relatively unchanged when compared to the MPEC Case. Nodes 1 and 2 contain a majority of the Marcellus shale play; hence prices there go up with the imposition of a tax on shale gas. Moreover, U.S. nodes 7 and 8 have high production, and it's profitable for these producers to sell at a lower price in their own market and at a higher price to the other nodes. However, imposing a tax on U.S. Node 7 increases prices at that particular node in 2025 when compared to the MPEC Case. Since the shale producer at node 7 is the Stackelberg leader, in this case it can derive more profits by passing the tax onto its own consumption node. Note that the prices under the two tax cases at node 7 ($4.94/MMBtu and $5.13/MMBtu in the ShaleTax and AllTax Cases, respectively) are still lower than the price for the Base Case ($5.72/MMBtu, when the shale producer at node 7 is not a Stackelberg player).

6 Conclusions

This paper provides a novel way to solve mathematical programs with equilibrium constraints. The new method has been shown to be computationally tractable, and able to solve MPECs where the lower level is a complementarity problem.

The method was applied to an example of a shale gas producer in the U.S. natural gas market acting as a dominant player. The results show that in the case of a Stackelberg structure, the profits of the producer are not negatively affected with the current proposals for taxes. However, with this structure the producers are able to pass the tax onto the consumer, as profits do not decrease with the implementation of tax but prices do go up. Moreover, if more resources are present, the producer is able to take advantage of them. While in actuality the Stackelberg player might not have such an advantage, this setup helps show how under this scenario, producers can manipulate the market.

Table 7 Prices in $/MMBTU in 2025

Region	Base	MPEC	MoreShale	ShaleTax	AllTax
Alaska	6.17	6.17	6.17	6.17	6.17
Canada	6.94	6.69	6.02	6.50	6.34
Mexico	6.66	6.65	5.63	6.70	6.92
U.S. Nodes 1 & 2	8.85	8.91	8.59	8.98	8.88
U.S. Nodes 3 & 4	7.48	7.52	7.02	7.48	7.37
U.S. Nodes 5 & 6	7.36	7.07	6.76	7.14	7.14
U.S. Node 7	5.72	4.88	4.59	4.94	5.13
U.S. Nodes 8 & 9	6.31	6.03	5.65	6.01	5.88

Appendix

Table 8 World Gas Model Nodes: Coverage of States and shale Basins

Shale Basin Name	States							WGM Nodes
Mancos	Utah							US_8
Hilliard-Baxter Mancos	Wyoming	Colorado						US_8
Niobrara	Colorado	Nebraska	Kansas					US_4, US_8
Cody	Montana							US_8
Mowry	Wyoming							US_8
Gammon	Montana	North Dakota	South Dakota					US_4, US_8
Excello-Mulky	Kansas	Oklahoma						US_4, US_7
New Albany	Illinois	Indiana	Kentucky					US_3, US_6
Antrim	Michigan	Indiana	Ohio					US_3
Utica	New York							US_2
Marcellus	New York	Pennsylvania	Ohio	West Virginia	Maryland	Virginia	Tennessee	US_2, US_3, US_5, US_6
Devonian	Ohio	Kentucky	West Virginia	Virginia	Tennessee	Alabama	Georgia	US_3, US_5, US_6
Chattanooga	Kentucky	Virginia	Tennessee	Alabama	Georgia			US_5, US_6
Conasauga	Alabama	Georgia						US_5, US_6
Floyd-Neal	Mississippi	Alabama						US_6
Fayetteville	Arkansas							US_7
Hayneville/Bossier	Louisiana	Texas						US_7
Woodford/Caney	Oklahoma							US_7
Barnett	Texas							US_7
Pearsall	Texas							US_7
Woodford	Oklahoma	Texas						US_7
Barnett and Woodford	New Mexico	Texas						US_7, US_8
Bend	Texas							US_7
Pierre	New Mexico	Colorado						US_8
Lewis	New Mexico	Colorado						US_8
Hermosa	Utah							US_8

References

Anitescu M, Tseng P, Wright S (2007) Elastic-mode algorithms for mathematical programs with equilibrium constraints: global convergence and stationarity properties. Math Program 110(2):337–371

Barnes T (2010) House passes shale gas production tax. Pittsburgh Post-Gazette. September 30th, 2010, http://www.post-gazette.com/pg/10273/1091447-454.stm

Bazaraa M, Sherali H, Shetty C (1993) Nonlinear programming: theory and algorithms, 2nd edn. John Wiley & Sons, NY, New York, pp 438–448

Beale E, Tomlin J (1970) Special facilities in a general mathematical programming system for non-convex problems using ordered sets of variables. In: Lawrence J (ed) OR 69: Proc. Fifth Int. Conf. Oper. Res. Tavistock Publications, London, pp 447–454

Beale E (1975) Some uses of mathematical programming systems to solve problems that are not linear. Opl Res Q 26:609–618

Chen Y, Hobbs B, Munson T, Leyffer S (2006) Leader-follower equilibria for electric power and NOx allowances markets. Comput Manag Sci 3(4):307–330

Cohen D (2009) A shale gas boom? Retrieved 4 22, 2011, from Energy Bulletin: http://www.energybulletin.net/node/49342

Cottle R, Pang J, Stone R (2009) The linear complementarity problem. SIAM, Philadelphia, PA

Fletcher R, Leyffer S (2004) Solving mathematical programs with complementary constraints as nonlinear programs. Optim Meth Software 19(1):15–40

Fletcher R, Leyffer S, Ralph D, Scholtes S (2006) Local convergence of SQP methods for mathematical programs with equilibrium constraints. SIAM J Optim 17(1):259–286

Fortuny-Amat J, McCarl B (1981) A representation and economic interpretation of a two-level programming problem. J Oper Res Soc 32(9):783–792

Gabriel S, Rosendthal K, Egging R, Avetisyan H, Siddiqui S (2012) Cartelization in gas markets: studying the potential for a "Gas OPEC. Energ Econ 34(1):137–152

Gabriel S, Leuthold F (2010) Solving discretely-constrained MPEC problems with applications in electric power markets. Energ Econ 32:3–14

Gabriel S, García-Bertrand R, Sahakij P, Conejo A (2006) A practical approach to approximate bilinear functions in mathematical programming problems by using Schur's decomposition and SOS type 2 variables. J Oper Res Soc 57:995–1004

GAMS (2009) Generalized Algebraic Modeling System, www.gams.com

Gibbons R (1996) Game theory for applied economists. Princeton University Press, Princeton, NJ

Golombek R, Gjelsvik E (1995) Effects of liberalizing the natural gas markets in Western Europe. Energ J 16(1):85–111

Gumus Z, Floudas C (2001) Global optimization of nonlinear bilevel programming problems. J Glob Optim 20:1–31

Hu J, Mitchell J, Pang J, Bennett K, Kunapuli G (2007) On the global solution of linear programs with linear complementarity constraints. SIAM J Optim 19(1):445–471

International Energy Agency (IEA) (2008) World Energy Outlook 2008, http://www.worldenergyoutlook.org/2008.asp

Leyffer S, Lopez-Calva G, Nocedal J (2006) Interior methods for mathematical programs with complementarity constraints. SIAM J Optim 17(1):52–77

Luo Z, Pang J, Ralph D (1996) Mathematical programs with equilibrium constraints. Cambridge University Press, Cambridge, U.K

Mitsos A (2010) Global solution of nonlinear mixed-integer bilevel programs. J Glob Optim 47(4):557–582

National Petroleum Council (NPC) (2007) "Topic paper #29: unconventional gas, http://www.npc.org/Study_Topic_Papers/29-TTG-Unconventional-Gas.pdf, July 18th, 2007

Renegar J (1994) Some perturbation theory for linear programming. Math Program, Series A 65(1):73–91

Renegar J (1995) Incorporating condition measures into the complexity theory of linear programming. SIAM J Optim 5(3):506–524

Scheel H, Scholtes S (2000) Mathematical programs with complementarity constraints: stationarity, optimality, and sensitivity. Math Oper Res 25(1):1–22

Skagen O (2010) Global gas reserves and resources: trends, discontinuities and uncertainties. SSB/NAE Workshop, Oslo, Norway

Steffensen S, Ulbrich M (2010) A new relaxation scheme for mathematical programs with equilibrium constraints. SIAM J Optim 20(5):2504–2539

Uderzo A (2010) Exact penalty functions and calmness for mathematical programming under nonlinear perturbations. Nonlinear Anal 73:1596–1609

Ye JJ, Zhu DL (1995) Optimality conditions for bilevel programming problems. Optimization 33:9–27