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A stochastic, two-level optimization model for compressed natural gas infrastructure investments in wastewater management

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Abstract: In this paper, we present a stochastic two-level optimization model whose upper-level problem depicts a wastewater treatment plant deciding on the size of compressed natural gas (CNG) filling stations and their locations. These upper-level decisions are integrated with operational decisions for the plant as well as downstream markets including agriculture, CNG transportation, residential natural gas, and electricity markets at the lower level. The two-level problem, expressed as a stochastic mathematical program with equilibrium constraints (SMPEC), is reformulated as mixed-integer linear program (MILP) using SOS1 transformations and linearizations. As a case study, the SMPEC is used to evaluate the options for CNG investment for a wastewater treatment plant located in the Washington, DC metro area. Our results indicate that the CNG produced from the wastewater treatment plant could meet approximately 20% of the expected total transportation demand in Washington, DC. In addition, CNG produced from the wastewater treatment plant could reduce CO_2 emissions by a significant amount. The CNG benefits are traded off with less on-site wastewater-derived power production.

Key Words: CNG; MPECs; waste-to-energy; stochastic model.

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1 Introduction

Compressed natural gas (CNG) is natural gas compressed to 200 bas which remains clear, odorless, and non-corrosive [1]. CNG is composed of 83 to 99 percent methane and has the highest energy/carbon ratio of any fuel. CNG is widely used as a transportation fuel in various parts of the world. Typically, most vehicles use CNG that has been compressed between 3,000 to 3,600 psi [2]. The CNG-capable vehicles range from taxis and delivery vans to city buses. The primary goal of using CNG over gasoline or diesel is the potential savings in fuel economies [3]. According to the U.S. Energy Information Administration (EIA) [4], CNG costs \$2.15/gallon of gasoline equivalent (GGE) compared with gasoline \$3.65/GGE and diesel \$3.56/GGE as of April 2014. The prices of CNG (\$/GGE) differ by state across the U.S. In addition, another advantage of CNG is that the emissions from burning CNG are relatively cleaner than from diesel or gasoline. According to the California Energy Commission, natural gas vehicles emit ozone-forming emissions approximately 80 percent less than those using gasoline [1].

Generally, CNG is produced from natural gas that can be extracted from three different types of sources: gas-and-condensate wells, coal bed methane wells, and oil wells. In addition to these sources, natural gas can also be generated from anaerobic digestion processes. Anaerobic digestion takes place in the absence of free oxygen. Places like landfills, wastewater treatment plants, or livestock manure lagoons are very common sites where biogas can be captured. Methane and carbon dioxide are the primary elements in biogas (methane about 40%). The important factors that control the anaerobic digestion process are temperature, moisture level, and nitrogen-to-carbon ratio. Natural gas from organic wastes can be converted to renewable natural gas (RNG); RNG is also called biomethane [5]. Organic waste from urban and rural areas include household trash, institutional food waste, animal by-products, etc. These organic wastes could be feedstock for biomethane production.

According to [5], there are more than 17,000 wastewater treatment plants in the U.S., but only approximately 1,300 plants have digesters to manage biosolids and manure. Although most of the wastewater treatment plants have operating anaerobic digesters, they are primarily used for controlling odor and killing pathogens not for generating biomass. However, the Blue Plains wastewater facility run by the District of Columbia Water and Sewer Authority (DC Water), one of the largest advanced wastewater treatment facilities in the world, is installing a combined-heat-and-power (CHP) facility as well as digesters to produce methane. The products gained from processing wastewater at DC Water include class B, class A biosolids,[1] as well as methane from the digesters, see Figure 1. This methane can then be used in a variety of ways such as: producing electricity on site, converting it to compressed natural gas and sold in the local transportation market (i.e., for District of Columbia buses), sold to the natural gas end-use sectors, or sold as high-end fertilizer. These options have been explored in a series of papers using both one- and two-level optimization models as well as considering both deterministic and stochastic versions of the model [6,7,8].

The new system at Blue Plains will include three Solar Mercury 50 low nitrogen oxide gas turbines, heat recovery steam generators, duct burners, a backup boiler, electrical equipment needed to operate in parallel with the utility grid and ancillary systems, and digester gas cleaning and compression equipment. The digesters are some of the largest in the world at 14 million liters (3.8 million gallons) each and can handle up to 450 dry tons of solids. The anaerobic digestion for the new system at Blue Plains will generate about 10 MW of power, enough to supply one-third of its demand. In addition, the maximum capacity of digester at Blue Plains can generate CNG up to 2.55 million cubic feet (MMcf) per day while total daily consumption in District of Columbia is 1.98 MMcf and there is just a fueling station that is exclusively for private access called Trillium CNG of Washington Metropolitan Area Transit Authority (WMATA).

Since the CNG production capacity at Blue Palins exceeds the total demand in District of Columbia, bioCNG from wastewater could provide options if demand for CNG increases in the future. However, in order to enter to CNG market, a significant investment in infrastructure cost is required and considering the various options. This is the primary motivation for the current paper.

[1] Class A biosolids have the total amount of pathogens below a detectable level and must meet the limitations of metal contaminants related to regulation 503, which is standard for the use or disposal of sewage sludge, [26]. Class B biosolids are less stringent in terms of pathogens but still require farm management practices and area restrictions before application [26,27].

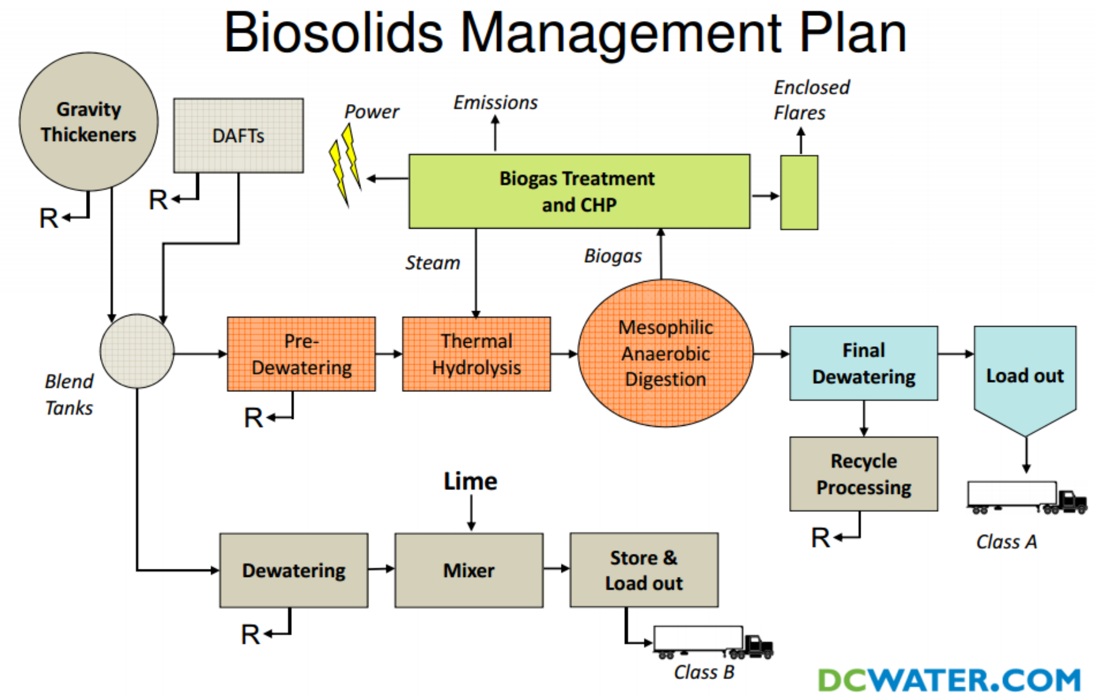

Figure 1: Biosolid management plan at Blue Plains[2]

The main contributions of the research reported in this paper are two-fold. First, we develop a novel SMPEC to analyze investments and operations aspects for advanced wastewater treatment plants considering a number of uncertainties such as fuel prices and biosolids inflow. This model is generalizable and can be applied to other wastewater treatment plants using a variety of scenario trees to represent uncertain data. Second, the SMPEC determines and optimal investment plan using the Blue Plains advanced wastewater treatment plant as a case study to validate the approach.

The remainder of the paper is as follows. Section 2 describes the methodology. The complete formulation of the SMPEC is presented in Section 3. Sections 4 and describe the case study and results. Lastly, Section 6 presents the main conclusions.

2 Methodology

Since an advanced wastewater treatment plant can have a strategic advantage relative to the CNG market as discussed earlier, the AWTP can be characterized as a dominant (i.e., Stackelberg) leader for that market. This is precisely the role it has in the model described below with a two-level Stackelberg to model the interaction between the AWTP and the relevant downstream markets. In this setting, the AWTP is the upper-level player (Stackelberg leader) and the independent suppliers associated with each market act as lower-level followers expressed as a stochastic MPEC. The general form of the SMPEC is as follows:

$$\begin{aligned} \min E\left\{f\left(x,y,\xi\right)\right\} \\ \text{s.t. } x \in X \\ (x,y,\xi) \in \Omega \\ y \in S(x) \end{aligned} \tag{1}$$

where x is the vector of upper-level fist stage decision variables, y is the vector of lower-level second-stage variables which is a solution to the equilibrium problem defined by $S(x)$. Here, X is the feasible region for x and Ω is the joint feasible region between the x and y variables. Solving stochastic MPECS is challenging

[2] http://www.virginiabiosolids.com/wp-content/uploads/2012/09/Peot-VWEA_DC_Water.pdf.

due to non-convexities in the last constraints (and others is present) and the large size of the problem due to consideration of many scenarios.

One approach is to transform (1) into a single-level problem using for example disjunctive constraints [9]. However, one disadvantage is that the computational time increases exponentially as the number of binary variables increase. An alternative is to use an SOS1 [10] approach suggested by [11] to transform the complementarity conditions of the lower-level problem and solve it as a mixed-integer program. As shown in [11], the SOS1 is numerically superior to the method of disjunctive constraints for the large-scale problems considered.

3 SMPEC modeling framework

In this section, a two-stage stochastic bilevel game, Stackelberg game, is formulated. As depicted in Figure 2, first-stage decisions involve the type of CNG station, and its location and the second-stage decisions are flows of quantities to four separate markets and operational decisions. In this framework, the market leader is the wastewater treatment plant modeled as a profit-maximizer facing uncertainties from markets i.e., natural gas and electricity prices and inputs such as wastewater inflows. The probability distribution for each uncertainty is shown in Figure 3 derived from historical data. The lower level involves equilibrium problems from the natural gas, electricity, CNG, and fertilizer markets. In addition, this paper considers three locations (market nodes) for CNG which are: 1) downtown Washington, DC, 2) on-site at the wastewater plant, and 3) Baltimore, Maryland. Each market has different inverse demand curves for CNG and thus the model must determine endogenously which markets to send the CNG to and at what levels. The CNG market representation and its network is shown in Figure 4. The upper-level player (the wastewater treatment plant) can service the three mentioned markets by investing in filling stations but the CNG transportation costs need to be considered if the installed CNG filling station is not onsite e.g., downtown Washington, DC or Baltimore, Maryland.

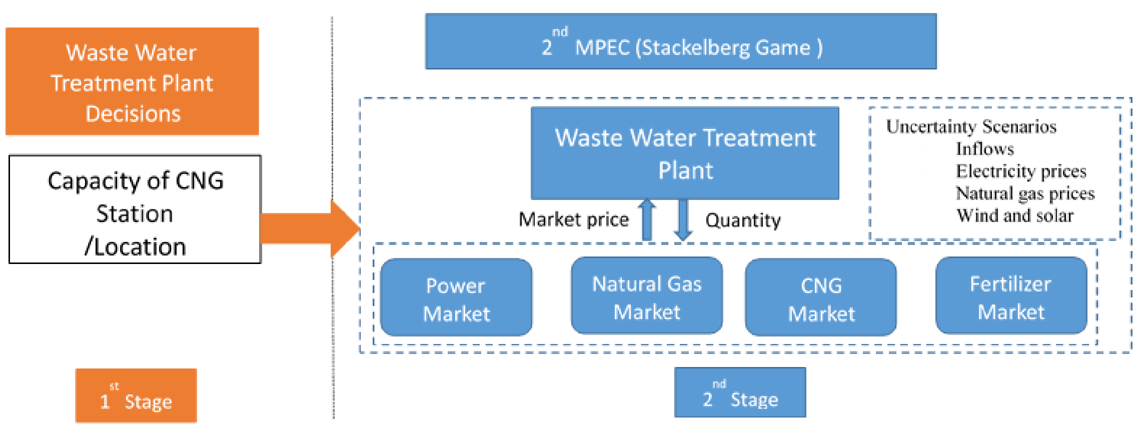

Figure 2: Modeling framework diagram

In addition to the investment decisions, as shown in Figure 3, the biosolids management decisions also considered to identify how much to produce of the following end-products: 1) biosolids class A and B, 2) biogas-and solar-based electricity, 3) bio-CNG and 4) bio-methane. [7] Besides CNG, electricity, natural gas, and fertilizer could be supplied to the relevant markets which define the market equilibrium model. Decisions made on one operation have a consequence on others. For example, if the advanced WWTP decides to use all biogas to produce CNG, there will be no more biogas to generate electricity. The next section discusses the complete model formulation.

3.1 Decision variables and parameters

The following is the description of the sets, variables and parameters used in the model with the main variables shown in Figure 3. Note that the model solves for values of only one typical day; hence, all the

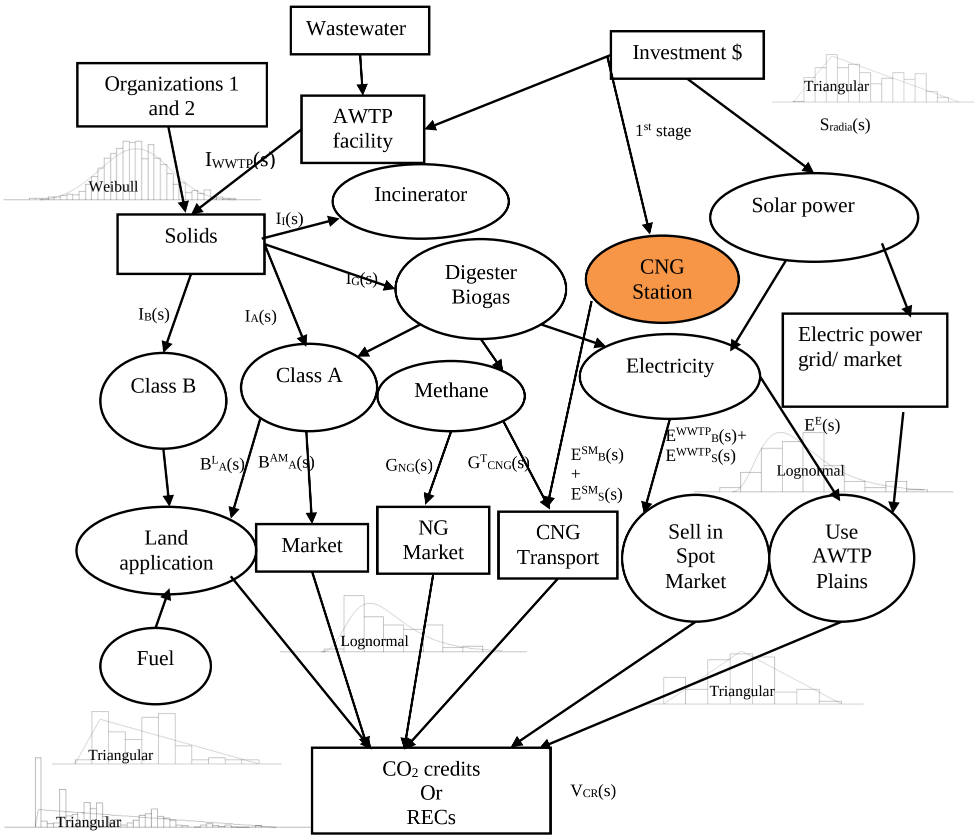

Figure 3: Flowchart of the stochastic optimization model for biosolids management program at the Blue Plains AWTP

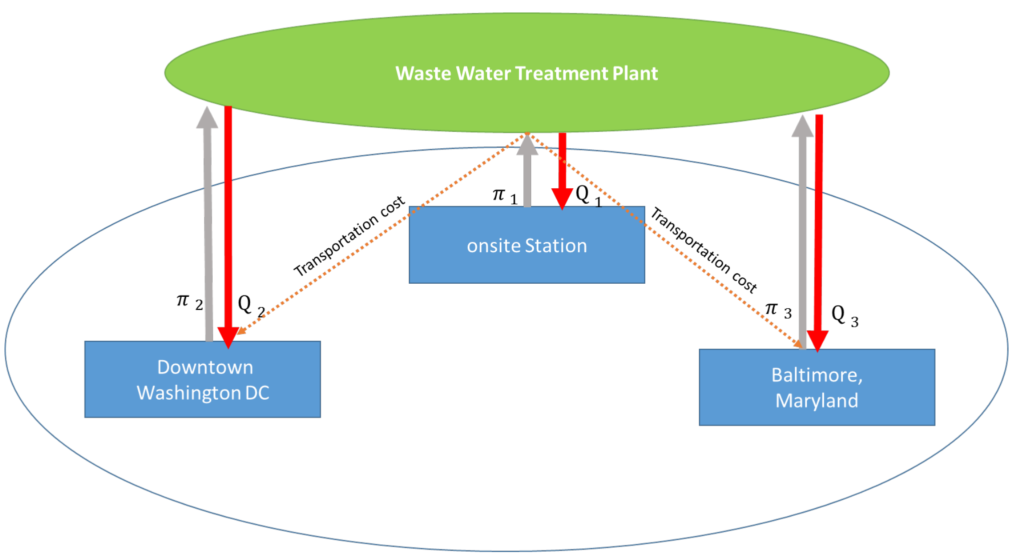

Figure 4: CNG market and network representations

variable values are in units per day. This model differs from the model in [7] in many aspects. The main purpose of the model in [7] is to find the optimal type of digester as part of the first-stage decisions. By contrast, the model in the current paper includes digester capacity as a fixed variable (decision made) and concentrates instead on the investment for CNG stations in the first-stage set of decisions.

Sets

$j \in \{1, 2, 3\}$	three segments for the digester cost curves
$s \in \{1, 2, ..6, 561\}$	scenarios
$c \in \{large, small\}$	options for two sizes of CNG filling stations
$m \in \{Onsite, Baltimore, downtown\ Washington, DC\}$	market nodes

3.1.1 Main upper-level variables[3]

Binary variable

$Build\_G_{c,m} = 1$	if CNG filling station size c is installed at node m; 0 otherwise

Continuous variables

$G^T_{CNG}(s)$	Total CNG production under scenario s (m^3)
$G^S_{CNG,c,m}(s)$	CNG sold by filling station c at location m under scenario s (m^3)
$I_G(s)$	solids used to produce biogas (dt)
$I_B(s)$	solids used to produce class B biosolids from lime stabilization for land application (dt)
$I_A(s)$	solids used to produce class A biosolids not from the digester (dt)
$I_I(s)$	solids incinerated (dt)
$I_{OR1}(s)$	solids brought in from organization 1 (dt)
$I_{OR2}(s)$	solids brought in from organization 2 (dt)
$G_E(s)$	biogas generated from biosolids for generating electricity (m^3)
$G_{NG}(s)$	methane gas transformed from biogas generated from the digestion process, called biomethane [28] and used in the residential natural gas sector (m^3)
$B^L_A(s)$	biosolids class A produced for land application (dt)
$B^{AM}_A(s)$	biosolids class A sold in the agricultural market (dt)
$E^E(s)$	electricity bought from external sources and used at the WWTP (kWh)
$E^{WWTP}_B(s)$	electricity generated from biogas and used at the WWTP (kWh)
$E^{SM}_B(s)$	electricity generated from biogas and sold to the spot market (kWh)
$E^{WWTP}_S(s)$	electricity generated from solar energy and used at the WWTP (kWh)
$E^{SM}_S(s)$	electricity generated from solar energy and sold to the spot market (kWh)
$NG^E_H(s)$	natural gas purchased from external sources (m^3)
$C_T(s)$	total net carbon dioxide equivalent (t)
$P_T(s)$	total energy purchased at WWTP (kWh)
$V_T(s)$	total WWTP value, which is the revenue minus costs ($)

[3]All variables are assumed to be nonnegative unless specified otherwise. Also, only the main primal variables are shown. The endogenously determined prices (dual variables) are not shown here but are described later in the text.

3.1.2 Parameters

$FCNG_c$	Installation fixed costs for CNG station type c (\$)
$OCNG_c$	Operating costs for CNG station type c (\$/m^3)
$\overline{CNG}_c$	Maximum capacity of CNG station type c (m^3)
$SCNG_{c,m}$	Shipping costs for CNG station type c from AWTP to market node m (\$/m^3)
$\overline{G}^T_{CNG}$	maximum amount of bio-CNG production (m^3)
CAP	maximum amount of class B production (dt)
$\overline{G}_{NG}$	maximum amount of bio-methane production (m^3)
$\overline{B}^{AM}_A$	maximum amount of class A biosolids sold in the agricultural market (dt)
$\overline{E}^{SM}_B$	maximum amount of electricity generated from biogas and sold to the grid (kWh)
$\overline{E}^{SM}_S$	maximum amount of electricity generated from solar radiation and sold to the grid (kWh)
S_{OR1}	maximum amount of solids from organization 1 (dt)
S_{OR2}	maximum amount of solids from organization 2 (dt)
S_{gas}	maximum amount of solids used to produce biogas (dt)
f_G	biogas production factor (m^3/dt)
f_{NG}	bio-methane production factor (average 60% methane gas is produced from biogas) (unitless)[4]
f_{CNG}	bio-CNG production factor (average 57.6% CNG is produced from biogas) (unitless)[5]
f_B	amount of dry tons of class A biosolids per dry ton of solids influent (dt/dt)
f_E	factor used to calculate generated electricity from biogas (kWh/m^3)
$WWTP_{NG}$	average daily amount of natural gas consumption at WWTP[6] from historical data (m^3/d)
f^E_C	factor used to calculate carbon dioxide emissions from electricity (t CO_2 e/kWh)
f^{NG}_C	factor used to calculate carbon dioxide emissions from natural gas used for heating at the Blue Plains facility (t CO_2 e/m^3)
f^I_C	factor used to calculate carbon dioxide emissions from incineration (t CO_2 e/dt)
f^{CNG}_C	factor used to calculate carbon dioxide offset from sold CNG for the transportation sector (t CO_2 e/m^3)
f^f_C	factor used to calculate carbon dioxide offset from biosolids used as fertilizer (t CO_2 e/dt)
f^t_C	factor used to calculate carbon dioxide emissions from transportating biosolids to the land application field (t CO_2 e/dt)
f^T_P	factor used to calculate fossil fuel consumption to transport class A and/or B biosolids to land application fields (kWh/dt)
f^G_P	factor used to calculate natural gas consumption at WWTP (kWh/m^3)
f^I_P	supplementary fuel for incineration process factor (kWh-\$/dt-liter)
f^T_I	factor used to calculate fossil fuel consumption for transportation class A and/or B biosolids to land application fields and to agricultural market in gallon per dry ton (liters/dt)

[4]The biogas (CH_4 + CO_2 + H_2O + trace gases) can be broken down into the following component shares: 55–65% methane gas (CH_4), 30–40% carbon dioxide gas (CO_2), and 0–5% water vapor, traces of hydrogen sulphide H_2S and hydrogen [12]. Consequently, in the model presented below, an average 60% of methane composition in biogas is used.

[5]The reduction of CNG from 100% of natural gas is due to further processing for gas quality outside of WWTP (http://www.environmental-expert.com/products/biogas-to-compressed-natural-gas-35510).

[6]The highest natural gas consumption obtained from the energy saving plan report of December, 2010.

f_E^{Gen}	electricity generation costs (\$/kWh)
$\gamma_{bio-CNG}$	CNG compression costs (\$/m^3)
$\gamma_{bio-methane}$	non-transportation natural gas production costs (\$/m^3)
f_A^{Com}	biosolids class A production costs (\$/dt)
f_{Ash}^I	ash from incineration disposal cost (\$/dt)
f_I^{TIP}	tipping fees (\$/dt of biosolids)
C_{allow}^{WWTP}	CO_2 e allowance (t)
S_{panel}	installation area of solar panels (m^2)
RES	credits from renewable electricity standard (\$/kWh)
f_{on}^{off}	parameter used to turn on REC or CO_2 credits (mutually exclusive options) and it is equal to 0 or 1, respectively (fixed for any given run)
REC	renewable energy credits (\$/t CO_2 e)
$\overline{q}_{ino}$	maximum amount of inorganic fertilizer in the market (dt)
$\overline{q}_{org}$	maximum amount of organic fertilizer in the market (dt)
$\overline{q}_{fossil}$	maximum amount of fossil fuel-based electricity sold to the grid (kWh)
$\overline{q}_{nuclear}$	maximum amount of nuclear-based electricity sold to the grid (kWh)
$\overline{q}_{hydro}$	maximum amount of fossil-fuel based electricity sold to the grid (kWh)
$\overline{q}_{CNG}$	maximum amount of CNG for transportation sold to the natural gas grid (m^3)
$\overline{q}_{NG}$	maximum amount of natural gas sold to the natural gas grid (m^3)
γ_{ino}	inorganic fertilizer production costs (\$/dt)
γ_{org}	organic fertilizer production costs (\$/dt)
γ_{fossil}	fossil fuel based-electricity production costs (\$/kwh)
$\gamma_{nuclear}$	nuclear based-electricity production costs (\$/kwh)
γ_{hydro}	hydropower based-electricity production costs (\$/kwh)
γ_{CNG}	CNG for transportation production costs (\$/m^3)
γ_{NG}	non-transportation natural gas production costs (\$/m^3)

3.1.3 Random parameters

$Pr(s)$	probability for each scenario
$I_{WWTP}(s)$	uncertain solids influent to digester (dt)
$E_{consump}(s)$	uncertain electricity consumption at WWTP (kWh)
$E_{purchased}(s)$	uncertain electricity purchasing prices (\$/kWh)
$NG_{purchased}(s)$	uncertain natural gas purchasing prices (\$/m^3)
$P_{fossil}(s)$	uncertain fossil fuel prices to transport class A and B bisolids (\$/liter)
$R_{CO_2}(s)$	uncertain carbon credits (\$/t CO_2 e)
$S_{radia}(s)$	uncertain solar radiation (kWh/m^2)
$S_{generate}(s)$	uncertain generated solar electricity cost (\$/kWh)

3.2 Lower-level problem

The objective of the lower-level separate optimization problems is to maximize expected profit (in dollars). There is one optimization problem for each of the relevant markets including fertilizer, electricity, residential natural gas and CNG for transportation. Markets are assumed to be perfectly competitive, so players are price-takers [13]. These prices are determined by market-clearing conditions for each market at the lower level which together with the KKT conditions of these separate optimization problems constitute the lower-level problem.

3.2.1 Lower-level optimization problem of selling CNG to the transportation sector

In this lower-level problem, the model assumes there is another aggregated CNG producer in each market m besides DC Water. In [7] the model only considered one market. The objective function of each aggregated CNG producer is to maximize expected profit of selling CNG to the consumers in each market. Profits are calculated as the difference between revenues using natural gas prices ($\$\pi_{CNG,m}(s)$ per m^3), and linear production costs ($\$\gamma_{CNG,m}$). The quantities of CNG actually sold should be less than or equal to the maximum amount of supply in the CNG transportation market in that particular market. Formulation (2) is the associated optimization problem for this lower-level problem for each CNG producer in market m.

$$\max_{q_{CNG}(s)} \sum_{s,m} Pr(s)\{\pi_{CNG,m}(s)q_{CNG,m}(s) - \gamma_{CNG,m}q_{CNG,m}(s)\} \tag{2a}$$

s.t.

$$q_{CNG,m}(s) \leq \bar{q}_{CNG,m} \qquad \big(\lambda_{CNG,m}(s)\big)\forall s \tag{2b}$$

$$q_{CNG,m}(s) \geq 0 \qquad \forall s \tag{2c}$$

where

$q_{CNG,m}(s)$ = amount of CNG sold to consumers in market m in m^3

$\lambda_{CNG,m}(s)$ = dual price of natural gas for transportation sector constraint

3.2.2 Lower-level optimization problem of selling class a biosolids to the fertilizer market

The U.S. Department of Agriculture categorizes plant nutrients (fertilizer) into three different groups: 1) single (nitrogen, phosphate) nutrient, 2) multiple (mono ammonium-phosphate) nutrients, 3) secondary and micronutrients (manure, compost, and sewage sludge),[7] dependent on the end-use purposes. This research didn't consider the end-use purposes but focused on compositions of fertilizer by categorizing them into two groups: 1) inorganic fertilizer and 2) organic fertilizer. The objective of this part of the lower-level problem is to maximize the expected profit of the fertilizer market. Considering both the inorganic and organic fertilizer producers, expected profits of each player are calculated from the difference of revenues based on fertilizer prices ($\$\pi_F(s)$ per dt), and linear production costs of inorganic and organic fertilizer ($\$\gamma_{ino}$, $\$\gamma_{org}$). In addition, the quantities of inorganic and organic fertilizer should be less than or equal to the maximum amount of supply in the fertilizer market. Problem (3) describes the optimization problem for the fertilizer markets.

$$\max_{q_{ino}(s),q_{org}(s)} \sum_{s} Pr(s)\{\pi_F(s)\big(q_{ino}(s) + q_{org}(s)\big) - \gamma_{ino}q_{ino}(s) - \gamma_{org}q_{org}(s)\} \tag{3a}$$

s.t.

$$q_{ino}(s) \leq \bar{q}_{ino} \qquad \big(\lambda_{ino}(s)\big)\forall s \tag{3b}$$

$$q_{org}(s) \leq \bar{q}_{org} \qquad \big(\lambda_{org}(s)\big)\forall s \tag{3c}$$

$$q_{ino}(s),\ q_{org}(s) \geq 0 \qquad \forall s \tag{3d}$$

[7] http://www.ers.usda.gov/data-products/fertilizer-use-and-price.aspx#26720.

where

$$q_{ino}(s) = \text{amount of inorganic fertilizer in dt}$$
$$q_{org}(s) = \text{amount of organic fertilizer in dt}$$
$$\lambda_{ino}(s) = \text{dual price of inorganic fertilizer constraint}$$
$$\lambda_{org}(s) = \text{dual price of organic fertilizer constraint}$$

3.2.3 Lower-level optimization problem of selling electricity to the grid

The objective function for this part of the lower-level problem is to maximize the expected profit of selling electricity to the grid; three types of power generators are considered: fossil fuel (coal, natural gas and petroleum), nuclear, and renewables (hydropower). Expected profits of each of the three players (fuel types) are calculated from the difference between revenues based on electricity sold ($\$\pi_E(s)$ per kWh), and linear production costs of fossil, nuclear and hydro-based electricity ($\$\gamma_{fossil}$, $\$\gamma_{nuclear}$, $\$\gamma_{hydro}$). The quantities of generated electricity from each source should be less than or equal to the maximum amount of supply in the power market. The associated optimization problem is shown in (4).

$$\max_{q_{fossil}(s) q_{nuclear}(s), q_{hydro}(s)} \sum_s Pr(s) \Big\{ \pi_E(s) \big(q_{fossil}(s) + q_{nuclear}(s) + q_{hydro}(s) \big) - \gamma_{fossil} q_{fossil}(s) - \gamma_{nuclear} q_{nuclear}(s) - \gamma_{hydro} q_{hydro}(s) \Big\} \quad (4a)$$

s.t.

$$q_{fossil}(s) \leq \overline{q}_{fossil} \qquad \big(\lambda_{fossil}(s)\big) \forall s \quad (4b)$$
$$q_{nuclear}(s) \leq \overline{q}_{nuclear} \qquad \big(\lambda_{nuclear}(s)\big) \forall s \quad (4c)$$
$$q_{hydro}(s) \leq \overline{q}_{hydro} \qquad \big(\lambda_{hydro}(s)\big) \forall s \quad (4d)$$
$$q_{fossil}(s), q_{nuclear}(s), q_{hydro}(s) \geq 0 \qquad \forall s \quad (4e)$$

where

$$q_{fossil}(s) = \text{amount of fossil fuel-based electricity in kWh}$$
$$q_{nuclear}(s) = \text{amount of nuclear-based electricity in kWh}$$
$$q_{hydro}(s) = \text{amount of hydropower-based electricity in kWh}$$
$$\lambda_{fossil}(s) = \text{dual price of fossil fuel-based electricity constraint}$$
$$\lambda_{nuclear}(s) = \text{dual price of nuclear-based electricity constraint}$$
$$\lambda_{hydro}(s) = \text{dual price of hydropower-based electricity constraint}$$

3.2.4 Lower-level optimization problem for selling natural gas to the residential natural gas sector

The objective in this lower-level problem is similar to the CNG one, namely maximizing the expected profit of selling natural gas to residential sector. Here the related gas prices are ($\$\pi_{NG}(s)$ per m^3), and the linear production costs are γ_{NG}. Quantities of natural gas sold should be less than or equal to the maximum amount of supply in this market. Formulation (5) depicts this lower-level optimization problem.

$$\max_{q_{NG}(s)} \sum_s Pr(s) \big\{ \pi_{NG}(s) q_{NG}(s) - \gamma_{NG} q_{NG}(s) \big\} \quad (5a)$$

s.t.

$$q_{NG}(s) \leq \overline{q}_{NG} \qquad \big(\lambda_{NG}(s)\big) \forall s \quad (5b)$$
$$q_{NG}(s) \geq 0 \qquad \forall s \quad (5c)$$

where

$$q_{NG}(s) = \text{amount of natural gas for the residential sector in m}^3$$
$$\lambda_{NG}(s) = \text{dual price of natural gas for the residential sector constant}$$

3.2.5 Market-clearing conditions for the lower-level markets

In addition to the lower-level optimization problems just described, there are market-clearing conditions (MCC) for each of the markets as shown in Appendix. For each market, these MCC stipulate that total supply (either from the lower- or upper-level or exogenously) must equal demand. The latter is described by linear demand function. Lastly, for each of these MCC, there is an associated Lagrange multiplier or price that is used by the lower-level players in each of the markets.

3.3 Mathematical formulation of the stochastic MPEC

As described above, this paper considers the AWTP as the strategic player at the upper-level of a stochastic MPEC, modeled as maximizing expected profit (expected total value) subject to investment, operational, and equilibrium constraints. The complete upper level of the stochastic MPEC is as follows:

$$Max \ \sum_s Pr(s)(revenues(s) - costs(s)) \qquad \$ \tag{6}$$

The revenues from different components are as follows:

The revenue from the fertilizer market: $$\pi_F(s)B_A^{AM}(s) \tag{7}$$

The revenue from selling electricity to grid by biogas base: $$\pi_E(s)E_B^{SM}(s) \tag{8}$$

The revenue from selling electricity to grid by solar base: $$E_S^{SM}(s)(\pi_E(s) + RES) \tag{9}$$

The revenue from selling natural gas to residential sector: $$\pi_{NG}(s)G_{NG}(s) \tag{10}$$

The revenue from selling CNG to transportation sector: $$\sum_{c,m} \pi_{CNG,m}(s)G_{CNG,c,m}^T(s) \tag{11}$$

The revenue from processing wastewater for other organization: $$f_I^{TIP}\big(I_{OR1}(s) + I_{OR2}(s)\big) \tag{12}$$

The revenue from renewable energy credit:
$$SC(s)\big(C_{allow}^{WWTP} - C_T(s)\big)f_{on}^{off} + REC\big(C_{allow}^{WWTP} - C_T(s)\big)\left(1 - f_{on}^{off}\right) \tag{13}$$

The upper-level costs are defined as follows:

CNG investment cost: $$\sum_{m,n} FCNG_m * Build\_G_{m,n} \tag{14}$$

Operating and transportation cost for CNG station: $$\sum_{c,m} (OCNG_{c,m} + SCNG_{c,m})G_{CNG,c,m}^T(s) \tag{15}$$

Cost of electricity and natural gas: $$\big(E_{purchased}(s)E^E(s)\big) + \big(NG_{purchased}(s)NG_H^E(s)\big) \tag{16}$$

Electricity, bio-CNG, and bio-methane costs:
$$\Big(S_{generate}(s)\big(E_S^{WWTP}(s) + E_S^{SM}(s)\big) + \big(\gamma_{bio\_CNG}G_{CNG}^T(s)\big) + \big(\gamma_{bio\_methane}G_{NG}(s)\big)\Big) \tag{17}$$

Ash disposal costs: $$\big(f_{ASH}^I \ I_I(s)\big) \tag{18}$$

Cost of transporting class A and B biosolids to land application fields:
$$\Big(f_I^T \ P_{fossil}(s)\big(B_A^L(s) + B_A^{AM}(s) + I_B(s)\big)\Big) \tag{19}$$

Transporting costs from organizations 1 and 2: $$\Big(f_I^T P_{fossil}(s)\big(I_{OR1}(s) + I_{OR2}(s)\big)\Big) \tag{20}$$

Supplementary fuel costs: $$\big(f_I^T \ P_{fossil}(s)I_I(s)\big) \tag{21}$$

Composting costs: $$\big(\gamma_{org}I_A(s)\big) \tag{22}$$

Constraints

The total sales of CNG to the market is equal to the total CNG sold from type c of CNG stations at market m.

$$G^T_{CNG}(s) = \sum_{c,m} G^S_{CNG,c,m}(s) \qquad \forall s \qquad \text{cu ft} \tag{23}$$

Constraint (24) is the capacity associated with the binary variable that determines if a small or large CNG station is chosen. The sales to the market is restricted by the maximum capacity.

$$G^S_{CNG,c,m}(s) \leq \overline{CNG}_{c,m} Build_{c,m} \qquad \forall c,m,s \qquad \text{cu ft} \tag{24}$$

Constraint (25) allows at most only one station built:

$$\sum_{c,m} Build\_G_{c,m} \leq 1 \tag{25}$$

Solids influent constraints

$$I_B(s) + I_A(s) + I_I(s) + I_G(s) = I_{WWTP}(s) + I_{OR1} + I_{OR2} \qquad \text{dt} \tag{26}$$

$$I_B(s) \leq CAP - I_A(s) - I_I(s) - I_G(s) \qquad \text{dt} \tag{27}$$

Constraints (28) and (29) present upper bound for biogas production from digesters.

$$I_G(s) \leq \sum_j x_j \qquad \text{dt} \tag{28}$$

$$I_G(s) \leq S_{gas} \qquad \text{dt} \tag{29}$$

Constraints (30) and (31) provide the bound on the maximum amount of solids from other organizations

$$I_{OR1} \leq S_{OR1} \qquad \text{dt} \tag{30}$$

$$I_{OR2} \leq S_{OR2} \qquad \text{dt} \tag{31}$$

Constraint (32) defines the maximum solids processing capacity in dt.

$$x_j \leq CAP \tag{32}$$

Constraint (33) presents the minimum solids processing capacity in dt.

$$x_j \geq l_j \tag{33}$$

Biogas production constraints

$$f_G I_G(s) = G_E(s) + G_{NG}(s) + G^T_{CNG}(s) \qquad \text{m}^3 \tag{34a}$$

$$G_{NG}(s) \leq f_{NG} f_G \; I_G(s) \qquad \text{m}^3 \tag{34b}$$

$$G^T_{CNG}(s) \leq f_{CNG} f_G \; I_G(s) \qquad \text{m}^3 \tag{34c}$$

$$G_{NG}(s) - \overline{G}_{NG}(s) \leq 0 \qquad \text{m}^3 \tag{34d}$$

$$G^T_{CNG}(s) - \overline{G}^T_{CNG}(s) \leq 0 \qquad \text{m}^3 \tag{34e}$$

Class A biosolids production constraints

$$B_A^L(s) + B_A^{AM}(s) = f_B\ I_G(s) + I_A(s) \qquad \text{dt} \qquad (35a)$$

$$B_A^{AM}(s) - \overline{B}_A^{AM}(s) \leq 0 \qquad \text{dt} \qquad (35b)$$

Electricity consumption constraints

$$E_{consump}(s) \leq E^E(s) + E_B^{WWTP}(s) + E_S^{WWTP}(s) \qquad \text{kWh} \qquad (36a)$$

$$E_B^{WWTP}(s) + E_B^{SM}(s) = f_E G_E(s) \qquad \text{kWh} \qquad (36b)$$

$$E_S^{WWTP}(s) + E_S^{SM}(s) = (S_{panel})\big(S_{radia}(s)\big) \qquad \text{kWh} \qquad (36c)$$

$$E_B^{SM}(s) - \overline{E}_B^{SM}(s) \leq 0 \qquad \text{kWh} \qquad (36d)$$

$$E_S^{SM}(s) - \overline{E}_S^{SM}(s) \leq 0 \qquad \text{kWh} \qquad (36e)$$

Natural gas residential sector consumption constraints

$$WWTP_{NG} \leq NG_H^E(s) + G_{NG}(s) \qquad \text{m}^3 \qquad (37)$$

Conservation of CO_2 e emissions

$$C_T(s) = \textit{emissions} - \textit{offsets} \qquad \text{ton} \qquad (38)$$

where

$$\begin{aligned} \text{Emissions } &= f_C^E E^E(s) + f_C^{NG} NG_H^E(s) + f_C^t\big(I_B(s) + B_A^L(s) + B_A^{AM}(s)\big) + \big(f_C^I I_I(s)\big) \\ \text{Offsets } &= f_C^E\big(E_B^{WWTP}(s) + E_B^{SM} + E_s^{WWTP}(s)\big) + f_C^{CNG} G_{CNG}^T(s) + f_C^{NG} G_{NG}(s) \\ &\quad + f_C^f\big(I_B(s) + B_A^L(s) + B_A^{AM}(s)\big) \end{aligned}$$

Conservation of CO_2 e emissions (38) defines the net total carbon dioxide equivalent emissions in tons. The CO_2 e emissions from AWTP operations ($f_C^E\ E^E(s)$), natural gas heating $f_C^{NG}(NG_H^E(s))$, transportation of biosolids ($f_C^t(I_B(s)+B_A^L(s)+B_A^{AM}(s))$) and incineration ($f_C^I\ I_I(s)$) and the offsets from renewable electricity generated ($f_C^E(E_B^{WWTP}(s) + E_B^{SM} + E_s^{WWTP}(s))$) and used at the AWTP, sold bio-CNG ($f_C^{CNG} G_{CNG}^T(s)$), sold bio-methane $f_C^{NG} G_{NG}(s)$, used/sold biosolids as fertilizer ($f_C^f(I_B(s) + B_A^L(s) + B_A^{AM}(s))$).

Conservation of energy purchased

$$\begin{aligned} P_T(s) = f_P^T\big(I_B(s) + B_A^L(s) + B_A^{AM}(s)\big) + f_P^T\big(I_{OR1}(s) + I_{OR2}(s)\big) \\ + f_P^G NG_H^E(s) + E^E(s) + f_P^I/P_{fossil}(s) I_I(s) \end{aligned} \qquad \text{kWh} \qquad (39)$$

Conservation of purchased energy (39) defines the total purchased energy of the AWTP including energy for transportation of class A and/or class B biosolids to land application sites ($f_P^T(I_B(s)+B_A^L(s)+B_A^{AM}(s))$), transportation of solids from organizations 1 and 2 ($f_P^T\ (I_{OR1}(s) + I_{OR2}(s))$), natural gas consumption ($f_P^G NG_H^E(s)$), electricity purchased from outside sources ($E^E(s)$), and supplementary fuel for incineration ($(f_P^I/P_{fossil}(s))I_I(s)$) in kWh. Besides the upper-level constraints, the model also includes Karush–Kuhn–Tucker (KKT) conditions of the lower-level individual optimization problems that give arise to SMPEC. More details on the necessary and sufficient KKT conditions and their transformation techniques can be found in the Appendix.

4 Case study of CNG supply in District of Columbia

In the District of Columbia area, both the residential and commercial natural gas prices have been gradually decreasing according to the U.S. Energy Information Administration [15]. This downward trend for natural gas prices is shown in Figure 5 indicating 16.49 dollars per thousand cubic feet ($/Mcf) in 2008 and $12.10/Mcf in 2012. Similarly, the commercial price was at $13.90/Mcf and $11.19 /Mcf in 2008 and 2012, respectively. However, the vehicle fuel price[8] fluctuated somewhat. The vehicle fuel price significantly decreased from $15.57 $/Mcf in 2008 to $4.17 in 2011, but then increased to $9.38/Mcf in 2012.

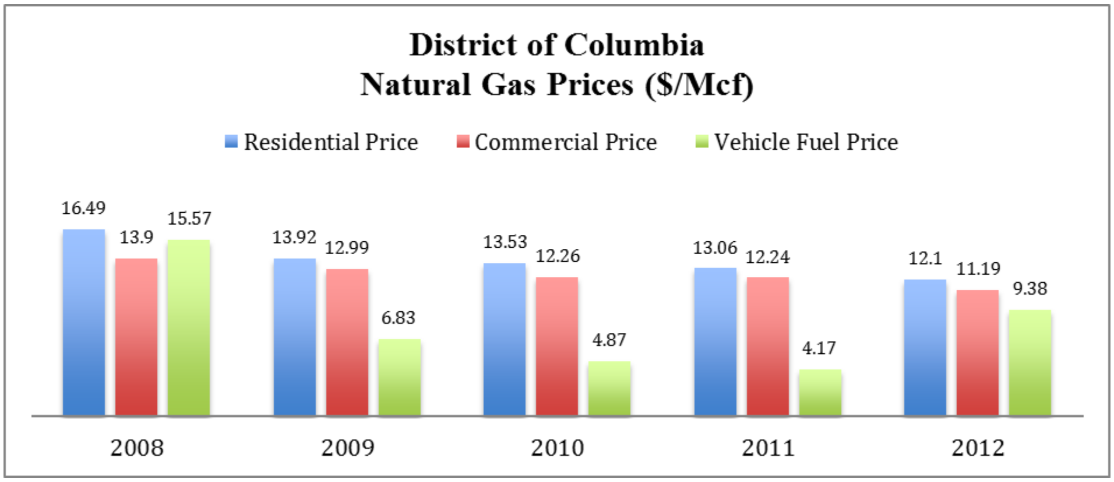

Figure 5: U.S. Energy Information Administration natural gas prices ($/Mcf)

In terms of CNG demand, as of 2012, the District of Columbia had 461 CNG buses operated by WMATA [16]. The daily consumption was 1.98 million cubic feet (MMcf). However, the CNG production capacity at AWTP is 2.55 MMcf per day. Thus, if feasible, DC Water could completely supply the CNG bus market for the District. Of course, this conclusion is predicated on the assumption that the methane obtained from the digesters going to produce electricity could be diverted to a separate stream for use as CNG to honor current contracts

Moreover, CNG fueling infrastructure is very limited [3]. Currently, there are no CNG commercial fueling stations in Washington, DC [17]. However, there is a fueling station that is exclusively for private access called Trillium CNG of Washington Metropolitan Area Transit Authority (WMATA), located at the Bladensburg Bus Garage at 2251 26th St NE [18]. The Fleet Management Administration of the DC Department of Public Works also has a private/government-only CNG fueling station at 1835 West Virginia Ave NE. Moreover, WMATA planned to have another CNG fueling station at Shepherd Parkway Bus Facility. This station is currently not yet accessible, and its actual location is to be determined.

In nearby states, there are five commercial CNG fueling stations in Virginia, two stations in Maryland, twenty-six stations in Pennsylvania, three stations in West Virginia, and one station in Delaware according to the U.S. Department of Energy [17]. Since there are only two private fueling stations in Washington, DC and the number of buses in operation will likely increase over time, DC Water has the potential to serve this market (e.g., buses and light-duty trucks) with its wastewater-derived CNG.

4.1 Natural gas filling stations data and economics

Historically, the number of CNG filling stations increased significantly after the Energy Policy Act of 1992 was passed. In the U.S., more than 1,000 CNG stations were installed due to the requirement of increasing light-duty alternative fuel vehicles. However, the number of CNG stations in the U.S. started declining in 1997 and resulted in less than 1,000 stations for the first time in a decade in 2004 because of high imported natural gas prices.

Currently, there are approximately 1,000 stations operating in the U.S. of which 54 percent have private access, and 46 percent have public access. In contrast, the large majority of the CNG fueling stations in

[8]Vehicle fuel prices are the average of liquefied natural gas (LNG) and CNG prices for transportation.

Canada are public access. A ratio of CNG to gasoline and diesel stations in the U.S. is one CNG station per one hundred and twenty station of gasoline station.

A CNG station cost will vary depending on many factors e.g., capacity needed, size of storage, and dispensing system. The typical installation costs for CNG stations may range from $600,000–$1,000,000 per station. It is important to note that CNG component costs include costs for the gas supply line, the compressor package, noise abatement, gas dryer, storage, the dispenser, card reader interface, engineering, construction, and contingencies. The component costs are quite similar, but the installation costs may vary by regions. The cost for public stations for two different capacities and operating costs per Mcf based on [19] is described in Table 1.

Table 1: CNG installation and operating costs as input to the model

	Small station	**Large Station**
Fixed costs[9]	$1,000,000	$1,150,000
Operating Costs	$0.013 per Mcf	$0.0146 per Mcf
Capacity	126,670 cubic feet /day	253,340 cubic feet /day

5 Results

The stochastic bilevel optimization problem (SMPEC) was coded in GAMS using the XPRESS solver on an Intel Core i7-3537U CPU at 2.0 GHz and 8 GB RAM. The KKT conditions of the lower-level problem were transformed using the SOS1 approach described in [11] giving arise to overall mixed-integer program.

It is important to note that the product of two variables $\left(\pi_{CNG}(s)G^{T}_{CNG}(s)\right)$ in the objective function represents a bilinear, hence non-convex term in the objective function and is thus something that needs to be convexified/linearized for computational reasons. The alternative we have chosen is to choose a discrete set of levels for the continuous variable $\left(G^{T}_{CNG}(s)\right)$, in the manner described in [20,21] and then linearize this bilinear revenue term. In this study, thirty valid CNG production levels for the wastewater treatment plant were defined. One may consider this as a selection of a discrete set of CNG production levels. Note that there are alternative ways to "convexify" these bilinear terms but they may depend on a special structure (e.g., [22]). The one we have chosen is generalizable under different forms of the stochastic MPEC model we have developed. In effect, the model selects the discrete level of CNG sold but allows for a continuous price determined from the lower level.

5.1 Base Case

The Base Case assumes no CNG investment for the AWTP. The Base Case is used as the reference and expected CNG consumption and expected prices have been calibrated to closely match the state of the market [15] for the year 2013. The calibration elements were the parameters of inverse demand functions. The idea is that the calibration technique slightly adjusts inverse demand parameters to make the model correctly describe the real-world historical data. Table 2 indicates that the percentage difference[10] between the SMPEC and [15] figures is fairly low.

Table 3 shows the numerical results from solving the stochastic MPEC. The maximum expected daily profit is –$158,444.02. The number is negative (–$151,258.2 per day, see Table 3) because the SMPEC only captures a subset of the AWTP's operations of the daily operating cost. For example, the model does not include revenue from clean water supplied to the community. As displayed in Table 3. This AWTP requires a lot of power for their operations. Of this, 448,700 kWh was bought from the grid, 225,930 kWh were generated from biogas and, 18,721 kWh was produced from solar power at this AWTP No electricity produced at the

[9] Fixed cost includes equipment, installation, and infrastructure costs.
[10] Percentage difference is the absolute value of the difference between reference and model output divided by the reference.

Table 2: SMPEC Baseline Scenarios outcomes for CNG prices and consumption in 2013

	Expected prices $/Mcf		% price	Expected consumption Mcf/day		% consumption
	SMPEC	EIA 2014	difference	SMPEC	EIA 2014	difference
Baltimore, Maryland	$11.69	$11.67	0.17%	678.46	676.71	0.25%
Washington, DC	$12.08	$11.89	1.60%	2,686.12	2,673.97	0.48%

Table 3: SMPEC Base Case operational outcomes

Variables	**Explanation**	**Value**
	Objective function (expected profit)	–$158,444.02
E^E	Expected electricity bought from external sources and used at the WWTP	448,700 (kWh)
E_B^{WWTP}	Expected electricity generated from biogas and used at the plant	225,930 (kWh)
E_S^{WWTP}	Expected electricity generated from solar power and used at the plant	18,721.84(kWh)
B_A^L	Expected amount of biosolids Class A produced for land application	165.862 (dt)
B_A^{AM}	Expected amount of biosolid Class A sold in the agricultural market	100.00 (dt)
E_B^{SM}	Expected amount of electricity generated from biogas and sold at grid market	0 (kWh)
E_S^{SM}	Expected amount of electricity generated from solar power and sold at grid market	0 (kWh)
G_{CNG}^T	Expected amount of bio-CNG generated from the digestion process	0 (Mcf)
G_{NG}	Expected amount of biogas from biogas generated from the digestion process	0 (kWh)
E_fossil	Expected amount of fossil fuel-based electricity	359,480 (kWh)
E_nuclear	Expected amount of nuclear-based electricity	84920 (kWh)
E_hydro	Expected amount of hydropower-based electricity	54482 (kWh)
NG_SM	Expected amount of natural gas for the residential sector	370.210 (Mcf)
Price_Fer	Expected fertilizer price	$249.600
Price_Ele	Expected electricity price	$0.139
Price_NG	Expected natural gas price	$0.003
f_inor	Expected amount of inorganic fertilizer	122,020 (dt)
f_org	Expected amount of organic fertilizer	1,607.923 (dt)

AWTP was sold to the grid because the AWTP tried to meet internal electricity demand before selling it to the rest of the grid.

The expected amount of biosolids of 165.862 dt were delivered to land application fields. The AWTP sold 100 dt of fertilizer produced from class A biosolids to the agricultural market with an expected price of $249.6 per ton. It is important to note that no biogas from AWTP was sold to the residential sector due to significant low expected prices ($3 per Mcf). In terms of CNG, none was supplied to the market since no investments for CNG were allowed for this case.

5.2 CNG investment scenarios

This section describes the scenarios defined in this study. First, we define the Base Case as the baseline for the comparisons with the other scenarios. The scenario descriptions are as follows:

- Base Case assumes no CNG investment for AWTPs
- Option 1 assumes the AWTP installs up to 1 CNG station
- Option 2 assumes the AWTP installs up to 2 CNG stations
- Option 3 assumes the AWTP installs up to 3 CNG stations

Table 4 presents a comparison of the results for four scenarios. Allowing investments in CNG improves the total profit of the AWTP as seen from the positive relative profit levels as compared to the Base Case (taken to be \$0). The results suggest that when more CNG stations are allowed and installed, the power E_B^{WWTP} generated by biogas at the AWTP is reduced substantially due to less availability of biogas as some of the biogas is instead converted to CNG and sold to the CNG market; see Figure 6. This leads to an increase in electricity purchased from outside sources, E^E. Lastly, one of the interesting results is that mode chose to invest in large CNG stations due to economies of scale although it require more fixed costs. This option resulted in the largest overall profit.

Table 4: Comparison of results for four scenarios relative to the Base Case (only variables different from the Base Case)

Variables	**Base Case**	**Option 1**	**Option 2**	**Option 3**
Profit difference per day[11]	0	+\$3,557.2	+\$6,700.6	+\$ 8,505.2
CNG station		large[12] onsite	large onsite large DC	large onsite large DC large MD
E^E (Expected electricity bought from external sources in kWh)	448,700	462,570	476,450	490,320
E_B^{WWTP} (Expected electricity generated from biogas and used at the plant in kWh)	225,930	212,050	198,170	184,300
G_{CNG}^T (Expected amount of bio-CNG generated from the digestion process in Mcf)	0	243.43	486.850	730.280

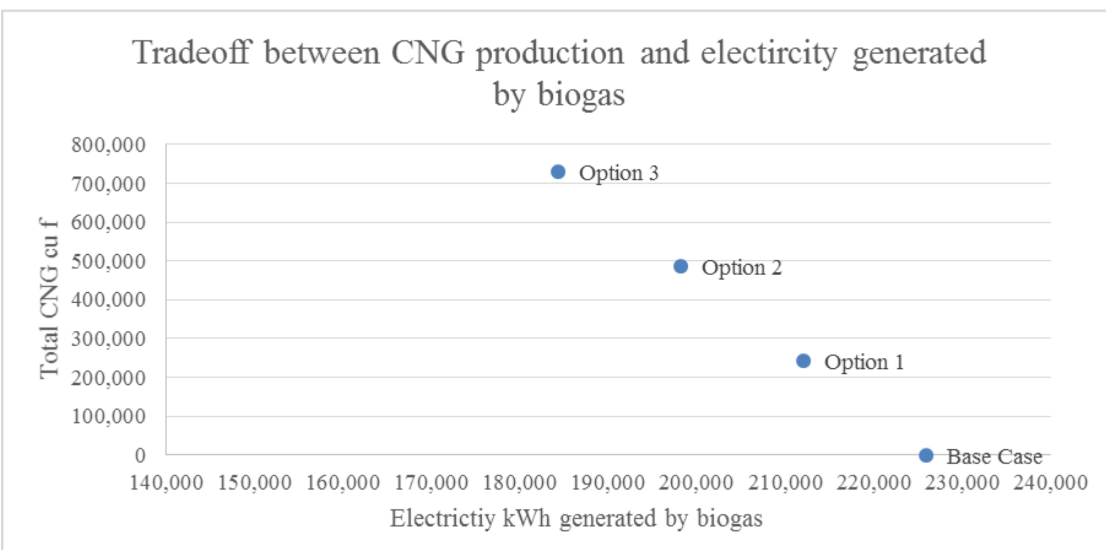

Figure 6: Tradeoff between electricity produced using biogas sources vs total CNG produced at AWTP

In terms of CO_2 emissions reduction, it is important to note that burning 1 gallon of diesel fuel produces 22.38 (10.15 kg) pounds of CO_2 emission, but only 14.46 pounds (6.46 kg) for CNG.[13] As shown in Table 5, CNG from the AWTP contributes significantly to decreasing CO_2 emissions. Moreover, Figure 7 presents the profit difference compared to CO_2 emissions reduction. Investing in CNG business not only has a financial

[11] Non-Base Case profit minus Base Case profit.
[12] The large CNG station has a capacity of 253,340 cubic feet/day.
[13] http://www.epa.gov/climatechange/.

benefit for the AWTP but also reveals an environmental advantage. The more CNG stations that are installed, the more CO_2 emission savings there will be, all else being equal.

Table 5: Comparison of CO_2 emissions reduction

	Total CNG produced by AWTP (Mcf)	**Diesel gallon equivalent (DGE[14])**	**CO_2 emissions reduction in pounds (kg) compared to diesel[15]**
Base	0	0	0(0)
option 1	243.43	1,691.15	+13,393.93 (6,075.38 kg)
option 2	486.85	3,382.23	+26,787.31 (12,150.52 kg)
option 3	730.28	5,073.39	+40,181.25 (18,225.91 kg)

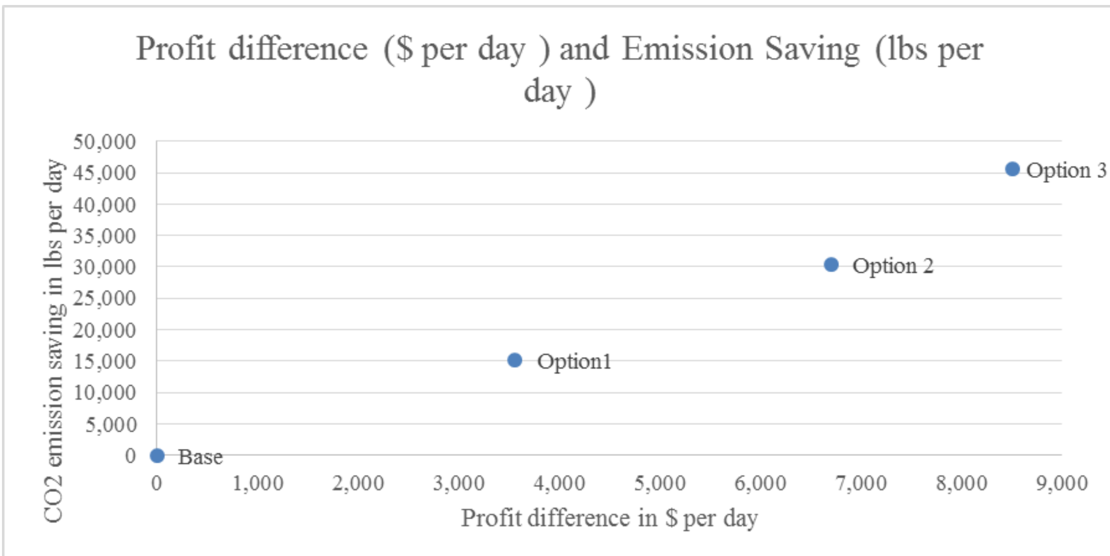

Figure 7: Profit difference in $ per day and emission saving in lbs per day

The results for expected consumption and prices are presented below. The investment scenarios produce higher expected prices e.g., $12/Mcf (Base Case) vs. $21/Mcf (Option 1) for the onsite market and lower total expected consumption e.g., 348.15 Mcf per day (Base Case) vs. 317.73 Mcf (Option 1) for the same market. The expected profit increases for the investment scenarios for Option 1 (+$3,557.23), Option 2 (+$6,700.65), and Option 3 (+$ 8,505.21) respectively, as compared to the Base Case (Table 4). This shows an advantage of being a Stackelberg leader and allowing more profits but affecting downstream markets disadvantageously for them. When the leader enters the market, the prices for some markets increase and the expected consumption simultaneously decreases. Lastly, we look at the results for Option 3. The AWTP supplies approximately 20% of expected total demand in Washington, DC market.

6 Conclusions

In this paper, we have introduced a novel stochastic two-level optimization model expressed as a mathematical program with equilibrium constraints (MPEC) for wastewater management at a large advanced wastewater treatment plant (AWTP). The numerical results indicate that the AWTP could become a potential supplier of compressed natural gas (CNG) for transport. The case study indicates that the CNG produced from the

[14] 111.47 cubic feet of CNG equals 1 DGE (http://www.nat-g.com/why-cng/cng-units-explained/).

[15] The difference of CO_2 emissions between burning CNG and diesel (3.69 kg) multiplied by number of CNG in gallon equivalent.

Table 6: Comparison of expected CNG prices

	Expected prices \$ per Mcf			
Market nodes	**Base**	**Option 1**	**Option 2**	**Option 3**
Onsite Market	\$12	\$21	\$21	\$21
Washington, DC	\$12	\$12	\$21	\$21
Baltimore, Maryland	\$11	\$11	\$11	\$20

Table 7: Comparison of CNG consumption

	Expected consumption in Mcf per day			
Market nodes	**Base**	**Option 1**	**Option 2**	**Option 3**
Onsite Market	348.15	317.73	317.73	317.73
Washington, DC	2,689.30	2,689.30	2,658.90	2,658.90
Baltimore, Maryland	678.51	678.51	678.51	646.82

AWTP can supply approximately 20% of the total demand in Washington, DC. In addition, CNG produced from AWTP can significantly reduce the amount of CO_2 emissions.

7 APPENDIX: KKT conditions and SOS1 transformation approach

Karush–Kuhn–Tucker (KKT) conditions of the lower-level individual optimization problems by market

Fertilizer market:

$$0 \leq Pr(s)\,(-\pi_F(s) + \gamma_{ino}) + \lambda_{ino}(s) \perp q_{ino}(s) \geq 0 \tag{40a}$$
$$0 \leq \overline{q}_{ino} - q_{ino}(s) \perp \lambda_{ino}(s) \geq 0 \tag{40b}$$
$$0 \leq Pr(s)\,(-\pi_F(s) + \gamma_{org}) + \lambda_{org}(s) \perp q_{org}(s) \geq 0 \tag{40c}$$
$$0 \leq \overline{q}_{org} - q_{org}(s) \perp \lambda_{org}(s) \geq 0 \tag{40d}$$

Electricity market:

$$0 \leq Pr(s)\,(-\pi_E(s) + \gamma_{fossil}) + \lambda_{fossil}(s) \perp q_{fossil}(s) \geq 0 \tag{40e}$$
$$0 \leq \overline{q}_{fossil} - q_{fossil}(s) \perp \lambda_{fossil}(s) \geq 0 \tag{40f}$$
$$0 \leq Pr(s)\,(-\pi_E(s) + \gamma_{nuclear}) + \lambda_{nuclear}(s) \perp q_{nuclear}(s) \geq 0 \tag{40g}$$
$$0 \leq \overline{q}_{nuclear} - q_{nuclear}(s) \perp \lambda_{nuclear}(s) \geq 0 \tag{40h}$$
$$0 \leq Pr(s)\,(-\pi_E(s) + \gamma_{hydro}) + \lambda_{hydro}(s) \perp q_{hydro}(s) \geq 0 \tag{40i}$$
$$0 \leq \overline{q}_{hydro} - q_{hydro}(s) \perp \lambda_{hydro}(s) \geq 0 \tag{40j}$$

CNG market:

$$0 \leq Pr(s)\,(-\pi_{CNG,n}(s) + \gamma_{CNG,n}) + \lambda_{CNG,n}(s) \perp q_{CNG,n}(s) \geq 0 \tag{40k}$$
$$0 \leq \overline{q}_{CNG,n} - q_{CNG,n}(s) \perp \lambda_{CNG,n}(s) \geq 0 \tag{40l}$$

Residental natural gas market:

$$0 \leq Pr(s)\,(-\pi_{NG}(s) + \gamma_{NG}) + \lambda_{NG}(s) \perp q_{NG}(s) \geq 0 \tag{40m}$$
$$0 \leq \overline{q}_{NG} - q_{NG}(s) \perp \lambda_{NG}(s) \geq 0 \tag{40n}$$

Market-clearing conditions of the relevant markets:

$$q_{ino}(s) + q_{org}(s) + B_A^{AM}(s) = 315,730.8 - 769.23\pi_F(s), (\pi_F(s)\ free) \tag{41a}$$

$$q_{fossil}(s) + q_{nuclear}(s) + q_{hydro}(s) + E_B^{SM}(s) + E_S^{SM}(s) = 0.4878 - 7x10^{-7}\pi_E(s), (\pi_E(s)\ free) \tag{41b}$$

$$q_{CNG,m}(s) + \sum_c G^T_{CNG,c,m}(s) = a_m - b_m\pi_{CNG,m}(s), = (p_{CNG}(s)\ free) \tag{41c}$$

$$q_{NG}(s) + G_{NG}(s) = 4.23x10^7 - 3x10^{-9}\pi_{NG}(s), (\pi_{NG}(s)\ free) \tag{41d}$$

The right-hand sides of (41) represent the inverse demand equations for each of the markets. These equations were determined from least-squares regression using data from the following sources: fertilizer market[16] [23], electricity market [24,25], CNG market[17,18] [24,25], residential natural gas market [24,25].

The SOS type 1 variables (SOS1) are used to transform the complemenarity conditions of the lower-level optimization problems into integer linear constraints. For example, constraints (40a) and (40b) were transformed and shown in (42).

$$zp^1_{ino}(s) = Pr(s)\{-\pi_F(s) + \gamma_{ino}\} + \lambda_{inor}(s) \tag{42a}$$
$$2SOS^{1+}_{ino}(s) + 2SOS^{1-}_{ino}(s) = zp^1_{ino}(s) + q_{ino}(s) \tag{42b}$$
$$2SOS^{1+}_{ino}(s) - 2SOS^{1-}_{ino}(s) = zp^1_{ino}(s) - q_{ino}(s) \tag{42c}$$
$$zp^2_{ino}(s) = \overline{q}_{ino} - q_{ino}(s) \tag{42d}$$
$$2SOS^{2+}_{ino}(s) + 2SOS^{2-}_{ino}(s) = zp^2_{ino}(s) + \lambda_{ino}(s) \tag{42e}$$
$$2SOS^{2+}_{ino}(s) - 2SOS^{2-}_{ino}(s) = zp^2_{ino}(s) - \lambda_{ino}(s) \tag{42f}$$
$$zp^1_{ino}(s), zp^2_{ino}(s) \geq 0 \tag{42g}$$
$$q_{ino}(s) \geq 0 \tag{42h}$$
$$\lambda_{ino}(s) \geq 0 \tag{42i}$$
$$SOS^{1+}_{ino}(s),\ SOS^{1-}_{ino}(s),\ SOS^{2+}_{ino}(s),\ SOS^{2-}_{ino}(s) \text{ are SOS1 variables}$$

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