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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.

1. Introduction

Compressed natural gas (CNG) is natural gas compressed to 200 bas which remains clear, odorless, and non-corrosive (California Energy Commission, 2014). CNG is composed of 83–99 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 3000 and 3600 psi (Alternative Fuel Systems Inc, 2014). 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 (Whyatt, 2010). According to the U.S. Energy Information Administration (EIA) (DOE, 2014a), 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 (California Energy Commission, 2014).

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);

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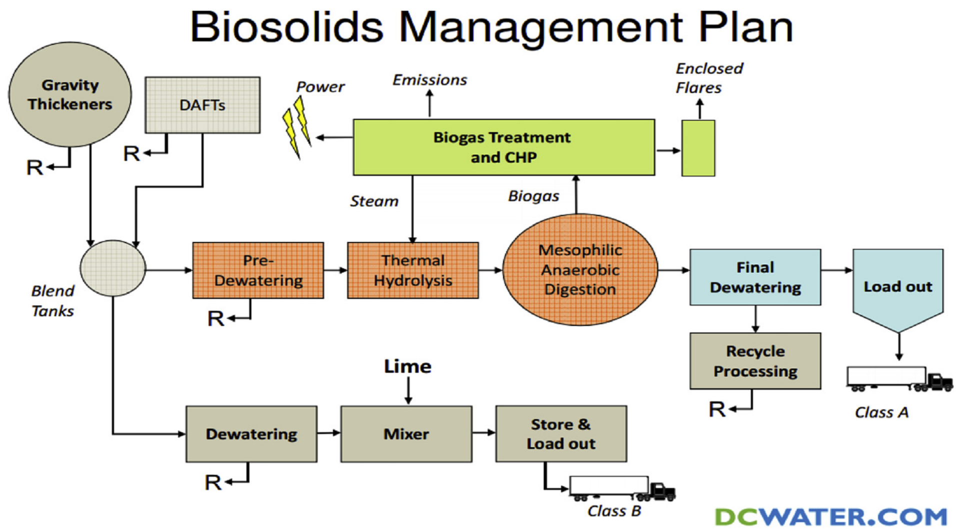

Fig. 1. Biosolid management plan at Blue Plains (The United States Environmental Protection Agency (EPA) eGRID 2006 Version 2.1, 2004).

RNG is also called biomethane (Vision et al., 2014). 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 Vision et al. (2014), there are more than 17,000 wastewater treatment plants in the U.S., but only approximately 1300 plants have digesters to manage biosolids and manure. Energy produced from wastewater treatment plants is a significant renewable energy source for household usage (Mamut and Badea, 2015). 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 Fig. 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 (Gabriel et al., 2013a; U-tapao Chalida, 2013; U-tapao et al., 2014).

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.

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. Section 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:

[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, (Energy information Administration (EIA)U.S. Department of Energy (2013)). Class B biosolids are less stringent in terms of pathogens but still require farm management practices and area restrictions before application ((Energy information Administration (EIA)U.S. Department of Energy (2013)) and The United States Environmental Protection Agency (EPA), 1994).

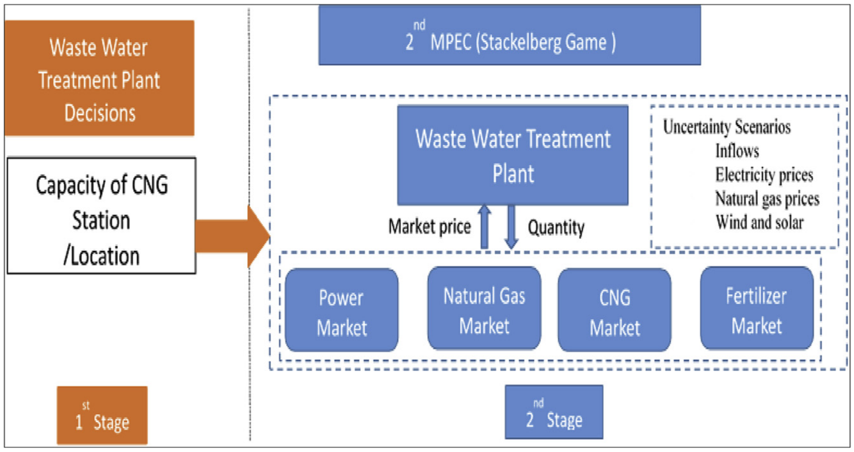

Fig. 2. Modeling framework diagram.

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

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 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 formulation (1) into a single-level problem using for example disjunctive constraints (Fortuny-Amat and McCarl, 1981). However, one disadvantage is that the computational time increases exponentially as the number of binary variables increase. An alternative is to use an SOS1 (Beale et al., 1970) approach suggested by Siddiqui and Gabriel (2012) to transform the complementarity conditions of the lower-level problem and solve it as a mixed-integer program. As shown in Siddiqui and Gabriel (2012), 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 Fig. 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 Fig. 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 Fig. 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.

In addition to the investment decisions, as shown in Fig. 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. (U-tapao Chalida, 2013) 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 Fig. 3. Note that the model solves for values of only one typical day; hence, all the variable values are in units per day. This model differs from the model in (U-tapao Chalida, 2013) in many aspects. The main purpose of the model in (U-tapao Chalida, 2013) 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
$s\ \varepsilon\ \{1, 2, \ldots 6, 561\}$ scenarios
$c\in\{large, small\}$ Options for two sizes of CNG filling stations
$m\in\{Onsite, Baltimore, downtown\ Washington\ D.C.\}$ Market Nodes

[2] All distributions displayed in this figure represent the random inputs to the model.
[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.

3.1.1. 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	
$G_{CNG}^{T}(s)$	total CNG production under scenario s (m^3)
$G_{CNG,c,m}^{S}(s)$	CNG sold by filling station c at location m under scenario s (m^3)
$G_E(s)$	amount of biogas produced from biosolids for power generation (m^3)
$G_{NG}(s)$	amount of bio-methane gas produced from digesters and sold to natural gas markets (m^3)
$B_A^L(s)$	amount of class A bipsolids generated for land application (dt)
$B_A^{AM}(s)$	amount of class A bipsolids sold in the agricultural market (dt)
$E^E(s)$	power purchased from electricity market and consumed at the plant (kWh)
$E_B^{WWTP}(s)$	power produced from biogas and consumed at the plant (kWh)
$E_B^{SM}(s)$	power produced from biogas and sold to the power market (kWh)
$E_S^{WWTP}(s)$	power produced from solar panels and used at the plant (kWh)
$E_S^{SM}(s)$	power produced from solar panels and sold to the grid (kWh)
$I_G(s)$	amount of solids utilized to generate biogas (dt)
$I_B(s)$	amount of solids used in lime stabilization process to generate class B biosolids and sent to land application (dt)
$I_A(s)$	amount of solids used to generate class A biosolids from other processes (not a digestion process) (dt)
$I_I(s)$	amount of solids for incineration process (dt)
$I_{OR1}(s)$	amount of solids transported from organization 1 (dt)
$I_{OR2}(s)$	amount of solids transported from organization 2 (dt)
$NG_H^E(s)$	natural gas bought from the gas markets (m^3)
$C_T(s)$	total net CO_2 e (t)
$P_T(s)$	total power bought at the plant (kWh)
$V_T(s)$	total net profit ($)
x	total solid processed by digester (dt)

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$)
$\overline{G}_{CNG}^{T}$	upper bound for CNG production (m^3)
CAP	upper bound for biosolids class B generation (dt)
$\overline{G}_{NG}$	upper bound for biogas-to-bio-methane conversion (m^3)
$\overline{B}_A^{AM}$	maximum amount of class A biosolids sold in the agricultural market (dt)
$\overline{E}_B^{SM}$	maximum amount of electricity generated from biogas and sold to the grid (kWh)
$\overline{E}_S^{SM}$	maximum amount of electricity generated from solar radiation and sold to the grid (kWh)
S_{OR1}	upper bound on solids transported from organization 1 (dt)
S_{OR2}	upper bound on solids transported from organization 2 (dt)
S_{gas}	limitation of solids for generating biogas (dt)
f_G	solids-to-biogas conversion factor (m^3/dt)
f_{NG}	biogas-to-bio-methane conversion factor
f_{CNG}	biogas-to-bio-CNG conversion factor (average 57.6% CNG is produced from biogas) (unitless)[4]
f_B	conversion factor to convert a dry ton of solids influent to class A biosolids
f_E	biogas-to-electricity conversion factor (kwh/m^3)
$WWTP_{NG}$	average daily demand for natural gas at AWTP[5] based on historical data (m^3/d)
f_C^E	CO_2 emission factor from electricity generation (t CO_2 e/kWh)
f_C^{NG}	CO_2 emission factor from heating (natural gas base) (t CO_2 e/m^3)
f_C^I	CO_2 emission factor from electricity generation from incineration (t CO_2 e/dt)
f_C^{CNG}	CO2 emission offset factor from sold CNG to the market (t CO_2 e/m^3)
f_C^f	CO2 emission offset factor from sold biosolids as fertilizer (t CO_2 e/dt)
f_C^t	CO_2 emission factor from sending biosolids to the land application field (t CO_2 e/dt)
f_P^T	fuel consumption factor for transporting class A and/or B biosolids to fields (kWh/dt)
f_P^G	natural gas consumption factor (kWh/m^3)
f_P^I	additional fuel for incineration process factor (kWh-$/dt-liter)
f_I^T	fossil fuel consumption factor for transporting class A and/or B biosolids to fields and to fertilizer market (liters/dt)
f_E^{Gen}	power production unit cost ($/kWh)
$\gamma_{bio-CNG}$	CNG production unit 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 disposal cost for incineration process ($/dt)
f_I^{TIP}	solids processing fees ($/dt of biosolids)
C_{allow}^{WWTP}	upper bound for CO_2 e (t)
S_{panel}	maximum available area for solar panel installation (m^2)
RES	renewable energy standard ($/kWh)
f_{on}^{off}	incidence parameter to choose REC or CO_2 credits (mutually exclusive options) and it is equal to 0 or 1, respectively (fixed for any given run)
REC	renewable energy credits ($/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$)
γ_{NG}	non-transportation natural gas production costs ($/$m^3$)
a_m	intercept of the inverse demand curve for market m
b_m	Slope of the inverse demand curve for market m

3.1.3. Random parameters corresponding to the distribution in Fig. 3

This section describes the random parameters corresponding to the distributions in Fig. 3. It is important to note that there may in fact be correlation between the random factors (e.g., natural gas and electric power prices). For simplicity though, we have assumed no correlation between the random variables nor any seasonality since just one average day is modeled.

[4] The reduction of CNG from 100% of natural gas is due to further processing for gas quality outside of WWTP (/www.mabiosolids.org).

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

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)
$R_{CO2}(s)$	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)

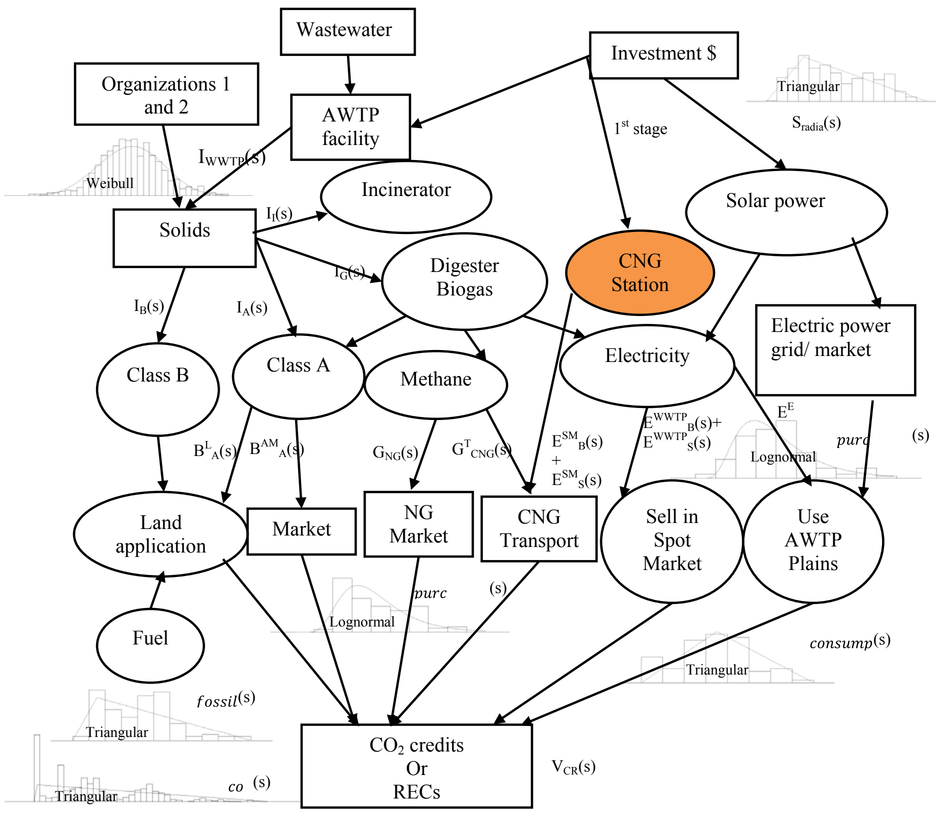

Fig. 3. Flowchart of the stochastic optimization model for biosolids management program at the Blue Plains AWTP.[2]

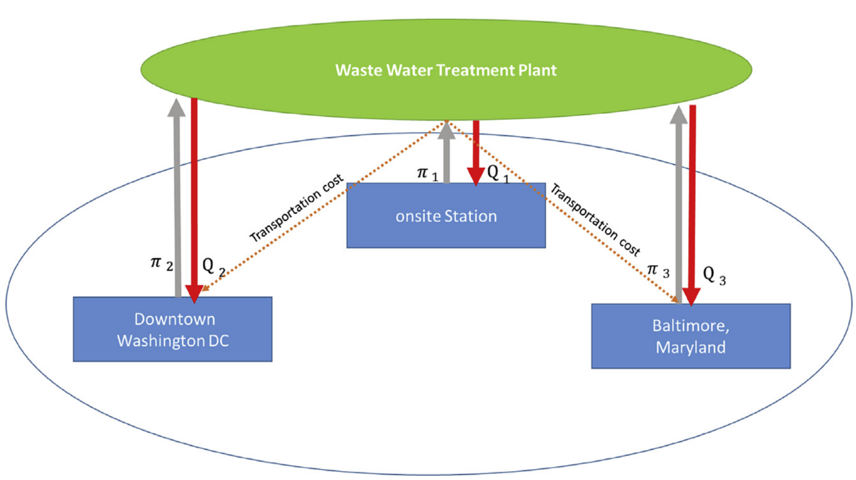

Fig. 4. CNG market and network representations.

We first describe the lower constraints for each market including the capacity constraints and supply demand constraints, then we focus on the upper level players' constraints which can be characterized in the following groups:

- Investment constraints e.g., number of CNG station equations (24) and (25)
- Capacity constraints e.g., (32)
- Energy conversion constraints equation (34)
- Energy balance constraints e.g., equation (39)
- Supply demand constraints e.g., equation (36)

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 (Shy, 1995). 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. Alternatively, one could "hardwire" the formulation for the lower level to be a social welfare maximization, then one would implicitly be always assuming a perfect competition approach at that level. Our approach, by contrast is flexible to allow both perfect competition as well as imperfect competition which is helpful in the lower-level markets considered. The reason is that from (40) and (41) (in the Appendix), the resulting lower-level problems separately and collectively constitute a mixed complementarity problem (MCP) (see Gabriel et al., 2013b) details) which also allows for non-optimization equilibria for future versions of this model.

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 U-tapao Chalida (2013) 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.

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

$$s.t.$$

$$q_{CNG,m}(s) \le \overline{q}_{CNG,m} \quad (\lambda_{CNG,m}(s)) \quad \forall s \tag{2b}$$

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

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) (http://www.environmental-expert.com/products/biogas-to-compressed-natural-gas-35510), 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.

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

$$s.t.$$

$$q_{ino}(s) \le \overline{q}_{ino} \quad (\lambda_{ino}(s)) \quad \forall s \tag{3b}$$

$$q_{org}(s) \le \overline{q}_{org} \quad (\lambda_{org}(s)) \, \forall s \tag{3c}$$

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

where

$q_{ino}(s)$ = amount of inorganic fertilizer in dt
$q_{org}(s)$ = amount of organic fertilizer in dt
$\lambda_{ino}(s)$ = dual price of inorganic fertilizer constraint
$\lambda_{org}(s)$ = 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 problem (4).

$$\max_{q_{fossil}(s),q_{nuclear}(s),q_{hydro}(s)} \sum_s \Pr(s)\left\{\pi_E(s)\left(q_{fossil}(s) + q_{nuclear}(s) + q_{hydro}(s)\right) - \gamma_{fossil} q_{fossil}(s) - \gamma_{nuclear} q_{nuclear}(s) - \gamma_{hydro} q_{hydro}(s)\right\} \tag{4a}$$

$$s.t.$$

$$q_{fossil}(s) \le \overline{q}_{fossil} \quad \left(\lambda_{fossil}(s)\right) \quad \forall s \tag{4b}$$

$$q_{nuclear}(s) \le \overline{q}_{nuclear} \quad (\lambda_{nuclear}(s)) \ \ \forall s \tag{4c}$$

$$q_{hydro}(s) \le \overline{q}_{hydro} \quad \left(\lambda_{hydro}(s)\right) \ \ \forall s \tag{4d}$$

$$q_{fossil}(s), q_{nuclear}(s), q_{hydro}(s) \ge 0 \ \ \forall s \tag{4e}$$

where

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

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

s.t.

$$q_{NG}(s) \le \overline{q}_{NG} \quad (\lambda_{NG}(s)) \ \ \forall s \tag{5b}$$

$$q_{NG}(s) \ge 0 \quad \forall s \tag{5c}$$

where

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

There is no implicit collusion between the players in each lower-level market. Rather, there is one optimization problem that is used to characterize the feedback between the upper-level (wastewater treatment plant) and the lower-level markets that it affects. These lower-level markets are perfectly competitive in the sense that no player in each market sees an inverse demand function and can therefore manipulate production to induce higher prices. If that were allowed, then the resulting model would be a stochastic EPEC (equilibrium problem with equilibrium constraints). Deterministic EPECS are hard enough to solve so for this version of our model we decided to stay with just a stochastic MPEC.

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. We applied a linearization procedure to the bilinear terms such as $\pi_F(s)B_A^{AM}(s)$, $\pi_E(s)E_B^{SM}(s)$, $\pi_E(s)E_S^{SM}(s)$, $\pi_{CNG}(s)G_{CNG}^T(s)$ and $\pi_{NG}(s)G_{NG}(s)$. Note that there are alternative ways to “convexify” these bilinear terms. The complete upper level of the stochastic MPEC is as follows:

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

The revenues from different components are as follows:

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

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

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

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

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

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

$$\text{The revenue from renewable energy credit}: \ SC(s)\left(C_{allow}^{WWTP} - C_T(s)\right)f_{0n}^{off} + REC\left(C_{allow}^{WWTP} - C_T(s)\right)\left(1 - f_{on}^{off}\right) \tag{13}$$

The upper-level costs are defined as follows:

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

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

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

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

Ash disposal costs : $\left(f^{I}_{ASH}\, I_I(s)\right)$ (18)

Cost of transporting class A and B biosolids to land application fields : $\left(f^{T}_{I}\, P_{fossil}(s)\left(B^{L}_{A}(s)+B^{AM}_{A}(s)+I_B(s)\right)\right)$ (19)

Transporting costs from organizations 1 and 2: $\left(f^{T}_{I}\, P_{fossil}(s)(I_{OR1}(s)+I_{OR2}(s)\right)$ (20)

Supplementary fuel costs : $\left(f^{T}_{I}\, P_{fossil}(s) I_I(s)\right)$ (21)

Composting costs : $\left(\gamma_{org}\, I_A(s)\right)$ (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*.

$$G^{T}_{CNG}(s)=\sum_{c,m} G^{S}_{CNG,c,m}(s) \quad \forall s \quad \text{cu ft} \tag{23}$$

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.

$$G^{S}_{CNG,c,m}(s) \le \overline{CNG}_{c,m} Build_{c,m} \ \forall c,m,s \quad \text{cu ft} \tag{24}$$

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

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

Solids influent constraints

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

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

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

$$I_G(s) \le x \quad \text{dt} \tag{28}$$

$$I_G(s) \le S_{gas} \quad \text{dt} \tag{29}$$

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

$$I_{OR1} \le S_{OR1} \quad \text{dt} \tag{30}$$

$$I_{OR2} \le S_{OR2} \quad \text{dt} \tag{31}$$

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

$$x \le CAP \tag{32}$$

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

$$x \ge l \tag{33}$$

Biogas and CNG production constraints

$$f_G\, I_G(s)=G_E(s)+G_{NG}(s)+G^{T}_{CNG}(s) \quad \text{m}^3 \tag{34a}$$

$$G_{NG}(s) \le f_{NG} f_G\, I_G(s) \quad \text{m}^3 \tag{34b}$$

$$G^{T}_{CNG}(s) \le f_{CNG} f_G\, I_G(s) \quad \text{m}^3 \tag{34c}$$

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

$$G^{T}_{CNG}(s) - \overline{G}^{T}_{CNG}(s) \le 0 \quad \text{m}^3 \tag{34e}$$

Constraint (34a) provides biogas mass balance; the biogas in qubic meter produced from solid influent equals biogas used in power generation, biogas used in natural gas production, and biogas used in CNG production. Constraints (34b, 34c, 34d, and 34e) specify the upper for biogas used for each product.

Class A biosolids production constraints

$$B^{L}_{A}(s)+B^{AM}_{A}(s)=f_B\, I_G(s)+I_A(s) \quad \text{dt} \tag{35a}$$

$$B^{AM}_{A}(s) - \overline{B}^{AM}_{A}(s) \le 0 \quad \text{dt} \tag{35b}$$

Constraint (34a) specifies amount of Class A biosolids transported to land application sites$B^{L}_{A}(s)$ or sold as a fertilizer to the market $B^{AM}_{A}(s)$ (35b) provides the upper bound for Class A bioslods sold to the market.

Electricity consumption constraints

$$E_{consump}(s) \le E^{E}(s)+E^{WWTP}_{B}(s)+E^{WWTP}_{S}(s) \quad \text{kWh} \tag{36a}$$

$$E^{WWTP}_{B}(s)+E^{SM}_{B}(s)=f_E G_E(s) \quad \text{kWh} \tag{36b}$$

$$E^{WWTP}_{S}(s)+E^{SM}_{S}(s)=(S_{Panel})(S_{radia}(s)) \quad \text{kWh} \tag{36c}$$

$$E^{SM}_{B}(s) - \overline{E}^{SM}_{B}(s) \le 0 \quad \text{kWh} \tag{36d}$$

$$E^{SM}_{S}(s) - \overline{E}^{SM}_{S}(s) \le 0 \quad \text{kWh} \tag{36e}$$

Conservation of power consumption is defined in equation (36). Uncertain power consumption $E_{consump}(s)$ is bounded by power purchased from outside sources $E^{E}(s)$, power produced by biogas$E^{WWTP}_{B}(s)$, and solar power$E^{WWTP}_{S}(s)$.Constraints(36b, 36c) denote the conversion for power generated by biogas and solar. equations (36d, 36e) provide the maximum on the power generation for biogas and solar respectively.

Natural gas residential sector consumption constraints

$$WWTP_{NG} \le NG^{E}_{H}(s)+G_{NG}(s) \quad \text{m}^3 \tag{37}$$

Conservation of CO_2 e emissions

$$C_T(s)=emissions - offsets \quad \text{ton} \tag{38}$$

where

$$\text{Emissions}=f^{E}_{C}\, E^{E}(s)+f^{NG}_{C} NG^{E}_{H}(s)+f^{t}_{C}\left(I_B(s)+B^{L}_{A}(s)+B^{AM}_{A}(s)\right) + \left(f^{I}_{C}\, I_I(s)\right)$$

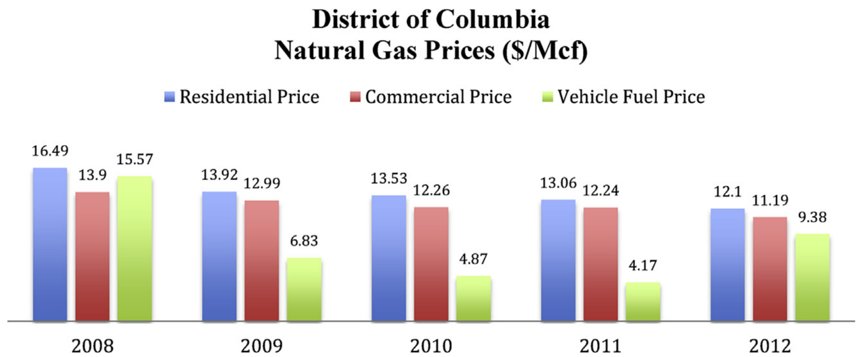

Fig. 5. U.S. Energy information administration natural gas prices ($/Mcf).

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

	Small station	Large station
Fixed costs[7]	$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

$$\text{Offsets} = f_C^E\left(E_B^{WWTP}(s) + E_B^{SM} + E_s^{WWTP}(s)\right) + f_C^{CNG}G_{CNG}^T(s) + f_C^{NG}G_{NG}(s) + f_C^f\left(I_B(s) + B_A^L(s) + B_A^{AM}(s)\right)$$

Constraint (38) specifies conservation of CO_2 e in tons. The CO_2 e emissions from AWTP wastewater treatment process $(f_C^E E^E(s))$, heating system using natural gas base $f_C^{NG}(NG_H^E(s))$, biosolids distribution $(f_C^t(I_B(s) + B_A^L(s) + B_A^{AM}(s)))$ and incineration $(f_C^I I_I(s))$. The CO_2 offsets are defined renewable power produced $(f_C^E(E_B^{WWTP}(s) + E_B^{SM} + E_s^{WWTP}(s)))$ and used at the AWTP, supplied CNG $(f_C^{CNG}G_{CNG}^T(s))$ to CNG market, supplied natural gas $f_C^{NG}G_{NG}(s)$ to natural gas market, used/sold biosolids as fertilizer $(f_C^f(I_B(s) + B_A^L(s) + B_A^{AM}(s)))$.

Conservation of energy purchased

$$P_T(s) = f_P^T\left(I_B(s) + B_A^L(s) + B_A^{AM}(s)\right) + f_P^T(I_{OR1}(s) + I_{OR2}(s)) + f_P^G NG_H^E(s) + E^E(s) + f_P^I \Big/ P_{fossil}(s) I_I(s) \quad \text{kWh} \tag{39}$$

Conservation of purchased energy in equation (39) specifies total energy consumption in kWh. The total energy can be characterized as follows: $(f_P^T(I_B(s) + B_A^L(s) + B_A^{AM}(s)))$ defines energy for transporting class A and/or class B biosolids to land application sites, $(f_P^T(I_{OR1}(s) + I_{OR2}(s)))$ represents energy used in transportation of solids from organizations 1 and 2, $(f_P^G NG_H^E(s))$ determines natural gas consumption at AWTP, $(E^E(s))$ includes electricity purchased from outside sources, and $((f_P^I/P_{fossil}(s))I_I(s))$ denotes supplementary fuel for incineration process.

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 the 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 (DOE, 2014c). This downward trend for natural gas prices is shown in Fig. 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[6] 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.

In terms of CNG demand, as of 2012, the District of Columbia had 461 CNG buses operated by WMATA (Metro Fact, 2012). 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 (Whyatt, 2010). Currently, there are no CNG commercial fueling stations in Washington, D.C. (DOE, 2014b) 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 (Find The Best, 2014). 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 (DOE, 2014b). 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 1000 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 1000 stations for the first time in a decade in 2004 because of high imported natural gas prices.

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

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

	Expected prices $/Mcf		% Price difference	Expected consumption Mcf/day		% Consumption difference
	SMPEC	EIA 2014		SMPEC	EIA 2014	
Baltimore, Maryland	$11.69	$11.67	0.17%	678.46	676.71	0.25%
Washington DC	$12.08	$11.89	1.60%	2686.12	2673.97	0.48%

Table 3
SMPEC Base Case operational outcomes.

Variables	Explanation	Value
	Objective function (expected profit)	-$158,444.02
E_B^{WWTP}	Expected electricity bought from external sources and used at the WWTP	448,700 (kWh)
	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	84,920 (kWh)
E_hydro	Expected amount of hydropower-based electricity	54,482 (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	1607.923 (dt)

Currently, there are approximately 1000 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 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 (Harklerod, 2013) is described in Table 1.

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 Siddiqui and Gabriel (2012) giving arise to an overall mixed-integer program.

It is important to note that the product of two variables ($\pi_{CNG}(s)G_{CNG}^T(s)$) 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. (This is just one of the bilinear terms, the others are mentioned in Section 3.3). The alternative we have chosen is to choose a discrete set of levels for the continuous variable ($G_{CNG}^T(s)$), in the manner described in (Gabriel et al., 2009; Gabriel and Leuthold, 2010) and then linearize this bilinear revenue term. In this study, thirty valid CNG production levels for the wastewater

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[9]	0	+$3557.2	+$6700.6	+$ 8505.2
CNG station		large[10] 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

[7] Fixed cost includes equipment, installation, and infrastructure costs.

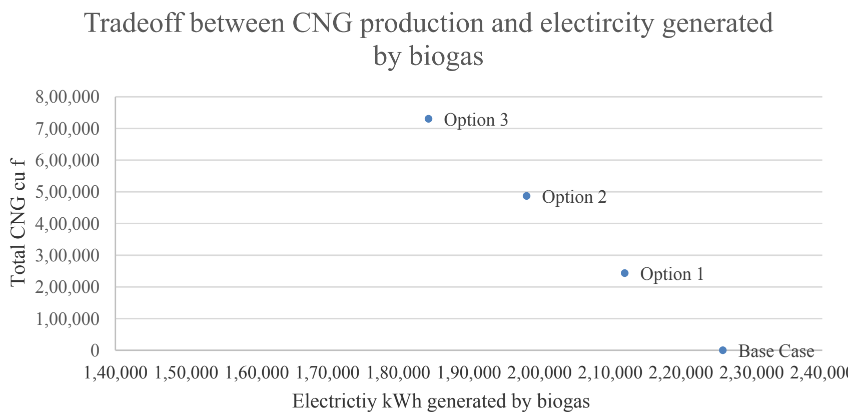

Fig. 6. Tradeoff between electricity produced using biogas sources vs total CNG produced at AWTP.

Table 5
Comparison of CO_2 emissions reduction.

	Total CNG produced by AWTP (Mcf)	Diesel gallon equivalent (DGE[11])	CO2 emissions reduction in pounds (kg) compared to diesel[12]
Base	0	0	0 (0)
Option 1	243.43	1691.15	+13,393.93 (6075.38 kg)
Option 2	486.85	3382.23	+26,787.31 (12,150.52 kg)
Option 3	730.28	5073.39	+40,181.25 (18,225.91 kg)

Table 6
Comparison of expected CNG prices.

Market nodes	Expected prices $ per Mcf			
	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.

Market nodes	Expected consumption in Mcf per day			
	Base	Option 1	Option 2	Option 3
Onsite Market	348.15	317.73	317.73	317.73
Washington, DC	2689.30	2689.30	2658.90	2658.90
Baltimore, Maryland	678.51	678.51	678.51	646.82

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 "(" these bilinear terms but they may depend on a special structure (e.g., (Ruiz and Conejo, 2009)). 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. We linearized all the bilinear terms in equations (7)–(11).

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 (DOE, 2014c) 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[8] between the SMPEC and (DOE, 2014c) 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 kW h was bought from the grid, 225,930 kW h were generated from biogas and, 18,721 kWh was produced from solar power at this AWTP No electricity produced at the 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

[8] Percentage difference is the absolute value of the difference between reference and model output divided by the reference.

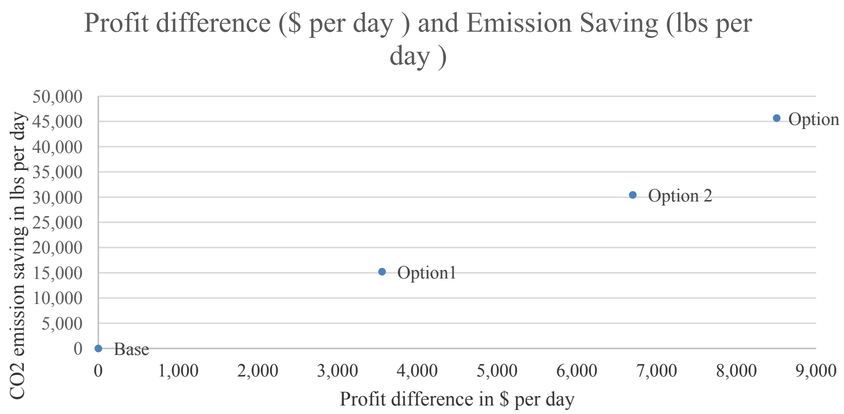

Fig. 7. Profit difference in $ per day and emission saving in lbs per day.

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 Fig. 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.

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 (http://www.ers.usda.gov/data-products/fertilizer-use-and-price.aspx#26720). As shown in Table 5, CNG from the AWTP contributes significantly to decreasing CO_2 emissions. Moreover, Fig. 7 presents the profit difference compared to CO_2 emissions reduction. Investing in CNG business not only has a financial 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 (see Tables 6 and 7).

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 (+$3557.23), Option 2 (+$6700.65), and Option 3 (+$ 8505.21) 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.

[9] Non-Base Case profit minus Base Case profit.

[10] The large CNG station has a capacity of 253,340 cubic feet/day.

[11] 111.47 cubic feet of CNG equals 1 DGE (http://www.nat-g.com/why-cng/cng-units-explained/).

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

6. Conclusions

In this paper, we have introduced a novel, large, 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). A Base Case was calibrated to match market conditions for the year 2013 and this case included no investment in compressed natural gas (CNG) by the AWTP.

Besides the Base Case, three other CNG investment scenarios were also developed and analyzed.

The other cases were as follows: Option 1 in which the AWTP could install at most 1 CNG station, Option 2 at most 2 CNG stations, and Option 3 at most 3 CNG stations.

The results indicate that it is most profitable for the AWTP to consider Option 3 with the most CNG stations potentially set up. This extra profit is derived from significantly more bio-CNG sold than all the other cases which results in somewhat less electricity generated for on-site use and the need for slightly more external purchases of electricity. It is also most environmentally beneficial for the AWTP to invest in CNG stations (Option 3) since it produces the largest CO_2 emissions reduction of the various cases."

APPENDIX A. KKT conditions and SOS1 transformation approach Karush–Kuhn–Tucker (KKT) conditions of the lower-level individual optimization problems by market

Fertilizer market:

$$0 \le Pr(s)(-\pi_F(s) + \gamma_{ino}) + \lambda_{ino}(s) \perp q_{ino}(s) \quad \ge 0 \tag{40a}$$

$$0 \le \overline{q}_{ino} - q_{ino}(s) \perp \lambda_{ino}(s) \ge 0 \tag{40b}$$

$$0 \le Pr(s)(-\pi_F(s) + \gamma_{org}) + \lambda_{org}(s) \perp q_{org}(s) \quad \ge 0 \tag{40c}$$

$$0 \le \overline{q}_{org} - q_{org}(s) \perp \lambda_{org}(s) \ge 0 \tag{40d}$$

Electricity market:

$$0 \le Pr(s)\Big(-\pi_E(s) + \gamma_{fossil}\Big) + \lambda_{fossil}(s) \perp q_{fossil}(s) \ \ge 0 \tag{40e}$$

$$0 \le \overline{q}_{fossil} - q_{fossil}(s) \perp \lambda_{fossil}(s) \ge 0 \quad (40f)$$

$$0 \le Pr(s)(-\pi_E(s) + \gamma_{nuclear}) + \lambda_{nuclear}(s) \perp q_{nuclear}(s) \ge 0 \quad (40g)$$

$$0 \le \overline{q}_{nuclear} - q_{nuclear}(s) \perp \lambda_{nuclear}(s) \ge 0 \quad (40h)$$

$$0 \le Pr(s)\Big(-\pi_E(s) + \gamma_{hydro}\Big) + \lambda_{hydro}(s) \perp q_{hydro}(s) \ge 0 \quad (40i)$$

$$0 \le \overline{q}_{hydro} - q_{hydro}(s) \perp \lambda_{hydro}(s) \ge 0 \quad (40j)$$

CNG market:

$$0 \le Pr(s)(-\pi_{CNG,n}(s) + \gamma_{CNG,n}) + \lambda_{CNG,n}(s) \perp q_{CNG,n}(s) \ge 0 \quad (40k)$$

$$0 \le \overline{q}_{CNG,n} - q_{CNG,n}(s) \perp \lambda_{CNG,n}(s) \ge 0 \quad (40l)$$

Residential natural gas market:

$$0 \le Pr(s)(-\pi_{NG}(s) + \gamma_{NG}) + \lambda_{NG}(s) \perp q_{NG}(s) \ge 0 \quad (40m)$$

$$0 \le \overline{q}_{NG} - q_{NG}(s) \perp \lambda_{NG}(s) \ge 0 \quad (40n)$$

Market-clearing conditions of the relevant markets:

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

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

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

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

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[13] (Mankiw, 2007), electricity market ((Mamut and Badea, 2015); (Bernstein and Griffin, 2006)), CNG market[14,15] ((Mamut and Badea, 2015); (Bernstein and Griffin, 2006)), residential natural gas market ((Mamut and Badea, 2015); (Bernstein and Griffin, 2006)).

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

$$zp^1_{ino}(s) = Pr(s)\{-\pi_F(s) + \gamma_{ino}\} + \lambda_{inor}(s) \quad (42a)$$

$$2SOS^{1+}_{ino}(s) + 2SOS^{1-}_{ino}(s) = zp^1_{ino}(s) + q_{ino}(s) \quad (42b)$$

$$2SOS^{1+}_{ino}(s) - 2SOS^{1-}_{ino}(s) = zp^1_{ino}(s) - q_{ino}(s) \quad (42c)$$

$$zp^2_{ino}(s) = \overline{q}_{ino} - q_{ino}(s) \quad (42d)$$

$$2SOS^{2+}_{ino}(s) + 2SOS^{2-}_{ino}(s) = zp^2_{ino}(s) + \lambda_{ino}(s) \quad (42e)$$

$$2SOS^{2+}_{ino}(s) - 2SOS^{2-}_{ino}(s) = zp^2_{ino}(s) - \lambda_{ino}(s) \quad (42f)$$

$$zp^1_{ino}(s),\ zp^2_{ino}(s) \ge 0 \quad (42g)$$

$$q_{ino}(s) \ge 0 \quad (42h)$$

$$\lambda_{ino}(s) \ge 0 \quad (42i)$$

$SOS^{1+}_{ino}(s),\ SOS^{1-}_{ino}(s),\ SOS^{2+}_{ino}(s),\ SOS^{2-}_{ino}(s)$ are SOS1 variables

Appendix B. Parameters

CAP = 1000 dt
$S_{OR1} = 60\ dt$[16]
$S_{OR2} = 50\ dt$[17]
$S_{gas} = 620$ dt (Metcalf & Eddy & AECOM, 2008)
$f_G = 339.94\ m^3/dt\ (12,012\ cf/dt)$[18]
$f_{NG} = 0.6$
$f_{CNG} = 0.579$
$f_B = 0.4838$ (Metcalf & Eddy & AECOM, 2008)
$f_E = 2.02\ kwh/m^3\ (0.057\ kwh/cf)$[19]
$WWTP_{NG} = 4874.39\ m^3/d\ (172,240\ cf/d)$[20]
$f_C^E = 0.00055$ t/kWh (The climate registry, 2008)
$f_C^{NG} = 0.00197\ t/m^3\ (0.000056\ t/cf)$ (The climate registry, 2008)
$f_C^I = 1.44$ t/dt (Brown et al., 2010)
$f_C^{CNG} = 0.001908\ t/m^3\ (0.000054\ t/cf)$ (The climate registry, 2008)
$f_C^f = 0.1$ t/dt (Brown, 2004)

[13] http://www.ers.usda.gov/data-products/fertilizer-use-and-price.aspx#26720.
[14] http://www.afdc.energy.gov/fuels/properties.html.
[15] Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) Model, version 1.7.2007. Input Fuel Specifications. Argonne National Laboratory. Chicago, IL., and www.afdc.energy.gov.

[16] 1,400,000 population, 1.4×10^{-4} wet tons per day produced sludge rate, and 70% water content.
[17] Wastewater influent 60 MGD and the solid production rate 0.82.
[18] The maximum biogas of approximately 4.4×10^6 cf/d comes from the digester design, which is equal to times each dry ton of solids influent.
[19] Calculated from the efficiency of one type of power generator using biogas (Metcalf & Eddy & AECOM, 2008).
[20] The highest natural gas consumption obtained from the energy saving plan report of December, 2010.

$f_C^t = 0.2$ t/dt (Brown, 2004)
$f_P^T = 73.5$ kWh/dt
$f_P^G = 2.02$ kWh/m^3 (0.057 kWh/cf)
$f_P^I = 26.58$ kWh/dt
$f_I^T = 0.56$ gal/dt
$f_E^{Gen} = \$0.00506$ per kWh
$\gamma_{bio-CNG} = \$0.1016$ per m^3 (\$0.0058 per cf)
$\gamma_{bio-methane} = \$0.1765$ per m^3 (\$0.005 per cf)
$f_A^{Com} = \$249.6$ per dt
$f_{Ash}^I = \$27.85$ per dt
$f_I^{TIP} = \$0$, \$50, \$100 per dt of biosolids influent to digester
$C_{allow}^{WWTP} = 346.2$ t
$S_{panel} = 14{,}944$ m^2
$RES = \$0.05$ per kWh[21]
$f_{on}^{off} = 0$
REC = \$1.89 per ton CO_2 e
$I_{WWTP}(s)$ = solids influent to digester (174–684 dt) fitted with a Weibull distribution function
$E_{consump}(s)$ = electricity consumption at WWTP (564,000–838,000 kWh) fitted with a triangular distribution function
$E_{purchased}(s)$ = electricity purchasing prices (\$ 0.03–0.136 per kWh) fitted with a lognormal distribution function
$NG_{purchased}(s)$ = natural gas purchasing prices (\$0.102–0.459 per m^3) or (\$0.0029–0.013 per cf)) fitted with a lognormal distribution function
$P_{fossil}(s)$ = fossil fuel prices to transport class A and B (\$0.38–1.32 per liter) or (\$1.43–5 per gallon) fitted with a triangular distribution function
$R_{CO2}(s)$ = carbon credits (\$0.05–8 per ton CO_2) fitted with a triangular distribution function
$S_{radia}(s)$ = solar radiation (0.19–2.65 kWh/m^2) fitted with a triangular distribution function
$S_{generate}(s)$ = generated solar electricity cost \$0.12, \$0.13 and \$0.15 per kWh.

Operation and Maintenance costs ($a_{i,j}$) in dollars.

Digester/segment	1	2	3
1	170.23	271.18	271.18
2	170.23	271.18	271.18
3	170.23	170.23	271.18
4	490.81	490.81	490.81
5	92.00	92.00	92.00

Minimum solids use to produce biogas ($l_{i,j}$) in dt.

Digester/segment	1	2	3
1	500	500.001	750.001
2	250	250.001	750.001
3	500	500.001	750.001
4	500	500.001	750.001
5	500	500.001	750.001

$\overline{q}_{ino} = 122{,}019$ dt[22]
$\overline{q}_{org} = 1899.8$ dt
$\overline{q}_{fossil} = 35{,}476$ kWh[23] (71.31% of average daily retail sales in 2012)
$\overline{q}_{nuclear} = 84{,}920$ kWh (16.85% of average daily retail sales in 2012)
$\overline{q}_{hydro} = 54{,}482$ kWh (10.81% of average daily retail sale in 2012)
$\overline{q}_{CNG} = 1.189$ m^3(42,293.15 cf)[24] (EIA 2013)
$\overline{q}_{NG} = 1.189$ m^3 (42,293.15 cf)
$\gamma_{ino} = \$224$ per dt[25]
$\gamma_{org} = \$249.6$ per dt[26]
$\gamma_{fossil} = \$0.047$ per kWh (EIA 2013)

Random parameter values	Low		Medium		High	
	Value	Probability	Value	Probability	Value	Probability
$I_{WWTP}(s)$ (dt)	196	0.295	241.5	0.283	474	0.422
$E_{consump}(s)$ (kWh)	615,500	0.321	701,000	0.429	786,500	0.250
$E_{purchased}(s)$ (\$/kWh)	0.038	0.260	0.080	0.659	0.129	0.081
$NG_{purchased}(s)$(\$/m^3)	0.148	0.338	0.226	0.407	0.364	0.255
$P_{fossil}(s)$ (\$/litter)	0.48	0.388	0.71	0.373	1.09	0.239
$R_{CO2}(s)$ (\$/ton CO_2)	0.125	0.037	1.30	0.467	5.20	0.496
$S_{radia}(s)$ (kWh/m^2)	0.29	0.180	0.87	0.400	2.03	0.420
$S_{generate}(s)$ (\$/kWh)	0.15	0.333	0.13	0.250	0.12	0.417

Note that the key cut-off value depends on two criteria.
- It should be about the 30th, 60th, or the 100th percentiles (for representativeness).
- The exact percentile is approximated by where a "bin" ends from the goodness-of-fit.

Digester fixed costs ($h_{i,j}$) in dollars.

Digester/segment	1	2	3
1	66,145.68	15,670.68	15,670.68
2	41,982.36	16,744.86	16,744.86
3	66,145.68	108,128.04	32,415.54
4	48,658.94	48,658.94	48,658.94
5	61,504.25	61,504.25	61,504.25

$\gamma_{nuclear} = \$0.025$ per kWh
$\gamma_{hydro} = \$0.011$ per kWh

[21] In (EIA, 2009) it was mentioned that the generated electricity from rooftop photovoltaic and small wind turbines will earn 1 credit per kWh after 2014, and gain \$0.05 per kWh as market value for each credit.

[22] U.S. department of agricultural (USDA) data from 2000 to 2010 <http://www.ers.usda.gov/data-products/fertilizer-use-and-price.aspx#26720>.

[23] An average daily amount of retail sales of electricity to the District of Columbia residential sector is 504,109.6 kWh (EIA 2013).

[24] http://www.eia.gov/oil_gas/natural_gas/data_publications/natural_gas_monthly/ngm.html.

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

[26] The composting process cost in 2008 is \$208 per dry ton of fertilizer, which included \$8 per dry ton for capital cost and \$200 per dry ton for operation and maintenance cost (EPA 2002; Harkness et al., 1994; Wang et al. 2009), and 20% of management cost was added.

γ_{CNG} = *\$0.671per m³(\$0.019 per cf) (included \$0.0058 per cf production unit, operation, and maintenance costs*[27] *and \$0.013 per cf natural gas*[28] *cost)*

γ_{NG} = \$0.459per m³ (\$0.013 per cf)

Appendix C. Probability for 6561 scenarios using in the stochastic model

The probability for each scenario is calculated by multiplying the probability of ten groups of uncertainty together (the details of each uncertainty probability are shown in Fig. C). Pr(s) denotes the probability for each scenario and is used to calculate expected values in the three objective functions.

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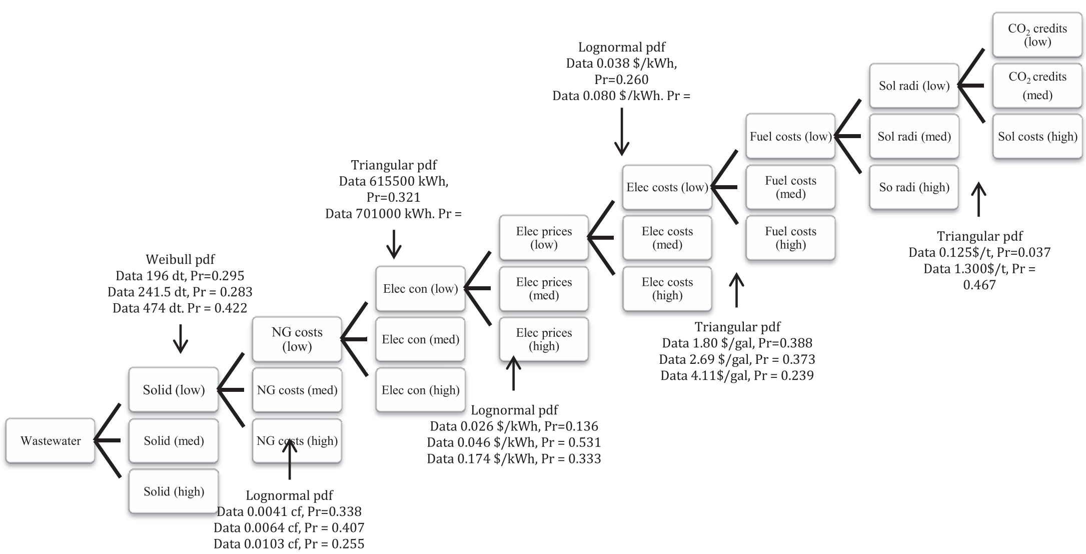

Fig. C. scenario tree show probability of uncertain data. Note that low = low amount, med = medium amount, high = high amount Solid = solid end products, NG = natural gas, Elec = electricity, Fuel = fossil fuel, Sol radi = solar radiation.

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