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A holistic planning model for sustainable water management in the shale gas industry

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ABSTRACT

To address water planning decisions in shale gas operations, we present a novel water management optimization model that explicitly takes into account the effect of high concentration of total dissolved solids (TDS), and its temporal variation in the impaired water. The model comprises different water management strategies: a) direct wastewater reuse, which is possible due to the new additives tolerant to high TDS concentration but at the expense of increasing the costs; b) wastewater treatment, taking separately into account pre-treatments, softening and desalination technologies and c) send to Class II disposal sites.

The objective is to maximize the "sustainability profit" determining flowback destination (reuse, degree of treatment or disposal), the fracturing schedule, fracturing fluid composition and the number of water storage tanks needed at each period of time.

Due to the rigorous determination of TDS in all water streams, the model is a non-convex MINLP model that is tackled in two steps: first, an MILP model is solved based on McCormick relaxations; next, the binary variables that determine the fracturing schedule are fixed, and a smaller MINLP is solved.

Finally, several case studies based on Marcellus Shale play are optimized to illustrate the effectiveness of the proposed formulation. The model identifies the best water management option to improve both economic and environmental criteria, resulting to be direct reuse the best one.

Keywords: water management, optimization, MINLP, planning, shale gas

1. INTRODUCTION

The global natural gas production is expected to increase around 62% by 2040. The largest component in the projected growth is due to shale gas production, which will increase from 342 billion cubic feet per day (bcf/d) in 2015 to 554 bcf/d by 2040.[1] Currently, only the United States, Canada, China, and Argentina have commercial shale gas production. However, Mexico and Algeria are expected to contribute to the projected growth due to the technological improvements made in the extraction techniques.[1,2]

It is well-known that the extraction of shale gas, apart from generating huge benefits, has associated environmental risks including many water-based concerns. The exploitation stages of a shale well include exploration, wellpad construction, well drilling, well treatment and completion, and production. The largest volume of water used is during well treatment and completion phase, when hydraulic fracturing occurs. Operators fracture shale gas wells in 8 to 23 stages, using from 190 to 38,000 m^3 of fracturing fluid per well depending on shale gas formation.[3] Fracturing fluid typically contains about 90% water, 9% propping agents and less than 1% of friction-reducing additives.[3,4] After a well is hydraulically fractured, the pressure of the wellhead is released allowing a portion of wastewater, called *flowback* water, return to the wellhead. Flowback water is recovered from few days to few weeks, containing total dissolved solids (TDS) ranging from 10,000 to 150,000 mg L^{-1}. The wastewater that continues generating over the life of the well (10 - 30 years) is called *produced water*. The TDS concentration in long-term produced water can reach 250,000 mg L^{-1}. Both wastewater volume and concentration of TDS are uncertain and vary with the geographical properties of the formation. As a rule of thumb, the volume of wastewater generated is 50 percent flowback water and 50 percent produced water.[3]

Current water management strategies include disposal of wastewater via Class II disposal wells, transfer to a centralized water treatment facility (CWT) or to mobile desalination treatment, or direct reuse in drilling the subsequent wells. The reused flowback is called *impaired water*.

Mechanical vapor compression is the most common and well-established desalination treatment employed in shale gas industry.[5–7] Besides, the emerging membrane distillation technology is gaining importance in the last years for desalinating shale water due to the utilization of low-grade heat sources for separating salts from water.[6–8]

Direct reuse of flowback water has been possible due to the development of salt-tolerant friction reducers.[3,9,10] Previous friction reducers were not compatible with salt-water, therefore they were not able to control friction pressure losses and associated pump pressure. Direct reuse in drilling the subsequent wells is currently the most popular option due to its operational simplicity for contractors.[11] Moreover, this practice has the potential to decrease the environmental issues associated with shale gas water management such as transportation, disposal or treatment. However, friction reducers expenses increase with the concentration of TDS. Operators must take into consideration that reusing impaired water, the concentration of TDS will increase over the time representing a major cost-barrier.

A rapid increase in publications on water management optimization in shale gas industry has been reported in the recent years. These publications cover various topics, including environmental impacts and uncertainty analysis in freshwater availability or flowback water production to identify its impact on the optimal decisions.

Yang et. al[12] proposed a discrete-time two-stage stochastic mixed-integer linear programming model to determine - in short-term operations - the optimal fracturing schedule and cost of transportation, storage, treatment and disposal cost under uncertain availability water. The model does not account for TDS concentration. They developed an extended model [13] accounting for TDS to consider long-term decisions for investments in water treatment, impoundments, and pipelines. However, to avoid non-linearities, they used an approximation by discretizing the TDS concentration. Bartholomew and Mauter[14] used the Yang et. al model[13] integrating human health and environmental impacts with multi-objective optimization. However, the authors do not consider return to pad operations and fixed the blending ratio a priori. Gao and You[15] proposed a mixed-integer linear fractional programming model to maximize the profit per unit of freshwater consumption. The authors include multiple transportation modes and water management options. Nevertheless, they also do not consider return to pad operations and they fixed the blending ratio and fracturing schedule a priori. Gao and You[16] also presented a mixed-integer nonlinear programming problem addressing the life-cycle economic and environmental optimization of shale gas supply chain network. Guerra et al.[17] presented an optimization framework that integrates the design and planning of the shale gas supply chain and water management. In this case, the fracturing schedule and sizing of storage facilities are out of the scope of the proposed framework. Moreover, they do not consider reusing water directly without treatment.

Lira-Barragán et. al[18] presented a mathematical model for synthesizing shale gas water networks accounting uncertainty in water demand for hydraulic fracturing and flowback water forecast. Lira-Barragán et. al[19] also developed an MILP mathematical programming formulation accounting for economics by minimizing the cost for the freshwater, storage treatment, disposal, and transportation, and minimizing freshwater usage and wastewater discharge as an environmental objective. However, in both works, the schedule is fixed in advance, and the wastewater is always treated.

Drouven and Grossmann[20] proposed an MILP model to identify the optimal strategies for impaired water overestimating the cost of friction reducers. The authors consider return to pad operations and assume that the water-blending ratio is unrestricted. However, the mathematical model does not take into account other water management strategies nor the salt concentration of impaired water.

Yizhon Chen et al.[21] developed a multi-level decision-making programming model for planning shale gas supply chain operations. The first level focused on mitigating GHG emissions, the middle level maximizes the system benefits and the lower level seeks to minimize the water usage. Lately, they published two works accounting uncertainties in the estimated ultimate recovery (EUR), greenhouse gas (GHG) emissions and flowback and produced water production, respectively, helping stakeholder to achieve supply chain satisfaction and to control GHG emissions.[22,23] The fracturing schedule is out of the scope of the proposed framework. Additionally, they do not include onsite-treatment option either storage solution.

This paper focuses on overcoming some of the limitations of the previous papers cited above. Specifically, we propose a holistic mixed-integer non-linear programming (MINLP) model that considers the TDS concentration of flowback and impaired water, as well as different water treatment solutions. The main novelties introduced in the mathematical model are the estimation of friction reducers expenses, as a function of TDS concentration to determine if the level of TDS in impaired water is an obstacle for reusing it in drilling and fracturing operations, and the rigorous handling at storage solution by determining the required number of tanks installed/uninstalled over the period of time. Additionally, the objective of the proposed model is to maximize the "sustainability profit"[24] in order to obtain a compromise solution among the three pillars of sustainability: social, economic, and environmental. The advantage of this metric is that multi-objective optimization is concentrated to a single-objective since all the indicators are expressed in monetary terms. Besides, the solution obtained is clear, understandable and intuitive for the stakeholders since different elements of the objective function can be easily compared. The rest of the paper is organized as follows: The problem statement is defined in section 2. In section 3, the mathematical MINLP model is described in detail. Section 4 describes the modeling and solution strategy. The results obtained from different case studies based on Marcellus shale play are presented in section 5. Finally, the last section summarizes the conclusions of the present work.

2. PROBLEM STATEMENT

The problem described in this paper can be stated as follows. Given are the following:

- A set of shale gas wells belonging to a specific wellpads including water requirements, fracturing time and crews available to perform the drilling and completion phase. Profiles for the flowback flowrate, TDS concentration and gas production curve per well are also provided.
- The capacity and the maximum number of fracturing tanks. Each storage unit includes the cost associated to move, demobilize and clean out the tank before removing it from the location and leasing cost.
- The capacity and the maximum number of freshwater tanks available to store the water required to complete each well.

- The capacity and the maximum number of impoundments. Freshwater can also be stored in freshwater impoundments.
- A set of freshwater sources available to supply the water for hydraulic fracturing operations and the water withdrawal cost.
- A set of Class II disposal wells to inject the wastewater and the corresponding cost of disposal.
- A set of treatment technologies to desalinate the flowback water onsite. The maximum capacity, treatment cost, leasing cost and the cost associated to move, demobilize and clean out are also given.
- A set of centralized water treatment (CWT) plants and the treatment cost and maximum capacity of each facility.
- Locations of the freshwater source, centralized water treatment (CWT), disposal wells and wellpads.
- Transportation costs of freshwater and wastewater via trucks.
- The cost of moving rigs, well drilling and completion, shale gas production and friction reducers are given.
- The sales price of shale gas per week for all prospective wells is provided.

The target is to determine the number of tanks leased at each time period, the fracturing schedule (wellpad fracturing start date), flowback destination (reuse, treatment or disposal), and type and location of onsite desalination treatment at each time period.

For this purpose, a shale gas water management superstructure, shown in Figure 1, is proposed.

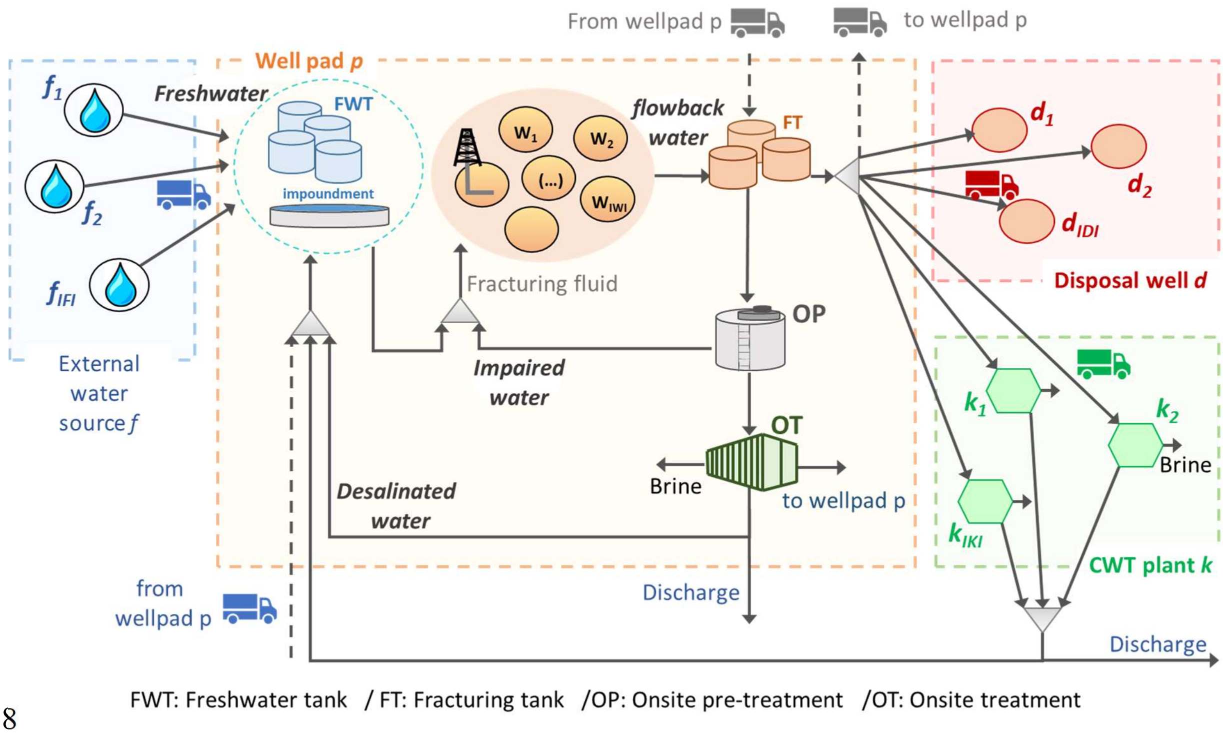

Figure 1. The proposed superstructure for shale gas water management operations.

The system comprises wellpads *p*, shale gas wells in each wellpad *w*, natural freshwater sources *f*, fracturing crew *c*, centralized water treatment technologies (CWT) *k*, and disposal wells *d*.

As commented before, part of the water used for hydraulic fracturing returns to the wellhead. This wastewater, called flowback water, is stored in portable fracturing tanks. After that, flowback water can be transported to a neighboring wellpad, CWT plants or Class II disposal wells. Also, it can be sent to a basic mobile treatment (pre-treatment) placed in each wellpad.

Pre-treatment can remove bacteria, suspended solids, oil and grease and certain ions depending on the final destination.[25] The pretreated water can be desalinated in onsite desalination units or can be used to fracture others wells in the same wellpad.

Mobile desalination treatment can be used two different technologies -membrane distillation (MD)[26] and/or multi-effect evaporation with mechanical vapor recompression

(MEE-MVR)[5,27]- to remove TDS contents. We consider that these technologies are designed to obtain the brine stream close to salt saturation conditions to maximize, at the same time, the freshwater recovered. Treatment cost restricts the selection of the desalination technology. Desalinated water from onsite treatment or CWT facility can be used as a fracturing fluid or discharged – after adequate water conditioning- for other uses. Freshwater is withdrawal from uninterruptible freshwater sources. This water, together with desalinated water, is stored in water impoundment and/or freshwater tanks (FWT).

The assumptions made in this work are as follows:

- A fixed time horizon is discretized into weeks as time intervals.
- The volume of water required to fracture each well is available at the beginning of well development, and includes the water used in drilling, construction and completion.
- Onsite pretreatment (OP) process provides adequate contaminant removal for the next operations.
- Friction reducers costs increase linearly with the concentration of salts.
- Transportation is only performed by trucks.

3. MATHEMATICAL PROGRAMMING MODEL

The optimization water management problem, which is detailed below, is formulated as an MINLP model that comprises: material balance in storage tanks, assignment constraints, logic constraints, mixers and splitters, and an objective function. Note that lower-case letters are used for variables and upper-case letters and Greek letters for parameters.

Set definition

To develop the mathematical model, the following sets are defined.

$$\begin{aligned}
&P = \{p \,/\, p \text{ is a wellpad}\}\\
&W = \{w \,/\, w \text{ is a well}\}\\
&T = \{t \,/\, t \text{ is a time period}\}\\
&N = \{n \,/\, n \text{ is a onsite water treatment}\}\\
&K = \{k \,/\, k \text{ is centralized water treatment plant}\}\\
&F = \{f \,/\, f \text{ is a freshwater source}\}\\
&C = \{c \,/\, c \text{ is a fracturing crew}\}\\
&D = \{d \,/\, d \text{ is a disposal}\}\\
&S = \{s \,/\, s \text{ is a storage tank type}\}\\
&RPW_p = \{w \,/\, w \text{ is a well in wellpad p}\}
\end{aligned}$$

Assignment constraint

Eq. (1) guarantees that at the time horizon each well can only be drilled once by one of the available fracturing crew *c*,

$$\sum_{t\in T}\sum_{c\in C} y^{hf}_{t,p,w,c} \le 1 \qquad \forall w \in RPW_p, p \in P \tag{1}$$

where $y^{hf}_{t,p,w,c}$ indicates that the well *w* in wellpad *p* is stimulating by fracturing crew *c* in time period *t*.

Eq. (2) ensures that there is no overlap in drilling and completions operations between different wells, namely, a fracturing crew cannot begin to fracture a new well until it has finished fracturing the previous one,

$$\sum_{p\in P}\sum_{w\in RPW_p}\sum_{tt=t-\tau_w+1}^{t} y^{hf}_{tt,p,w,c} \le 1 \qquad \forall t \in T, c \in C \tag{2}$$

where τ_w is a parameter that indicates the time required to fracture well *w* by fracturing crew *c*.

Shale water composition and water recovered

After a well is drilled and hydraulically fractured, a portion of the water injected is returned to the wellhead. Well drilling and construction typically take from one to five weeks[3], therefore the flowback water will come out τ_w weeks after a well is selected to be fractured,

$$\sum_{c \in C} y^{hf}_{t,p,w,c} = y^{fb}_{t+\tau_w,p,w} \qquad t \le T - \tau_w, \forall w \in RPW_p, p \in P \tag{3}$$

where $y^{fb}_{t,p,w,c}$ represents the time period when the flowback water comes out. The binary variable $y^{fb}_{t,p,w,c}$ is treated as a continuous variable -with bounds between 0 and 1- since its integrality is enforced by constraint (3). This practice permits save time and resources due to any binary (integer) variable will eventually could be branched during the optimization. Although in modern MI(N)LP solvers this situation is somewhat minimized due to constraint propagation techniques, more rigorous selection of branching variables, etc., it could still have an important effect on solver performance.

The shale gas water recovered and composition from each wellpad, once the well is hydraulically fractured, is calculated with Eqs. (4-5),

$$f^{well}_{t,p,w} = \sum_{tt=0}^{tt \le t-1} F^{well}_{t-tt,p,w} \cdot y^{fb}_{tt+1,p,w} \qquad \forall t \in T, w \in RPW_p, p \in P \tag{4}$$

$$c^{well}_{t,p,w} = \sum_{tt=0}^{tt \le t-1} C^{well}_{t-tt,p,w} \cdot y^{fb}_{tt+1,p,w} \qquad \forall t \in T, w \in RPW_p, p \in P \tag{5}$$

where, $F^{well}_{t,p,w}$ and $C^{well}_{t,p,w}$ are parameters that indicate flowback flowrate and TDS concentration, respectively.

Eqs. (6-7) correspond to the mass and salt balance of flowback water collected from the wells belonging the wellpad p,

$$f^{pad}_{t,p} = \sum_{w \in RPW_p} f^{well}_{t,p,w} \qquad \forall t \in T, p \in P \tag{6}$$

$$c_{t,p}^{pad} \cdot f_{t,p}^{pad} = \sum_{w \in RPW_p} C_{t,p,w}^{well} \cdot F_{t,p,w}^{well} \qquad \forall t \in T, p \in P \tag{7}$$

Mass and salt balance in storage tanks

The level of the storage tank in each time period ($st_{t,p,s}$) depends on the water stored in the previous time period ($st_{t-1,p,s}$), the mass flowrates of the inlet streams belonging to the storage tank s ($f_{t,p,s}^{i}$), and the mass flowrates of the outlet streams belonging to the storage tank *s* ($f_{t,p,s}^{o}$). Note that subsets ISs and OSs represent the set of inlet and outlet streams that belong storage tank s.

$$st_{t-1,p,s} + \sum_{i \in IS_s} f_{t,p,s}^{i} = st_{t,p,s} + \sum_{o \in OS_s} f_{t,p,s}^{o} \qquad \forall t \in T, p \in P, s \in S \tag{8}$$

The salt mass balance in fracturing tank (FT) is described by the following equation,

$$st_{t-1,p,s} \cdot c_{t-1,p} + \sum_{i \in IS} f_{t,p,s}^{i} \cdot c_{t,p}^{i} = \left(st_{t,p,s} + \sum_{o \in OS} f_{t,p,s}^{o} \right) \cdot c_{t,p} \qquad \forall t \in T, p \in P, s \in \{ft\} \tag{9}$$

Storage balances

Flowback water and freshwater are stored in portable leased tanks at wellpad p. Eq. (10) describes the storage balance of tank *s* in wellpad *p* in time period *t*,

$$n_{t,p,s} = n_{t-1,p,s} + n_{t,p,s}^{ins} - n_{t,p,s}^{unins} \qquad \forall t \in T, p \in P, s \in S \tag{10}$$

where $n_{t,p,s}$ is the total number of tanks, $n_{t,p,s}^{ins}$ and $n_{t,p,s}^{unins}$ represent the number of installed or uninstalled tanks in a specific time period.

The amount of water stored, $st_{t,p,s}$, is bounded by the capacity of one tank, CST_s , and the number of tanks installed, $n_{t,p,s}$. Besides, the storage tanks should handle the wastewater that returns to the wellhead from one day. Therefore, as the time horizon is discretized into weeks, the variable $\theta_{t,p,s}$, which is equal to the inlet wastewater or freshwater divided by the number of days in a week, is introduced to avoid oversizing the tanks,

$$st_{t,p,s} + \theta_{t,p,s} \le CST_s \cdot n_{t,p,s} \qquad \forall t \in T, p \in P, s \in \{ft\} \tag{11}$$

$$N_s^{LO} \cdot y_{t,p,s}^{st} \le n_{t,p,s}^{ins} \le N_s^{UP} \cdot y_{t,p,s}^{st} \qquad \forall t \in T, p \in P, s \in S \tag{12}$$

N_s^{LO} and N_s^{UP} are lower and upper bounds of the number of tanks installed. $y_{t,p,s}^{st}$ indicates the installation of each tank *s* on wellpad *p* at time period *t*.

The total freshwater stored also depends on the number of freshwater impoundments installed,

$$n_{t,p}^{im} = n_{t-1,p}^{im} + n_{t,p}^{im,ins} \qquad \forall t \in T, p \in P \tag{13}$$

$$N^{im,LO} \cdot y_{t,p}^{im} \le n_{t,p}^{im,ins} \le N^{im,UP} \cdot y_{t,p}^{im} \qquad \forall t \in T, p \in P \tag{14}$$

$$st_{t,p,s} + \theta_{t,p,s} \le CST_s \cdot n_{t,p,s} + V^{imp} \cdot n_{t,p}^{im} \qquad \forall t \in T, p \in P, s \in \{fwt\} \tag{15}$$

where V^{imp} is the capacity of an impoundment.

Water Demand

The amount of water required per wellpad ($f_{t,p}^{dem}$) can be supplied by a mixture of fresh ($f_{t,p}^{fre}$) or impaired water ($f_{t,p}^{imp}$),

$$f_{t,p}^{dem} = f_{t,p}^{fresh} + f_{t,p}^{imp} \qquad \forall t \in T, p \in P \tag{16}$$

The fracturing water ($f_{t,p,w}^{dem}$) required in each well is given by constraint (17),

$$f_{t,p}^{dem} = \sum_{w \in RPW_p} f_{t,p,w}^{dem} \qquad \forall t \in T, p \in P \tag{17}$$

The following constraint indicates that the water available at each well, when the well is fractured must be greater or equal than the water demand of each well (WD_w),

$$f_{t,p,w}^{dem} \geq WD_w \cdot \sum_{c \in C} y_{t,p,w,c}^{hf} \qquad \forall t \in T, w \in RPW_p, p \in P \tag{18}$$

Onsite treatment

Mass balance around onsite pretreatment technology is described in Eq.(19). The total inlet wastewater that enters in the pretreatment in wellpad p in time period t is equal to the outlet pretreated stream plus the sludge stream.

$$f_{t,p}^{pre,in} = f_{t,p}^{pre,out} + f_{t,p}^{on,slud} \qquad \forall t \in T, p \in P \tag{19}$$

The relation between the inlet and outlet mass flowrate is modeled by using the recovery factor (α^{pre}),

$$f_{t,p}^{pre,out} = \alpha^{pre} \cdot f_{t,p}^{pre,in} \qquad \forall t \in T, p \in P \tag{20}$$

After pretreatment, the water can be used as a fracturing fluid ($f_{t,p}^{imp}$) or/and can be sent to a desalination unit ($f_{t,p}^{on,in}$),

$$f_{t,p}^{pre,out} = f_{t,p}^{imp} + f_{t,p}^{on,in} \qquad \forall t \in T, p \in P \tag{21}$$

The total and salt balances around the onsite desalination treatment are given by Eqs. (22-23). In order to achieve the outlet stream close to ZLD conditions, the outlet brine salinity (C^{zld}) is fixed to 300 g·kg^{-1} (close to salt saturation condition of ~350 g·kg^{-1}).

$$f_{t,p}^{on,out} + f_{t,p}^{on,brine} = f_{t,p}^{on,in} \qquad \forall t \in T, p \in P \tag{22}$$

$$f_{t,p}^{on,brine} \cdot C^{zld} = f_{t,p}^{on,in} \cdot c_{t,p} \qquad \forall t \in T, p \in P \tag{23}$$

Two options have been considered for TDS reduction such as MSMD and MEE-MVR. The onsite desalination treatment is also leased. Hence, onsite treatment balance is described in the following equations,

$$n_{t,p,n}^{on} = n_{t-1,p,n}^{on} + n_{t,p,n}^{on,ins} - n_{t,p,n}^{on,unins} \qquad \forall t \in T, p \in P, n \in N \tag{24}$$

where $n_{t,p,n}^{on}$ is the total number of onsite treatment leased in time period t on wellpad p using a desalination technology n, $n_{t,p,s}^{on,ins}$ and $n_{t,p,s}^{on,unins}$ represent the number of installed or uninstalled onsite treatment in a specific time period.

The number of onsite treatment leased depends on the total number of portable treatments available ($N_n^{on,UP}$).

$$N_n^{on,LO} \cdot y_{t,p,n}^{on} \le n_{t,p,n}^{on,ins} \le N_n^{on,UP} \cdot y_{t,p,n}^{on} \qquad \forall t \in T, p \in P, n \in N \tag{25}$$

Eq (26) represents the mass balance through the desalination unit,

$$f_{t,p}^{on,in} = \sum_{n \in N} f_{t,p,n}^{on,in} \qquad \forall t \in T, p \in P \tag{26}$$

The selection of the treatment unit in each time period is represented by Eq. (27). If an onsite desalination unit n is selected in time period t on wellpad p, the integer variable $n_{t,p,n}^{on}$ is equal to the number of tanks needed in time period t on wellpad p. The inlet flowrate is bounded for the maximum and minimum capacity of each treatment unit multiply by the total number of tanks leased. On the contrary, if the onsite treatment n is not needed in time period t on wellpad p, the integer variable $n_{t,p,n}^{on}$ takes the value of zero, and consequently, the inlet flowrate is also zero.

$$F_n^{on,LO} \cdot n_{t,p,n}^{on,ins} \le f_{t,p,n}^{on,in} \le F_n^{on,UP} \cdot n_{t,p,n}^{on,ins} \qquad \forall t \in T, p \in P, n \in N \tag{27}$$

The flow directions for the desalinated water are given by Eq.(28),

$$f_{t,p}^{on,out} = f_{t,p}^{on,fwt} + f_{t,p}^{on,des} + \sum_{pp \in P} f_{t,p,pp}^{pad,fwt} \qquad \forall t \in T, p \in P \tag{28}$$

where $f_{t,p}^{on,fwt}$ is the desalinated water sent to freshwater tank, $f_{t,p}^{on,des}$ is the water discharged on the surface and $f_{t,p,pp}^{pad,fwt}$ is the desalinated water used as a fracturing fluid in the same or other wellpad.

Centralized water treatment

In this section, mass balances are performed in the CWT facility. Eq. (29) shows the relationship between the inlet and outlet streams, and Eq. (30) constraints the inlet flowrate of CWT *k* with the maximum flowrate allowed.

$$f_{t,k}^{cwt,out} = \alpha_k^{rec} \cdot \sum_{p \in P} f_{t,p,k}^{cwt,in} \qquad \forall t \in T, k \in K \tag{29}$$

$$\sum_{p \in P} f_{t,p,k}^{cwt,in} \le F_k^{cwt,UP} \qquad \forall t \in T, k \in K \tag{30}$$

The freshwater mass balance at the end of CWT k is given by Eq.(31),

$$f_{t,k}^{cwt,out} = \sum_{p \in P} f_{t,p,k}^{cwt,fwt} + f_{t,k}^{cwt,des} \qquad \forall t \in T, k \in K \tag{31}$$

Sustainability profit – Objective function

The objective function, which is to be maximized, comprises the economic-profit ($p^{Economic}$), eco-cost (c^{Eco}) and social-profit (p^{Social}).

$$max : sp = p^{Economic} - c^{Eco} + p^{Social} \tag{32}$$

Economic profit consists of revenues from natural gas minus the sum of the following expenses: drilling and production cost, wastewater disposal cost, storage tank cost, freshwater cost, friction reducer cost, wastewater and freshwater transport cost and onsite and offsite treatment cost.

$$p^{Economic} = r^{gas} - (e^{drill} + e^{dis} + e^{sto} + e^{source} + e^{fr} + e^{trans} + e^{ondes} + e^{cwt} + e^{crew}) \tag{33}$$

The revenues of shale gas sales can be represented by Eq. (34),

$$r^{gas} = \sum_{t \in T} \sum_{p \in P} \sum_{w \in RPW_p} \sum_{tt=0}^{tt \le t-1} F_{t-tt,p,w}^{gas} \cdot y_{tt+1,p,w}^{fb} \cdot \alpha_t^{gas} \tag{34}$$

where $F_{t,p,w}^{gas}$ is the gas production and α_t^{gas} is the gas price forecast in time period *t*.

Drilling, completion and production cost are defined by Eq. (35),

$$e^{drill} = \sum_{t\in T}\sum_{p\in P}\sum_{w\in RPW_p}\sum_{c\in C}\alpha^{drill}\cdot y^{hf}_{t,p,w,c} + \sum_{t\in T}\sum_{p\in P}\sum_{w\in RPW_p}\alpha^{prod}\cdot f^{gas}_{t,p,w} \tag{35}$$

Disposal expenses only include the disposal costs α^{dis}_{d} which depend on the place where the class II disposal well is located,

$$e^{dis} = \sum_{t\in T}\sum_{p\in P}\sum_{d\in D}\alpha^{dis}_{d}\cdot f^{dis}_{t,p,d} \tag{36}$$

Fracturing, impaired water and freshwater tanks are typically leased, the cost is made up of leasing cost (α^{sto}_{s}) and mobilize, demobilize and cleaning cost (β^{sto}_{s}) as follows,

$$e^{sto} = \sum_{t\in T}\sum_{p\in P}\sum_{s\in S}\left(\alpha^{sto}_{s}\cdot n_{t,p,s} + \beta^{sto}_{s}\cdot n^{ins}_{t,p,s}\right) + \sum_{t\in T}\sum_{p\in P}\alpha^{im}\cdot n^{im,ins}_{t,p}\cdot V^{im} \tag{37}$$

Where α^{im} represents the cost of the impoundments construction. The freshwater cost includes the withdrawal cost from the diverse sources *f*,

$$e^{source} = \sum_{t\in T}\sum_{p\in P}\sum_{f\in F}\alpha^{source}_{f}\cdot f^{source}_{t,p,f} \tag{38}$$

The friction reducers costs are given by Eq.(39). They depend on the TDS concentration and the flowrate used for hydraulic fracturing,

$$e^{fr} = \sum_{t\in T}\sum_{p\in P}\left(\alpha^{fr}\cdot c_{t,p} + \beta^{fr}\right)\cdot f^{imp}_{t,p} \tag{39}$$

Transportation expenses by truck involve the sum of the following transfers: (1) from wellpad *p* to disposal location *d*, (2) from freshwater source *f* to wellpad *p*, (3) from wellpad *p* to offsite treatment *k*, and (4) from wellpad *p* to wellpad *pp*.

$$e^{truck} = \alpha^{truck}\cdot\sum_{t\in T}\sum_{p\in P}\left(\begin{array}{l}\sum\limits_{d\in D} f^{dis}_{t,p,d}\cdot D^{pad-dis}_{p,d} + \sum\limits_{f\in F} f^{source}_{t,p,f}\cdot D^{pad-source}_{f,p} \\ + \sum\limits_{k\in K}\left(f^{cwt,in}_{t,k} + f^{cwt,fwt}_{t,p,k}\right)\cdot D^{pad-cwt}_{p,k} \\ + \sum\limits_{pp\in P}\left(f^{pad}_{t,p,pp} + f^{pad,imp}_{t,p,pp}\right)\cdot D^{pad-pad}_{p,pp}\end{array}\right) \tag{40}$$

where $D^{pad-d}_{p,d}$, $D^{pad-sourc}_{p,f}$, $D^{pa}_{p,k}$ and $D^{pad-pad}_{p,pp}$ are the distances from wellpad *p* to disposal site *d*, source *f*, CWT facility and wellpad *pp*.

Pretreatment expenses depend on the wastewater destination. Obviously, requirements to desalinate the water in thermal treatment or membrane treatments are more restrictive than the requirements to reuse it in fracturing operations. As described in Eq. (41), α^{reuse} represents the pretreatment cost aiming its reuse, and α^{treat} the pretreatment cost aiming to remove TDS by desalination technologies. Onsite TDS removal unit cost includes desalination cost (α_n^{on}), mobilize, desmobilize and cleaning cost (β_n^{on}) and leasing cost (α_n^{on}).

$$e^{ondes} = \sum_{t \in T} \sum_{p \in P} [\alpha^{reuse} \cdot f_{t,p}^{imp} + \alpha^{treat} \cdot f_{t,p}^{on,in} + \sum_{n \in N} (\alpha_n^{on} \cdot n_{t,p,n}^{on} + \beta_n^{on} \cdot n_{t,p,n}^{on,inst})] \tag{41}$$

The CWT cost is given by Eq. (42) and it depends on the cost that the treatment plant imposes for treating the flowback water from shale gas operations (α_k^{cwt}).

$$e^{cwt} = \sum_{t \in T} \sum_{p \in P} \sum_{k \in K} \alpha_k^{cwt} \cdot f_{t,p,k}^{cwt,in} \tag{42}$$

The cost of moving crews and rigs depends if the candidate well is going to be fractured in the same or other wellpad. With that purpose, the binary variable $y_{t,p,c}^{crew}$ is equal to one if at least one well is drilled in wellpad p in time period t by crew c,

$$y_{t,p,c}^{crew} \geq \sum_{w \in RPW_p} y_{t,p,w,c}^{hf} \qquad \forall t \in T, p \in P, c \in C \tag{43}$$

$$\sum_{p \in P} y_{t,p,c}^{crew} \leq 1 \qquad \forall t \in T, c \in C \tag{44}$$

Clearly, if the fracturing crew c in time period t is on the same wellpad in time period t-1, the fracturing expenses are equal to zero.

$$e^{crew} = \sum_{t \in T} \sum_{p \in P} \sum_{c \in C} \alpha^{crew} \cdot (y_{t,p,c}^{crew} - y_{t-1,p,c}^{crew}) \tag{45}$$

Eco-cost is a robust indicator from cradle-to-cradle LCA calculations in the circular economy that includes eco-costs of human health, ecosystems, resource depletion and global warming. The terms are calculated by using eco-cost coefficients.[28] In our problem, the eco-cost term includes natural gas extraction, freshwater withdrawal, desalination, disposal and transportation. The eco-cost to be minimized is defined by Eq. (46),

$$c^{Eco} = \sum_{r\in R} \mu_r \cdot q_r + \sum_{g\in G} \mu_g \cdot q_g + \sum_{r\in R} \mu_r^T \cdot D \cdot q_r + \sum_{g\in G} \mu_g^T \cdot D \cdot q_g \tag{46}$$

where r and g are indices for raw materials and products, respectively. μ represents eco-cost of raw materials and products and μ^T is the eco-cost of transportation. All coefficients are proportional to mass flows (q).

Social profit, displayed by Eq. (47), comprises social security contributions paid for the employees to fracture a well (SS), plus the social transfer by hiring people (SU), minus social cost (SC).[24] We only contemplate the number of jobs on a fracturing crew and the working hours per employee needed to fracture a specific well. Once the well is completed, the number of jobs generated by maintenance team or truck drivers are not contemplated.

$$\begin{gathered} p^{Social} = SS + SU + SC = \\ \sum_{t\in T}\sum_{p\in P}\sum_{w\in RPW_p}\sum_{c\in C} y_{t,p,w,c}^{hf} \cdot \left[\mathrm{N}^{jobs} \cdot (S^{Gross} - S^{Net}) + \mathrm{N}^{jobs} \cdot C^{UNE,State} - \mathrm{N}^{jobs} (C^{EMP,State} + C^{Company}) \right] \cdot \tau_w^{hf} \end{gathered} \tag{47}$$

where N^{jobs} is the number of new jobs needed to fracture a well, S^{gross} and S^{net} are the average gross and net salaries paid for each employee, $C^{UNE,State}$ is the average social transfer for unemployed people, $C^{EMP,State}$ is the state social transfer (i.e child allowance, state scholarship, health insurance) and $C^{company}$ is company's social charge (i.e team building events, excursions, cultural activities).

4. SOLUTION STRATEGY

The optimization problem is modeled using total flows and salt composition as variables. This proposed MINLP model -Eqs. (1)-(47)- involves bilinear terms in the salt water mass balances: Eqs. (7), (9), (23) and (39). These terms are the source of the non-convexity in the model. An advantage of using this representation is that the bounds of the variables present in the non-convex bilinear terms can be easily determined. If local solvers are selected to solve the MINLP problem, we may converge to a local solution. Global optimization solvers can in principle be used but may not reach a solution for a large scale non-convex MINLP problems in a reasonable period of time. Thus, we propose the following decomposition strategy in order to achieve a trade-off between the solution quality vs time.

- The original MINLP is relaxed using under and over estimators of the bilinear terms, McCormick convex envelope[29], which leads to an MILP. To this aim, the bilinear terms in constraints (7), (9), (23) and (39) are replaced by the following equations. The solution of this MINLP yields an upper bound (UB) to the original MINLP.

$$\left.\begin{array}{l} s \geq c \cdot F^{LO} + C^{LO} \cdot f - C^{LO} \cdot F^{LO} \\ s \geq C^{UP} \cdot f + c \cdot F^{UP} - C^{UP} \cdot F^{UP} \end{array}\right\} Underestimators$$
$$\left.\begin{array}{l} s \leq c \cdot F^{UP} + C^{LO} \cdot f - C^{LO} \cdot F^{UP} \\ s \leq C^{UP} \cdot f + c \cdot F^{LO} - C^{UP} \cdot F^{LO} \end{array}\right\} Overstimators \qquad (48)$$

  where s is the corresponding bilinear term and flow and C^{LO}, F^{LO}, C^{UP} and F^{UP} are the lower and upper bound of salt concentrations and flows.

- The binary variables obtained in the previous MILP, that determine the fracture schedule ($y^{hf}_{t,p,w,c}$), are fixed into the original MINLP, resulting in a smaller MINLP involving the binary variables $y^{st}_{t,p,s}$ and $y^{on}_{t,p,n}$.

The mathematical model is implemented in GAMS 25.0.1.[30] The relaxed MILP problem is solved with Gurobi 7.5.2[31] and the MINLP problem with DICOPT 2[32] using CONOPT 4[33] to solve the NLP sub-problems. DICOPT cannot guarantee a global solution, however, we calculate the optimality gap, defined by Eq. (49), to obtain the deviation of this solution with respect to the global optimum,

$$gap = \frac{UB - LB}{UB} \tag{49}$$

The relaxed MILP problem has 3,273 binary variables, 21,373 continuous variables and 20,600 constraints. In the reduced non-convex MINLP, the binary variables decrease to 2,337 by using the solution of the relaxed MILP problem that provides the fracturing schedule for the non-convex MINLP. The reduced non-convex MINLP has 14,607 continuous variables and 9,361 constraints. The model has been solved on a computer with a 3 GHz Intel Core Dual Processor and 4 GB RAM running Windows 10.

5. CASE STUDIES

The case studies shown in Table 1 based on Marcellus Play illustrate the capabilities of the proposed optimization model. They are composed by 20 wells grouped in 3 wellpads, one year discretized at one week per time period, three Class II disposal wells, four interruptible sources of freshwater, two CWT plants and one fracturing crew. The difference between interruptible sources, disposal wells and CWT plants lies in the geographical location. Data of the problem -cost coefficients and model parameters- are given in Supporting Information (Tables S.1-S.4). Gross and net salaries paid for each employee are obtained from the Bureau of Labor Statistics.[34] Our goal is to determine the optimal planning solution from well drilling and construction to the end of flowback water generation. Therefore, we consider the natural gas production and wastewater generated in the first twelve weeks, which is the critical period for shale gas water management. In this phase, the coordination among different contractors is crucial since the water is recovered in a short time period. In this work, we assume that 50% of the water used to fracture a well (water demand per well), which ranges from 4,800 to 18,600 m^3, is recovered as flowback water. Additionally, we consider that the TDS concentration depends on each well and increases with time ranging from 3,000 to 200,000 ppm.

Table 1. Case studies description

Case study	**Description**
Case 1	All water management options are allowed: reuse the flowback water with a ligth treatment, desalinate the water in onsite treatment or CWT facility, reuse the desalinated water as a fracturing fluid and disposal in class II disposal wells.
Case 2	Disposal in class II disposal wells is the only water management option allowed.
Case 3	Wastewater can be sent to onsite desalination treatment or CWT facility.
Case 4	The highest estimated cost for friction reducers is assumed for the whole range of salinity concentrations. Thus Eq. (39) is replaced by: $E^{fr} = \sum_{t \in T} \sum_{p \in P} \gamma^{fr} \cdot f^{imp}_{t,p}$ (50)
Case 5	All water management options, as in Case 1, are permitted. However, return to pad-operations is not allowed and wells are fractured in order; well 2 cannot be fractured before well 1. Accordingly, the following constraint is added: $\sum_{t \in T} t \cdot y^{hf}_{t,p,w,c} \le \sum_{t \in T} t \cdot y^{hf}_{t,p,ww,c} \qquad w < ww, \forall w \in RPW_p, p \in P$ (51)

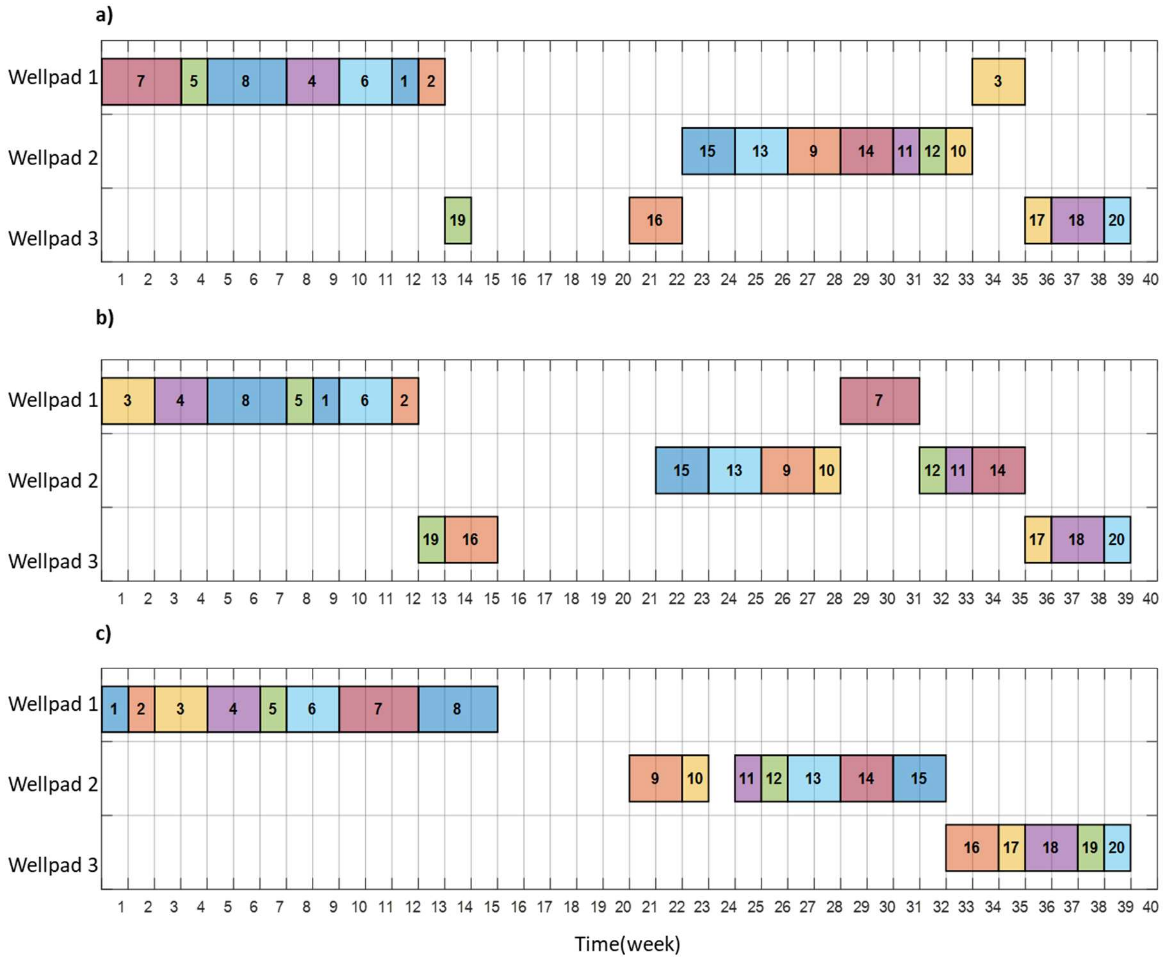

Figure 2. Fracturing schedule obtained after economic, social and environmental optimization of the shale gas planning model: (a) Case 1; (b) Cases 2,3 and 4; (c) Case 5.

For each case study, the optimal fracturing schedule and the sustainability profit, which is a weighted sum of three objectives eco-cost, social-profit and economic-profit, are shown in Figure 2 and Table 2, respectively. It should be mentioned that all wells are fractured before time period forty starts to allow that all the flowback water is considered by the model. Figure 2 highlights that the same fracturing schedule is obtained for Cases 2, 3 & 4, where the economic-profit, driven by the maximization of shale gas revenues, controls the sustainability profit. In Case 1, the fracturing schedule maximizes the total water reused for fracturing purposes, reducing the eco-cost to \$17,490k and increasing the economic-profit (due to cost reduction is greater than revenues decrease) to \$16,909k, which is the lowest of the five cases (see Table 2). Therefore, in this case, the water management selected is direct reuse to fracture other wells, and once all wells been fractured, the wastewater is desalinated in onsite treatments.

Additionally, although the cost of moving a fracturing crew from one wellpad to another is significant, the optimal facturing schedule (Figure 2) reveals that raising the number of these movements increase the sustainability profit (Table 2). For example, in the optimal fracturing schedule for Case 1, fracturing crew moves from wellpad 1 to wellpad 3, before fracturing all wells belonging wellpad 1, and again, before wellpad 2 completion, fracturing crew travel from wellpad 3 to 2 (in total there 4 transitons). The underlying logic for this unexpected crew's shift schedule are twofold: the shale gas price forecast and the well gas production.

Table 2. Contribution of each objective (eco cost, social profit and economic profit) to the weighted average objective (sustainability profit, k$).

	Case 1	**Case 2**	**Case 3**	**Case 4**	**Case 5**
Sustainability profit	840	-16,325	- 57	709	-1,629
Eco-cost	17,490	22,584	17,599	17,502	17,495
Social-profit	1,421	1,421	1,421	1,421	1,421
Economic-profit	16,909	4,838	16,120	16,789	14.444
Gap MILP-MINLP (%)	0.86	1.99	4.21	0.36	0.86

Reusing the flowback water for subsequent fracturing requires to add costly friction reducers. However, we can realize comparing the results obtained of Case 2&3 vs Case 1 (see Table 3) that reusing the wastewater yields large savings in freshwater transportation cost, and treatment and withdrawal cost of the impaired water. It is important to highlight that although 90,580 m^3 of impaired water is reused, freshwater is still necessary (132,720 m^3) as the flowback only represents 50% of the water injected into the well. Figure 3 shows the freshwater and impaired water used for each case study.

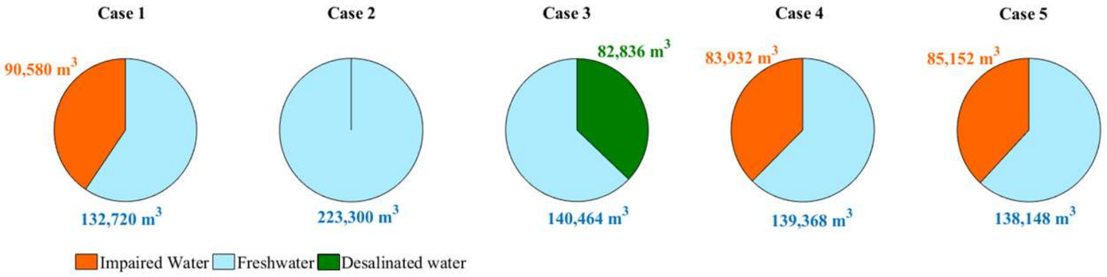

Figure 3. Total impaired water and freshwater used for all case studies.

In Case 4, where the friction reducers cost assumed is the highest, the impaired water used as fracturing fluid decreases by 7.3 % with respect Case 1. This fact highlights the influence of the cost of friction reducers in the planning decisions. In addition, the suitanibility profit for Case 4 ($709k) decreases by 13% with respect Case 1. However, the former is a viable solution (i.e., a positive sustanbility profit) among economic, environmental and social criteria. As Case 4 was designed at the worst case (i.e., the highest friction reducer cost), an additional benefit of its solution is that exhibits a good performance even if the concentration of TDS would increase due to the use of impaired water over the time, which implies a higher fiction reducer cost.

In case studies 2, 3 & 5, a compromise solution is not found. Therefore, the sustainability profit is negative, and no wells should be fractured. Nevertheless, in these cases, we enforce that all wells must be fractured at the end of the time period in order to compare the results obtained with case studies 1 & 4.

In Case 2, where the only water management option considered is water disposal, is the worst scenario studied, being the sustainability profit equal to - \$16,325k. Both eco and economic costs are too high compared with other case studies. Hence, the results highlight that injecting wastewater into Class II disposal wells should be excluded for wells based on Marcellus play. When only desalination is allowed (Case 3), both economic-cost and eco-cost decrease significantly compared with Case 2. However, sustainability profit still remains negative equal to - \$57k. In this case, part of desalinated water is reused to fracture other wells. This allows important economic and environmental savings in transportation and water withdrawal. Finally, it is interesting to mention that in Case 5, where the fracturing schedule is restricted to be sequential, is the second worst scenario. Although the wastewater reused (85,152 m^3) is close to the impaired water of the first scenario (90,580 m^3), the revenue obtained from natural gas decreases 9% compare with the revenue obtained from Case 1. This result clearly shows the dependency of the fracturing schedule on the price and production forecast of natural gas.

It should be noted that in all cases, water-related costs range from 5 to 13% of the revenue of shale gas production. Figure 4 displays the percentage contribution of each water-related cost (additives, freshwater withdrawal, disposal, storage, transportation, and desalination) of the total water cost and Table 3 details economic-cost and eco-cost of each case study. Regarding economic criterion, the cost of drilling and production for Cases 1, 3, 4 & 5 represent the highest contribution of the total cost, and in Case 2, the disposal cost is the highest one (\$10,165k). Regarding the environmental criterion, the eco-cost of natural gas production is equal to \$17,375k, which is significantly higher than the others eco-cost calculated (see Table 3).

Table 3. Detailed description of Economic-cost and Eco-cost from the five case studies (k$).

		Case 1	**Case 2**	**Case 3**	**Case 4**	**Case 5**
Economic-cost	Cost moving crew	415	498	498	498	249
	Cost drilling and production	9,523	9,523	9,523	9,523	9,523
	Cost friction reducers	167	0	0	252	157
	Cost freshwater acquisition	262	472	291	271	269
	Cost disposal	0	10,165	0	0	0
	Cost storage	370	457	666	381	289
	Cost transport	833	2,903	811	857	784
	Cost onsite-treatment	243	0	900	293	280
	Cost CWT	0	0	47	0	0
Eco-cost	Eco-cost freshwater acquisition	28	50	31	29	30
	Eco-cost disposal	0	4,931	0	0	0
	Eco-cost desalination	22	0	129	30	29
	Eco-cost natural gas production	17,375	17,375	17,375	17,375	17,375
	Eco-cost transportation	66	228	64	67	62

Transportation cost decreases reusing the wastewater to fracture other wells (see Table 3 Cases 1, 4 & 5 vs Cases 2 & 3). However, it still represents a high contribution to the final economic and environmental water-related cost (see Figure 4). Except from Case 2, which disposal constitute the highest eco and economic percentage, transportation represents around 45% of the total water-related economic-cost, and around 80-60% of the eco-cost.

Other authors include transportation of freshwater via pipelines to avoid impacts such as road damages, traffic accidents and CO_2 emissions.[13,16] Nevertheless, in this work, we only consider truck hauling since it provides enough flexibility to guarantee freshwater supply without the uncertainty of pipelines construction permits.

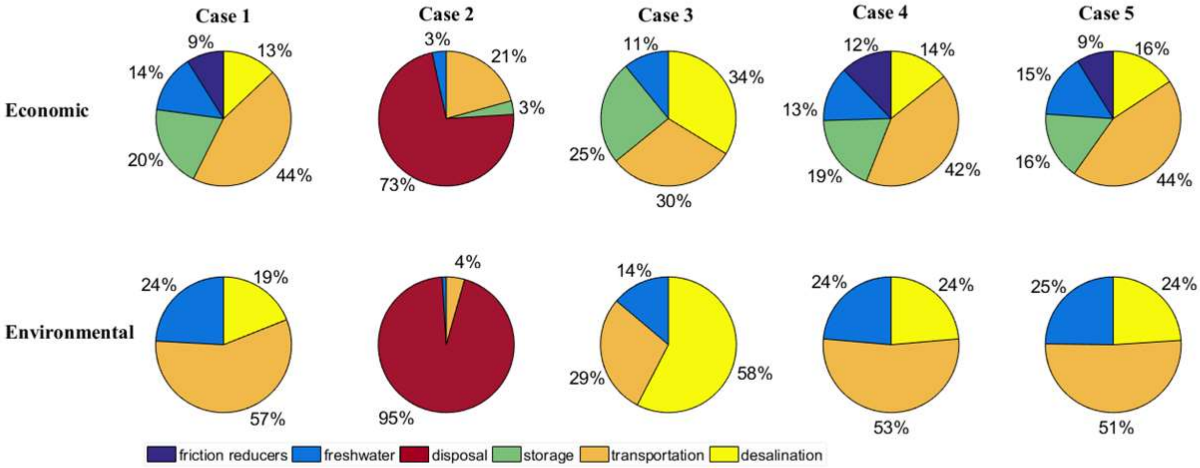

Figure 4. Comparison of all cases of the contribution percentage of each economic and environmental cost of the total water-related cost.

Despite the concern over the usage of freshwater for well fracturing, economic-cost and eco-cost of water withdrawal only represent around 15% of the total water-related cost. However, it is important to take into consideration that freshwater withdrawal is an issue in water-scarce areas, where the water demand is high. In these areas, producers must deal with higher water withdrawal cost, environmental impact and with the competition to gain water withdrawal permits.

The results obtained also provides a realistic cost storage estimation. We rigorously calculate the number of tanks leased in each time period considering installing, uninstalling, clean out and leasing costs. Figure 5 displays, for Case 1, the number of fracturing tanks and freshwater tanks leased over the time for each wellpad. Simplifying the storage solution and considering that the maximum capacity needed is available from the first to the last time period, as other authors have assumed[13,18], the storage cost increases by 53%, changing the planning decisions. Note that once the storage tanks are installed, it is more profitable to pay the leasing cost of the storage until all the wells belonging to the wellpad p have been fractured than install and uninstall them over the time. For example, see wellpad 3 in Figure 2 (a), where well 19 and 16 are fractured in time period 13 and 20, and wells 17, 18 and 20 in time period 35, 36 and 38. That means that freshwater tanks would not be required from time period 20 to 35, however, they remain installed.

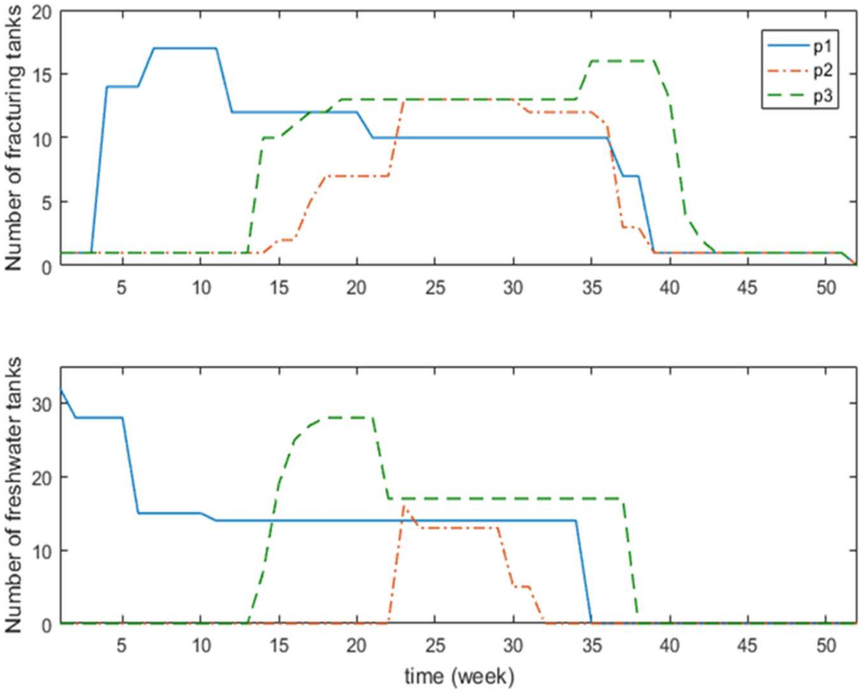

Figure 5. Number of fracturing tanks and freshwater tanks leased over the time for each wellpad in case study 1.

6. CONCLUSIONS

An MINLP mathematical model has been proposed accounting for economic, environmental and social objectives in shale gas production, considering the TDS concentration of flowback and impaired water. The sustainability profit, a new weighted sum objective expressed in monetary value, helps the decision-makers towards more economic and sustainable decisions. The goal is to maximize this objective function to find a compromise solution among the three pillars of sustainability: the economic-profit, the eco-cost and the social-profit. The economic indicator includes revenue from natural gas and cost related to drilling and production, storage, freshwater withdrawal, friction reducer, transportation, disposal and treatment. The environmental indicator takes into consideration cost of transportation, treatment, disposal, water withdrawal and shale gas extraction. Finally, the social indicator includes social security contributions, social effects due to the new jobs created and social cost.

This work also includes a study of the effect of friction reducers cost as a function of TDS concentration to determine if reusing impaired water is a cost barrier. Additionally, the rigorous calculation of storage solution permits operators to know the number of tanks that should be leased in each time period, and hence, it provides a more realistic cost storage estimation.

To solve the non-convex MINLP model effectively we use a decomposition technique. First, the original problem is relaxed using McCormick convex envelopes obtaining a relaxed MILP. Then, the fracturing schedule is fixed, and the reduced MINLP is solved. The multi-objective problem is solved using the weighted sum method saving time efforts. In this sense, there is no need to solve the large problem many times (a exponential increase with the number of objectives), which is required to obtain a Pareto frontier in a 3-dimensional space.

We apply our model to different case studies based on Marcellus Play. Different assumptions are analyzed in each case study to gain a clear understanding of the nature of the problem. The results reveal that reusing flowback water is compulsory to obtain a compromise solution among the three pillars of sustainability: economic, environmental and social criteria. Furthermore, the solution unveils that the level of TDS in reused water is not an obstacle to use it as fracturing fluid in shale gas operations, although the concentration increases over the time, and consequently the cost of the friction reducers. Regarding the wastewater management alternatives, it has been also shown that onsite desalination is the most cost-effective once water demand for fracturing new wells would be less than the volume of water produced by active wells. Finally, it should be noted that transportation is the highest water-related contribution to both economic and environmental impacts.

It is worth mentioning that the results obtained provide realistic planning decisions for the particular cases studies analyzed in this work. Nevertheless, shale gas water management decisions are highly dependent on local regulations, geographical location of the basin and local shale rock formation characteristics. For example, in Australia, where shale gas reservoirs are in remote dry locations, disposal in evaporation ponds might be economic and sustainable. Therefore, in this situation maybe there is no interest in treat the water. In an eventual shale gas exploitation in Europe, the class II disposal is likely to be forbidden and the sites will be close to populated areas. A policy of wastewater direct reuse and desalination treatment will be mandatory in order to reduce costs, environmental impacts and gain a favorable public perception (social impact). To sum up, the mathematical model proposed would be a useful and robust tool, which would help to take the best decisions under different circumstances.

SUPPORTING INFORMATION

Input data used in the case study: cost coefficients, model parameters, eco-cost and social coefficients.

ACKNOWLEDGMENTS

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NOMENCLATURE

Parameters

$C_{t,p,w}^{well}$	Concentration of flowback water forecast for well w on wellpad p in time period t, kg·kg^{-1}
C^{con}	Outlet salinity for desalination treatments, kg·kg^{-1}
CST_s	Capacity of storage tank s, m^3
$D_{p,d}^{pad-dis}$	Distance from wellpad p to disposal well d, km
$D_{f,p}^{pad-source}$	Distance from source f to wellpad p, km
$D_p^{pad-off}$	Distance from wellpad p to offsite-treatment, km
$D_{p,pp}^{pad-pad}$	Distance from wellpad p to wellpad pp, km
$F_{t,p,w}^{well}$	Flowback water forecast for well w on wellpad p in time period t, m^3·week^{-1}
$F_n^{on,UP}, F_n^{on,LO}$	Maximum and minimum onsite capacity for treatment wt, m^3·week^{-1}

$F_k^{cwt,UP}$	Maximum centralize water treatment capacity k, $m^3 \cdot week^{-1}$
$F_{t,p,w}^{gas}$	Production gas flow forecast for well w on wellpad p in time period t, $m^3 \cdot week^{-1}$
N_s^{UP}, N_s^{LO}	Upper and lower bound of tanks s installed
$N^{im,UP}, N^{im,LO}$	Upper and lower bound of impoundments installed
$N^{on,UP}, N^{on,LO}$	Upper and lower bound of onsite treatment leased
V^{im}	Capacity of an impoundment, m^3
WD_w	Water demand of well w, m^3
τ_w	Time to fracture well w, week
α^{pre}	Pretreatment recovery factor
α^{rec}	Centralized water treatment recovery factor
α^{drill}	Drilling and completion cost, $
α^{prod}	Shale gas production cost, $\$ \cdot m^{-3}$
α_d^{dis}	Disposal coefficient cost coefficient for disposal d, $\$ \cdot m^{-3}$
α_s^{sto}	Storage leasing cost coefficient for storage tank s, $\$ \cdot week^{-1} \cdot tank^{-1}$
α^{im}	Impoundment construction cost, $\$ \cdot m^{-3}$
α_f^{source}	Freshwater cost coefficient in freshwater source f, $\$ \cdot m^{-3}$
α^{fr}	Friction reducer cost coefficient, $\$ \cdot m^{-3}$
α^{truck}	Trucking cost coefficient, $\$ \cdot km^{-1} \cdot m^{-3}$
α^{reuse}	Pretreatment cost coefficient aiming its reuse, $\$ \cdot m^{-3}$
α^{treat}	Pretreatment cost coefficient aiming its desalination, $\$ \cdot m^{-3}$
α^{crew}	Cost of moving crews, $

α_n^{on}	Onsite desalination cost coefficient for treatment n, $·m^{-3}
α_k^{cwt}	Cost coefficient of centralized water treatment k, $·m^{-3}
α_t^{gas}	Natural gas price forecast in time period t, $·m^{-3}
β_s^{sto}	Mobilize, demobilize and cleaning cost coefficient for storage tank s, $
β^{fr}	Friction reducer cost coefficient, $
β_n^{on}	Maintenance cost coefficient for onsite desalination treatment n, $
γ^{fr}	Overestimated cost of friction reducers, $·m^{-3}

Integer variables

$n_{t,p,s}$	Number of tank type s on wellpad p on time period t
$n_{t,p,s}^{ins}$	Number of tank type s installed on wellpad p on time period t
$n_{t,p,s}^{unis}$	Number of tank type s uninstalled on wellpad p on time period t
$n_{t,p}^{im}$	Number of impoundments on wellpad p on time period t
$n_{t,p}^{im,ins}$	Number of impoundments installed on wellpad p on time period t
$n_{t,p,n}^{on}$	Number of onsite treatment n on wellpad p on time period t
$n_{t,p,n}^{on,ins}$	Number of onsite treatment n installed on wellpad p on time period t
$n_{t,p,n}^{on,unis}$	Number of onsite treatment n uninstalled on wellpad p on time period t

Binary variables

$y_{t,p,w,c}^{hf}$	Indicates if well w on wellpad p is stimulating using fracturing crew c in time period t
$y_{t,p,s}^{st}$	Indicates if storage tank type s are installed on wellpad p in time period t
$y_{t,p,n}^{on}$	Indicates if onsite treatment n is used on wellpad p in time period t

$y_{t,p,c}^{crew}$	Indicates if at least one well is drilled in wellpad p in time period t with fracturing crew c

Variables

$c_{t,p}^{pad}$	Salt concentration on wellpad p in time period t, kg·kg^{-1}
$c_{t,p}$	Salt concentration in fracturing tanks on wellpad p in time period t, kg·kg^{-1}
$c_{t,p}^{i}$	Salt concentration of the inlets flows in fracturing tanks on wellpad p in time period t, kg·kg^{-1}
e^{drill}	Drilling and production expenses, $
e^{dis}	Disposal expenses, $
e^{sto}	Storage freshwater and wastewater expenses, $
e^{source}	Freshwater acquisition expenses, $
e^{fr}	Friction reducer expenses, $
e^{trans}	Transport expenses, $
e^{ondes}	Onsite treatment expenses, $
e^{cwt}	Centralized water treatment expenses, $
e^{drill}	Drilling and production expenses, $
e^{crew}	Moving crew expenses, $
$f_{t,p,w}^{well}$	Flowrate of produced water on well w wellpad p in time period t, m^3·week^{-1}
$f_{t,p}^{pad}$	Flowrate of produced water on wellpad p in time period t, m^3·week^{-1}
$f_{t,p}^{pre,in}$	Onsite pretreatment inflow in wellpad p in time period t, m^3·week^{-1}
$f_{t,p,f}^{source}$	Flowrate of freshwater from natural source f to wellpad p in time period t, m^3·week^{-1}

$f_{t,p}^{on,fwt}$	Flowrate of desalinated water from onsite treatment to freshwater tanks in wellpad p in time period t, $m^3 \cdot week^{-1}$
$f_{t,pp,p}^{pad,fwt}$	Flowrate of desalinated water from wellpad pp to freshwater tanks in wellpad p in time period t, $m^3 \cdot week^{-1}$
$f_{t,p}^{on,des}$	Flowrate of freshwater used in hydraulic fracturing in wellpad p in time period t, $m^3 \cdot week^{-1}$
$f_{t,p}^{imp}$	Flowrate of impaired water used in hydraulic fracturing in wellpad p in time period t, $m^3 \cdot week^{-1}$
$f_{t,p}^{dem}$	Flowrate of water demand in wellpad p in time period t, $m^3 \cdot week^{-1}$
$f_{t,p}^{pre,out}$	Onsite pretreatment outflow in wellpad p in time period t, $m^3 \cdot week^{-1}$
$f_{t,p}^{on,slud}$	Slud flowrate after onsite desalination process in wellpad p in time period t, $m^3 \cdot week^{-1}$
$f_{t,p}^{on,in}$	Onsite desalination inflow in wellpad p in time period t, $m^3 \cdot week^{-1}$
$f_{t,p}^{on,out}$	Onsite desalination outflow in wellpad p in time period t, $m^3 \cdot week^{-1}$
$f_{t,p,d}^{on,brine}$	Brine flowrate after onsite desalination process in wellpad p in time period t, $m^3 \cdot week^{-1}$
$f_{t,p}^{on,fresh}$	Flowrate of desalinated water from onsite treatment on wellpad p in time period t sent to discharge, $m^3 \cdot week^{-1}$
$f_{t,k}^{cwt,in}$	Inlet flow in centralized water treatment k in time period t, $m^3 \cdot week^{-1}$
$f_{t,k}^{cwt,out}$	Outlet flow in centralized water treatment k in time period t, $m^3 \cdot week^{-1}$

$f_{t,p,k}^{cwt,fwt}$	Desalinated water from centralized water treatment k to freshwater tank on wellpad p in time period t, $m^3 \cdot week^{-1}$
$f_{t,k}^{cwt,des}$	Desalinated water from centralized water treatment k to discharge in time period t, $m^3 \cdot week^{-1}$
$f_{t,p,s}^{i}$	Outlet flow in tank s in wellpad p in time period t, $m^3 \cdot week^{-1}$
$f_{t,p,s}^{o}$	Inlet flow in tank s in wellpad p in time period t, $m^3 \cdot week^{-1}$
r^{gas}	Total gas revenue, \$
$st_{t,p,s}$	Level of water in tank type s on wellpad p in time period t, m^3
$y_{t,p,w}^{fb}$	Indicates when the water starts to come out on well w on wellpad p in time period t

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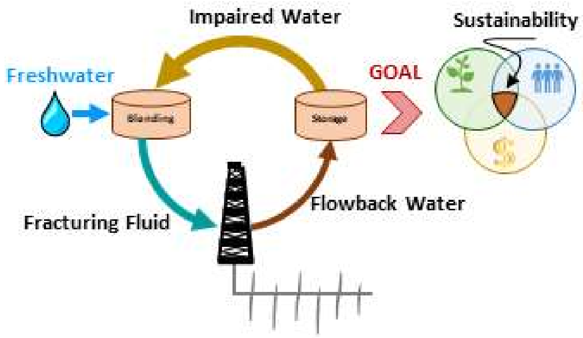
Table of Contents Graphic



Supporting Information

The following tables (Tables S.1-S.4) details the parameters used in the mathematical model for the case study: cost coefficients, model parameters, eco-cost and social coefficients.

Table S.1. Costs coefficient

Parameter	Value	Units	Ref
Drilling cost (α^{drill})	270,000	\$	1
Production cost (α^{prod})	0.014	\$/m^3	1
Disposal cost (α_d^{dis})	90 - 120	\$/m^3	2
Truck cost (α^{truck})	0.15	\$/km/m^3	2
Storage cost (α_s^{sto})	70	\$/week/tank	*
Impoundment cost (α^{im})	3.86	\$/m^3	3
Pretreatment cost ($\alpha^{reuse}, \alpha^{treat}$)	0.8 - 2	\$/m^3	4
Desalination cost (α_n^{on})	6 - 15	\$/m^3	5,6
Demobilize, mobilize and clean out cost (β_n^{on})	2,000	\$/week	*
Centralized water treatment (α_k^{cwt})	42 - 84	\$/m^3	2
Demobilize, mobilize and clean out cost (β_s^{sto})	1,500	\$	*
Friction reducer cost (α^{fr})	0.18 - 0.30	\$/m^3	*
Freshwater withdrawal cost (α_f^{source})	1.76 - 3.5	\$/m^3	3
Moving crew cost (α^{crew})	83,000	\$	*

*Provided by a company

Table S.2. Model parameters

Parameter	Value	Units	Ref
CST_s	60	m^3	*
$C_{t,p,w}^{well}$	3,000 - 200,000	ppm	[7]
C^{con}	300	g kg^{-1}	[5]
$F_n^{on,UP}$	4,000	m^3 week^{-1}	*
$F_k^{cwt,UP}$	16,700	m^3 week^{-1}	*
N_s^{UP}	100	-	*
$N^{im,UP}$	3	-	*
$N_n^{on,UP}$	3	-	*
V^{im}	120	m^3	*
WD_w	4,800 - 18,600	m^3 week^{-1}	[7]
τ_w	1-5	weeks	[7]

*Provided by a shale gas company

Table S.3. Eco-cost coefficients [8]

Raw material (μ_r)	**Eco-cost**	**Interpretation**
Freshwater	0.19 € m^{-3}	water scarcity
Products (μ_g)	**Eco-cost**	**Interpretation**
Desalinated water to discharge	1 € m^{-3}	Water from drilling is treated and returned to natural resource
Desalinated water to reuse	1 € m^{-3}	Water from drilling is treated and used for new drilling operations
Disposal water	37 € m^{-3}	Disposal
Natural gas at extraction	0.05 € m^{-3}	Natural gas extraction
Transport (μ_g^T, μ_r^T)	**Eco-cost**	**Interpretation**
Transport	0.01 € m^{-3} km^{-1}	Truck plus container

Table S.4. Social coefficients

Parameter	**Value**	**Units**	**Ref**
N^{jobs}	145	-	[9]
S^{Gross}	857	\$ $week^{-1}$	[10]
S^{Net}	685	\$ $week^{-1}$	[10,11]
$C^{UNE,State}$	125	\$ $week^{-1}$	[12]
$C^{EMP,State}$	12.5	\$ $week^{-1}$	[12]
$C^{company}$	6.5	\$ $week^{-1}$	[12]

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