Sustainable Optimal Strategic Planning for Shale Water Management

Alba Carrero-Parreño[a], Juan A. Reyes-Labarta*[a,b], Raquel Salcedo-Díaz[a,b], Rubén Ruiz-Femenia[a,b], José A. Caballero[a,b], Ignacio E. Grossmann[c]

[a]*Institute of Chemical Process Engineering, University of Alicante, Ap Correos 99, Alicante 03080, Spain*
[b]*Department of Chemical Engineering, University of Alicante, Ap Correos 99, Alicante 03080, Spain*
[c]*Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, U.S.A.*

**** Corresponding author at.** Institute of Chemical Process Engineering, University of Alicante, Ap Correos 99, Alicante 03080, Spain. Phone: +34 965903867. ja.reyes@ua.es*

ABSTRACT

In this work, we introduce a non-convex MINLP optimization model for water management in shale gas production. The superstructure includes direct reuse in the same or neighboring wellpads, treatment in mobile units and in centralized water treatment (CWT) facility, and transport to Class II disposal wells. We consider four different water qualities: flowback water, impaired water, desalinated water and freshwater. Additionally, water blending ratios are unrestricted and friction reducers expenses are calculated accounting for impaired water contamination. The objective is to optimize the fracturing schedule, the number of tanks needed at each time period, flowback destination (reuse, treated or disposal), and fracturing fluid composition by maximizing the "sustainability profit". The problem is tackled in two steps. First, we solve an MILP model based on McCormick relaxations. Second, a smaller MINLP is solved in which the binary variables that determine the fracturing schedule are fixed. The capabilities of the proposed mathematical model are validated against several case studies based on Marcellus Shale play.

INTRODUCTION

Natural gas production worldwide is expected to increase 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 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 of a shale gas well includes exploration, wellpad construction, well drilling, well treatment and completion, and production. The largest volume of water used is during well treatment and completion where 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 fluids typically contain about 90% water, 9% propping agent and less than 1% of friction-reducing additives.[3,4] After the well is hydraulically fractured, the pressure of the wellhead is released allowing a portion of wastewater, called *flowback* water, return to the wellhead. Flowback 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 *produce water*. The TDS concentration in long-term produce water can reach 250,000 mg L^{-1}. Both wastewater volume and concentration of TDS is uncertain and varies 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 produce water.[3]

Current water management strategies include disposal of wastewater via Class II disposal wells, transfer to a centralized water treatment facility (CWT) or direct reuse in drilling the subsequent wells. The reused flowback is called *impaired water*. This water management strategy has been possible due to the development of salt-tolerant friction reducers.[3,5,6] 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.[7] Moreover, this practice has the potential to decrease the environmental issues associated with shale gas water management such as transportation, disposal or treatment. However, the cost of friction reducers increases 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.

Several works have been reported on the optimization of shale gas water management. Yang et. al[8] proposed a discrete-time two-stage stochastic mixed-integer linear programming model to determine - in short-term operations - the optimal fracturing schedule and transportation, storage, treatment and disposal cost under uncertain availability water. The model does not account for TDS concentration. They developed an extended model [9] 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[10] used the Yang et. al model[9] 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[11] 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[12] 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.[13] presented an optimization framework that integrates water management and the design and planning of the shale gas supply chain. 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[14] 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[15] also developed an MILP mathematical programming formulation accounting for economics by minimizing the cost for the freshwater, treatment, storage, disposals, and transportation, and minimizing freshwater usage and wastewater discharge as an environmental objectives. However, in both works the schedule is fixed in advance, and the wastewater is always treated. Recently, Drouven and Grossmann[16] 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 account for other water management strategies nor the salt concentration of impaired water.

This paper focuses on overcoming some of the limitations of the previous papers cited above. Specifically, we propose a 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 this work comprise: (a) estimation of friction reducers expenses as a function of TDS concentration to determine if the level of TDS in impaired water is an impediment for reusing it in fracturing operations; (b) distinction of four types of water: impaired water, flowback water, desalinated water and freshwater; and (c) rigorous handling at storage solution by determining the required number of tanks installed/uninstalled over the time period.

The objective of the proposed model is to maximize the “sustainability profit”[17] in order to obtain a compromise solution between economic, environmental and social aspects. The advantage of this metric is that multi-objective optimization can be reduced to a single-objective since all the indicators are expressed in monetary terms.

The rest of the paper is organized as follows: Section 2 describes the problem statement. In section 3, the mathematical MINLP model is described in detail. In section 4, the modeling and solution strategy are described. The results obtained from different case studies based on Marcellus play are presented in section 5. Finally, the last section summarizes the conclusions of the present work.

PROBLEM STATEMENT

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

- A set of shale gas wells belonging 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 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 problem is to determine: wellpad fracturing start date (fracturing schedule), number of tanks leased at each time period, flowback destination (reuse, treatment or disposal), and type and location of onsite desalination treatment at each time period.

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

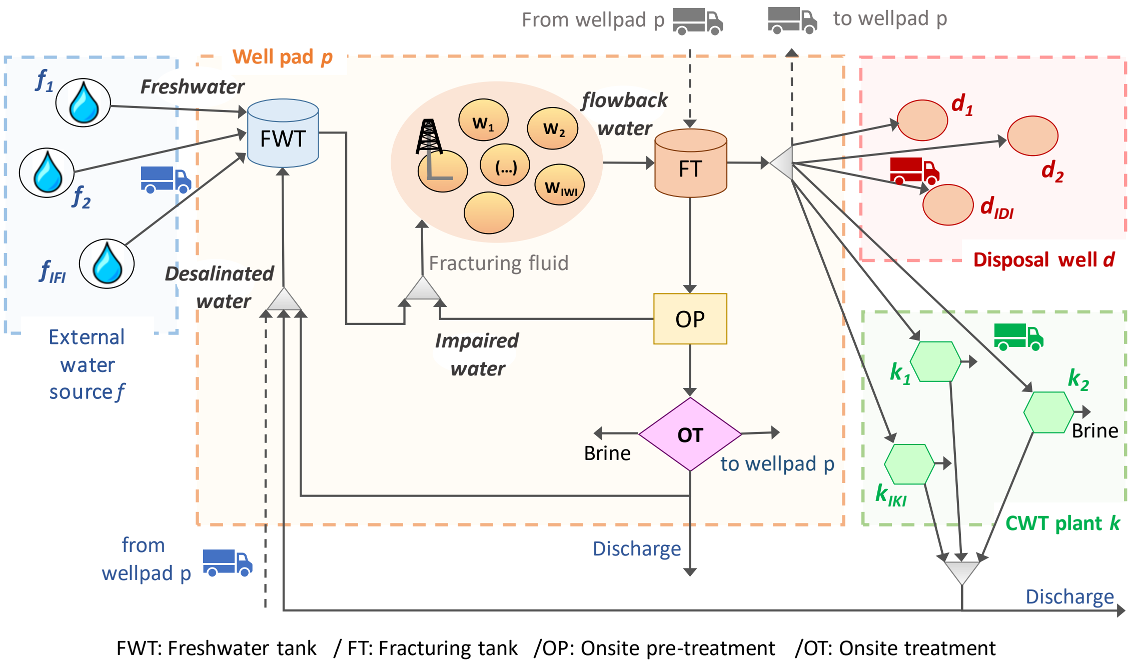

Figure 1. General superstructure of shale gas water management operations.

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

As commented before, after hydraulic fracturing, a portion of the water called *flowback water* returns to the wellhead. The flowback water is stored onsite in fracturing tanks (FT) before basic treatment (pre-treatment) in mobile units, or else transported to CWT facility, Class II disposal, or to a neighboring wellpad. Pre-treatment includes technologies to remove suspended solids, oil and grease, bacteria and certain ions that can cause the scale to form on equipment and interfere with fracturing chemical additives.[18] After pre-treatment, the water can be used directly as a fracturing fluid in the same or neighboring wellpad, or it can be desalinated in the onsite TDS removal technologies.

Two desalination technologies can be selected such as multi-stage membrane distillation (MSMD)[19] and multi-effect evaporation with mechanical vapor recompression (MEE-MVR)[20,21]. We consider that the outflow brine salinity in the onsite treatment is close to salt saturation conditions to achieve zero liquid discharge (ZLD) operation, maximizing at the same time the recovered freshwater. Costs restrict the type of desalination unit that can be used for TDS removal. The onsite desalinated water can also be used as a fracturing fluid in the same wellpad, transported to the next wellpad, or discharged for other uses. The flowback water can also be transported and treated in CWT plants. Desalinated water from CWT plants can select the same routes as the desalinated water in onsite technologies. Natural freshwater is obtained from an uninterruptible freshwater source. Desalinated water and natural freshwater are stored in freshwater tanks (FWT) and/or water impoundment.

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.

MATHEMATICAL PROGRAMMING MODEL

The optimization problem is formulated as an MINLP model that includes: assignment constraints, material balance in storage tanks, mixers and splitters, logic constraints, and an objective function. The mathematical problem is detailed below.

Set definition

The following sets are defined to develop the MINLP model.

$P = \{ p \,/\, p \text{ is a wellpad} \}$

$W = \{ w \,/\, w \text{ is a well} \}$

$T = \{ t \,/\, t \text{ is a time period} \}$

$N = \{ n \,/\, n \text{ is a onsite water treatment} \}$

$K = \{ k \,/\, k \text{ is centralized water treatment plant} \}$

$F = \{ f \,/\, f \text{ is a freshwater source} \}$

$C = \{ c \,/\, c \text{ is a fracturing crew} \}$

$D = \{ d \,/\, d \text{ is a disposal} \}$

$S = \{ s \,/\, s \text{ is a storage tank type} \}$

$RPW_p = \{ w \,/\, w \text{ is a well in wellpad p} \}$

Assignment constraint

Eq. (1) ensures that at the time horizon each well can be fractured 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) guarantees that there is no overlap in the hydraulic fracturing operations between different wells,

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

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 hydraulically fractured, a portion of the water injected is returned to the wellhead,

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

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 since its integrality is enforced by constraint (3).

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 at week, respectively.

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

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

$$c^{pad}_{t,p} \cdot f^{pad}_{t,p} = \sum_{w \in RPW_p} C^{well}_{t,p,w} \cdot F^{well}_{t,p,w} \qquad \forall t \in T, p \in P \tag{7}$$

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 the storage tank s, and the mass flowrates of the outlet streams belonging the storage tank *s*.

$$st_{t-1,p,s} + \sum_{i \in IS} f^{i}_{t,p,s} = st_{t,p,s} + \sum_{o \in OS} f^{o}_{t,p,s} \quad \forall t \in T, p \in P, s \in S \tag{8}$$

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

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

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,

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

where $n_{t,p,s}$ is the total number of tanks, $n^{ins}_{t,p,s}$ and $n^{unins}_{t,p,s}$ 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. As the time horizon is discretized into weeks, the storage tank should handle the inlet water that comes from one day. Therefore, $\theta_{t,p,s}$ represents the inlet water in the storage tank divided by the number of days in a week to avoid oversizing the tanks,

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

$$N^{LO}_{s} \cdot y^{st}_{t,p,s} \le n^{ins}_{t,p,s} \le N^{UP}_{s} \cdot y^{st}_{t,p,s} \qquad \forall t \in T, p \in P, s \in S \tag{12}$$

N^{LO}_{s} and N^{UP}_{s} are lower and upper bounds of the number of tanks installed. $y^{st}_{t,p,s}$ 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,

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

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

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

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 ($f_{t,p}^{fresh}$) 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),

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

The relation between 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 desalination technology ($f_{t,p}^{on,in}$),

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

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.

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

The number of onsite treatment leased depends on the total number of portable treatments available.

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

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 following equation Eq. (27) represents the selection of treatment units and their maximum capacity.

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

The flow directions for the desalinated water are given by Eq.(28). $f_{t,p}^{on,fwt}$ 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,

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

Centralized water treatment

In this section, mass balances are performed in the CWT facility. Eq. (29) shows the relationship between 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 to be maximized includes 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 includes 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 $\alpha_t^{gas}$is the gas price forecast in time period t.

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

$$E^{drill} = \sum_{t\in T}\sum_{p\in P}\sum_{w\in RPW_p}\sum_{c\in C}\alpha^{drill}\cdot y_{t,p,w,c}^{hf} + \sum_{t\in T}\sum_{p\in P}\sum_{w\in RPW_p}\alpha^{prod}\cdot f_{t,p,w}^{gas} \tag{35}$$

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

$$E^{dis} = \sum_{t\in T}\sum_{p\in P}\sum_{d\in D}\alpha_d^{dis}\cdot f_{t,p,d}^{dis} \tag{36}$$

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

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

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

$$E^{source} = \sum_{t\in T}\sum_{p\in P}\sum_{f\in F}\alpha_f^{source}\cdot f_{t,p,f}^{source} \tag{38}$$

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

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

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*.

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

where $D_{p,d}^{pad-dis}$, $D_{p,f}^{pad-source}$, $D_{p,k}^{pad-cwt}$ and $D_{p,pp}^{pad-pad}$ 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 1 if at least one well is drilled in wellpad *p* in time period *t* by crew *c*,

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

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

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

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.[22] 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 includes social security contributions paid for the employed people to fracture a well (SS), plus the social transfer by hiring people (SU), minus social cost (SC).[17] We only take into account the number of jobs on a fracturing crew and the time that they are working to fracture a specific well. Once the well is completed, the number of jobs generated by truck drivers or maintenance team are not considered. The social-profit is defined by Eq. (47),

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

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).

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 nonconvexity 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[23], 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.

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

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 model is implemented in GAMS 25.0.1.[24] The relaxed MILP problem is solved with Gurobi 7.5.2 [25] and the MINLP problem with DICOPT 2 [26] using CONOPT 4 [27] to solve the NLP sub-problems. Although DICOPT cannot guarantee a global solution, we calculate the optimality gap defined by Eq. (49) to obtain the deviation of this solution with respect to the global optimum,

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

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 Appendix A (Table A.1 – A.4). Gross and net salaries paid for each employee are obtained from the Bureau of Labor Statistics. [28] Our goal is to determine the optimal water management during the flowback water process. Therefore, we consider the natural gas production and wastewater generated in the first twelve weeks. Flowback water generation is the critical period for shale gas water management. In this phase, the coordination between different contractors is crucial since the water is recovered in a short time period. The inlet TDS concentration increase with time ranging from 3,000 to 200,000 ppm. We assume that 50% of the water used to fracture a well, which ranges from 4,800 to 18,600 m^3, is recovered as flowback water.

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.

Table 1. Case study description

Case study	Description
Case 1	All water management options are allowed: reuse the flowback water with a little treatment, desalinate the water in onsite treatment or CWT, 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.
Case 4	The cost of friction reducers is overestimated. Eq. (50) is replaced by the following equation: $$E^{fr} = \sum_{t\in T}\sum_{p\in P}\gamma^{fr}\cdot f_{t,p}^{imp} \qquad (50)$$
Case 5	All water management options, as in Case 1, are allowed. However, return to pad-operations is not allowed and wells are fractured in order; well 2 cannot be fractured before well 1. To do this, the following constraint is added: $$\sum_{t\in T} t\cdot y_{t,p,w,c}^{hf} \le \sum_{t\in T} t\cdot y_{t,p,ww,c}^{hf} \qquad w<ww, \forall w\in RPW_p, p\in P \qquad (51)$$

The optimal fracturing schedule for each case study is shown in Figure 2. All wells are fractured before time period forty. This allows to treat the flowback water and extract the natural gas that comes from all wells in the first twelve weeks.

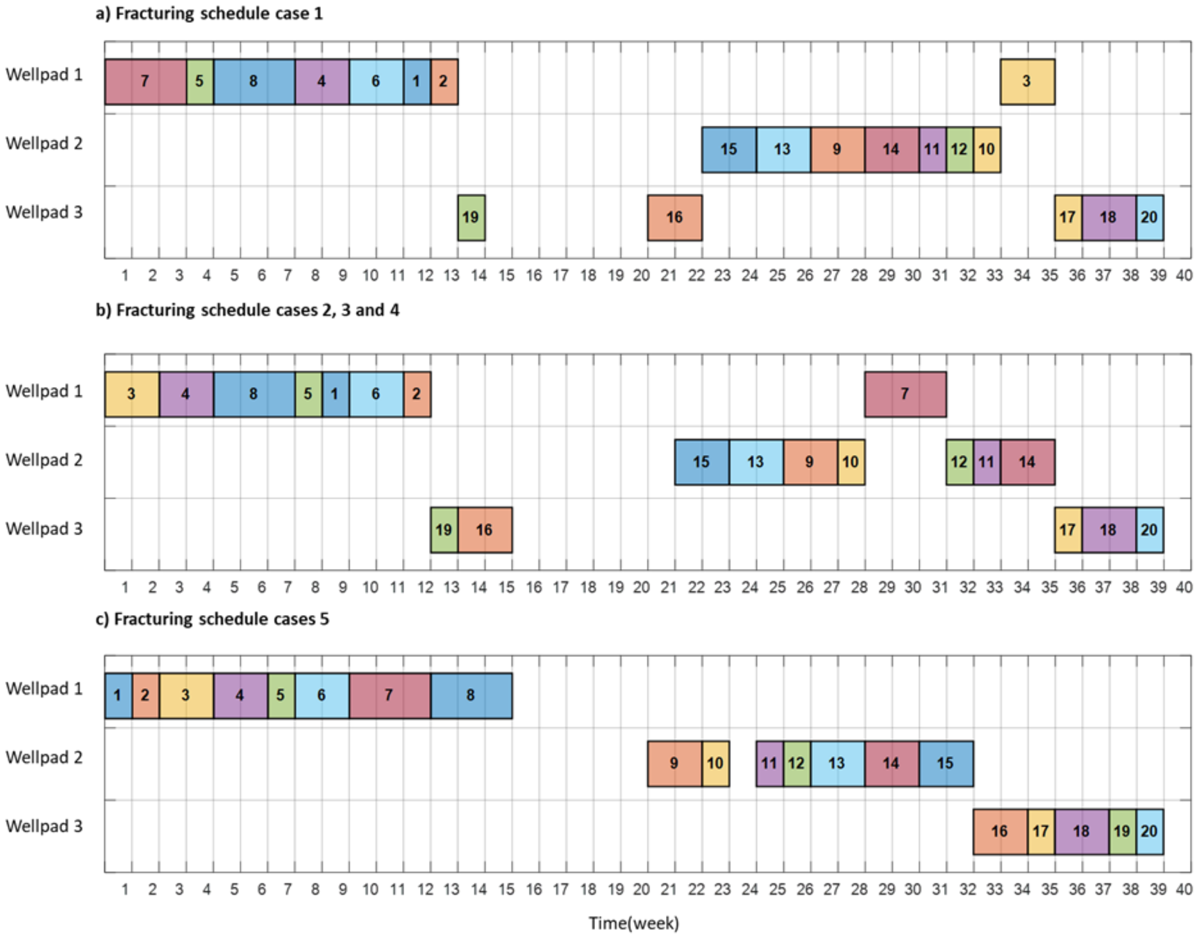

Figure 2. Fracturing schedule for all case studies.

The fractured schedule for Cases 2, 3 & 4 is the same since the model maximizes the revenue. A different schedule with lower revenue would reduce the cost to compensate the change in the revenue. This happens in Case 1, the maximization of the water reuse to fracture other wells compensate to obtain another fracture schedule with lower revenue but lower cost.

In all cases, the optimal solution shows that the fracturing schedule includes return to pad-operations, except in Case 5 where it is prohibited. Therefore, moving the crew from one wellpad to another without fracturing all wells that belong to the candidate wellpad is profitable. Return to pad-operations always must take into consideration to the optimal shale gas fracturing schedule.

The various items of the objective function are shown in Table 2. The negative values of the objective function mean that the result obtained is not a sustainable or viable solution.

Table 2. Disaggregated result of the objective function: sustainable profit, eco profit, social profit and economic profit (k$).

	Case 1	**Case 2**	**Case 3**	**Case 4**	**Case 5**
Sustainable 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

Case 1 has the highest sustainable profit value equal to $840k where the economic profit, eco-cost and social profit are equal to $16,909k, $17,490k and $1,421k, respectively. Although the environmental component has a high negative value, the model can find a compromise solution between economic, environmental and social criteria. The reuse of the flowback water to fracture other wells is the selected option for water management. Once all wells have been fractured, the water management option selected is to desalinate the wastewater with onsite desalination treatment. Reuse the flowback water to fracture other wells implies the need to use costly friction reducers. However, we can realize comparing the results obtained of Case 2&3 vs Case 1 (see Table 3) that reusing the water to fracture other wells yields large savings in transport, treatment and water withdrawal costs. 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 use for each case study. As can be seen, when the cost of friction reducers is overestimated, the impaired water used as fracturing fluid decreases 7.5%. This is because the lower cost obtained if the same amount of water in Case 1 is reused, does not compensate the higher revenue achieved with the fracturing schedule obtained in Case 4.

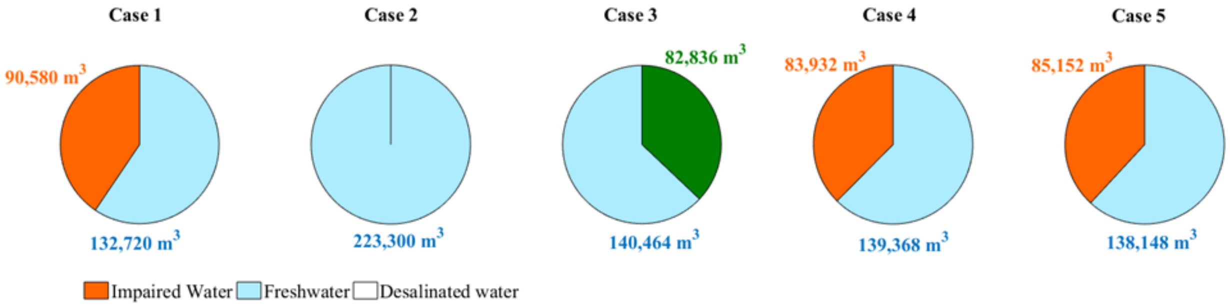

Figure 3. Total impaired water and freshwater used for all case studies.

In Case 1 the producer would spend $167k on tolerant additives, while overestimating the price of friction reducers this cost would rise to $252k. It should be noted that in Case 4 a compromise solution between economic, environmental and social criteria is also found, although the sustainable profit decreases 13%. Therefore, if the concentration of TDS increases over the time due to the use of impaired water as a fracturing fluid, reusing it to fracture other wells will be the best water management option.

In the other case studies (Cases 2, 3 & 5), a compromise solution is not found. Therefore, the sustainable profit is negative, and no wells should be fractured. However, 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 the others case studies. The worst scenario studied is Case 2, where the only water management option available is to send the wastewater to Class II disposal wells. The sustainable profit is equal to - $16,325k. Both eco and economic costs to send flowback water to disposal is too high compared with other water management options. Therefore, disposal wastewater into Class II disposal wells should be excluded for wells based on Marcellus play. Case 3, where desalination is the only water management strategy allowed, has lower economic and eco impact than disposal, although the sustainable profit still remains negative equal to - $57k. In this case, part of desalinated water is reused to fracture others 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. Hence, the fracturing schedule is highly dependent on the price and production of the natural gas forecast.

In Table 3, the different costs from the five case studies are reported in detail. Water-related costs range from 5 to 13% for the different case studies of the revenue of shale gas production. Regarding economics, the cost of drilling and production represents for Cases 1, 3, 4 & 5 the highest contribution of the total cost. In Case 2, the disposal cost yields the highest contribution in the total cost ($10,165k), however, it is close to the drilling and production cost equal to $9,523k. Regarding the environmental criterion, the eco-cost of natural gas production is equal to $17,375k, which is significantly higher than the others calculated eco-cost (see Table 3).

Table 3. Detailed description of costs from the five case studies (k$).

	Case 1	**Case 2**	**Case 3**	**Case 4**	**Case 5**
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 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

Figure 4 displays the percentage contribution of each water cost – additives, freshwater withdrawal, disposal, storage, transportation and desalination - of the total water-related cost.

Transportation cost decreases reusing the wastewater to fracture other wells (see Table 3 Cases 1, 4 & 5 vs Cases 2 & 3). However, they still represent a high contribution to the final economic and environmental water cost (see Figure 4). Except for Case 2 that disposal represent 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.[9],[12] However, in this work we analyze the water strategy with only truck hauling since it provides enough flexibility to guarantee freshwater supply without the uncertainty of pipelines construction permits.

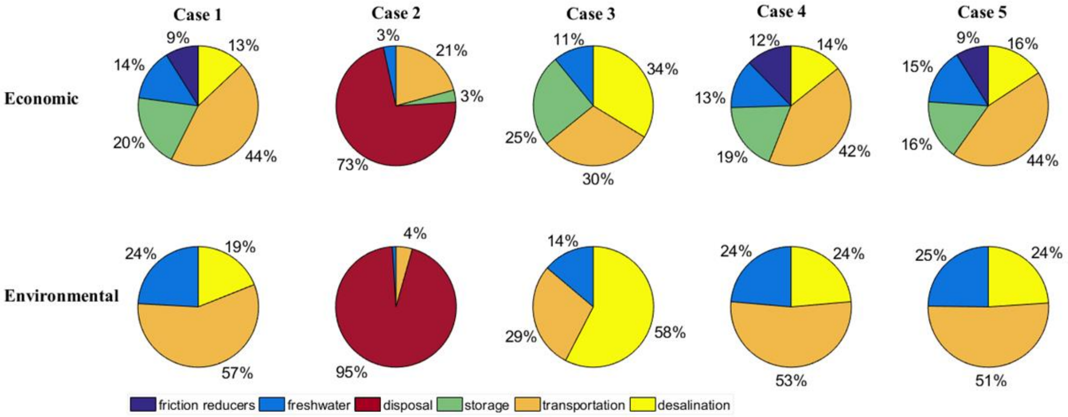

Figure 4. Comparison of all cases of the contribution percentage of each economic and environmental cost of the total water-related cost.

Despite the concern of the usage of freshwater for well fracturing, economic and environmental 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.

Note that the total water storage cost is significant in the optimization of water management (see Figure 4). In this work, we rigorously calculate the number of tanks in each time period considering installing, uninstalling, clean out and leasing costs. 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 [9,14], the storage cost increases by 53%.

Figure 5 displays the number of fracturing tanks and freshwater tanks over the time for each wellpad in Case 1. 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 to install and uninstall them over the time. 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 over these times periods.

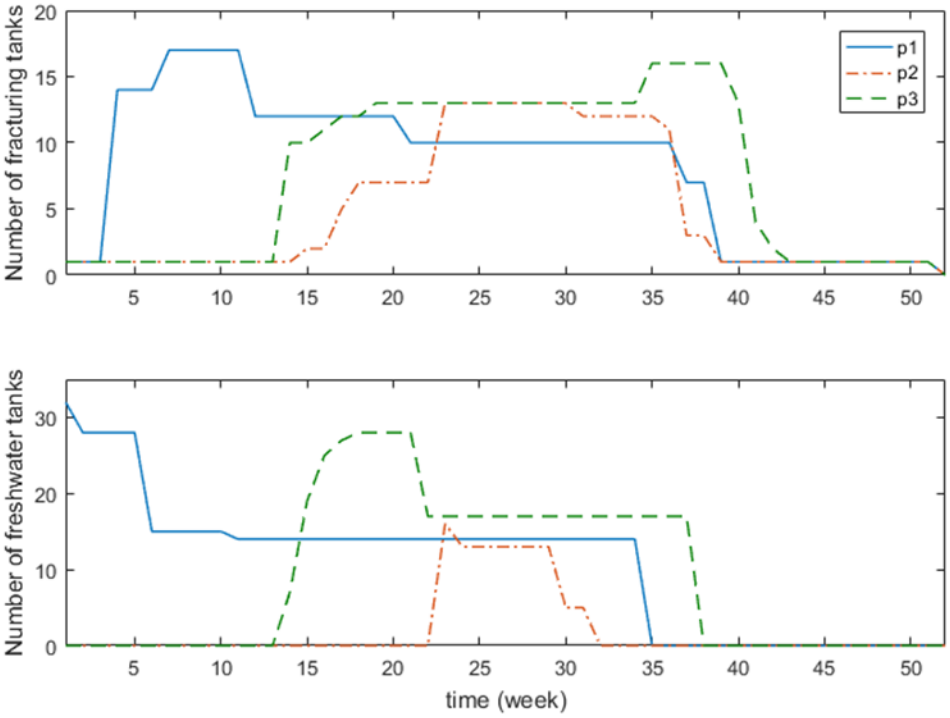

Figure 5. Number of fracturing tanks and freshwater tanks over the time for each wellpad in Case 1.

CONCLUSIONS

An MINLP 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 new objective function expressed in monetary value, helps the producers to make sustainable, viable and economic decisions. The goal is to maximize the objective function to find a compromise solution between the three pillars of sustainability. 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. The social indicator includes social security contributions, social effects due to the new jobs created and social cost. The inclusion of friction reducers cost function of TDS concentration allows to determine if reusing impaired water is a cost barrier. Additionally, the rigorous calculation of storage solution permits to operators to know the number of tanks that should be leased in each time period.

The proposed decomposition technique solves the MINLP model effectively. 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.

We have presented 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 possible to obtain a compromise solution between economic, environmental and social criterium. The level of TDS in impaired water is not an obstacle to reusing it for fracturing purposes, although the concentration increases over the time, and consequently the cost of the friction reducers. Also, it has been shown that onsite desalination treatment can be cost-effective for operators once no more wells are available to be fractured. Finally, it should be noted that transportation is the highest water-related contribution to both economic and environmental impacts.

ACKNOWLEDGMENTS

This project has received funding from the European Union’s Horizon 2020 Research and Innovation Program under grant agreement No. 640979 and from the Spanish «Ministerio de Economía, Industria y Competitividad» CTQ2016-77968-C3-02-P (FEDER, UE).

NOMENCLATURE

Parameters

$C_{t,p,w}^{well}$	Concentration of flowback water forecast for well w on wellpad p in time period t
C^{con}	Outlet salinity for desalination treatments
CST_s	Capacity of storage tank s
$D_{p,d}^{pad-dis}$	Distance from wellpad p to disposal well d
$D_{f,p}^{pad-source}$	Distance from source f to wellpad p
$D_p^{pad-off}$	Distance from wellpad p to offsite-treatment
$D_{p,pp}^{pad-pad}$	Distance from wellpad p to wellpad pp
$F_{t,p,w}^{well}$	Flowback water forecast for well w on wellpad p in time period t
$F_n^{on,UP}, F_n^{on,LO}$	Maximum and minimum onsite capacity for treatment wt
$F_k^{cwt,UP}$	Maximum centralize water treatment capacity k
$F_{t,p,w}^{gas}$	Production gas flow forecast for well w on wellpad p in time period t
N_s^{UP}, N_s^{LO}	Upper and lower bound of tanks s installed

$N_s^{im,UP}, N^{im,LO}$	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
WD_w	Water demand of well w
τ_w	Time to fracture well w
α^{pre}	Pretreatment recovery factor
α^{rec}	Centralized water treatment recovery factor
α^{drill}	Drilling and completion cost
α^{prod}	Shale gas production cost
α_d^{dis}	Disposal coefficient cost coefficient for disposal d
α_s^{sto}	Storage leasing cost coefficient for storage tank s
α^{im}	Impoundment construction cost
α_f^{source}	Freshwater cost coefficient in freshwater source f
α^{fr}	Friction reducer cost coefficient
α^{truck}	Trucking cost coefficient
α^{reuse}	Pretreatment cost coefficient aiming its reuse
α^{treat}	Pretreatment cost coefficient aiming its desalination
α^{crew}	Cost of moving crews
α_n^{on}	Onsite desalination cost coefficient for treatment n
α_k^{cwt}	Cost coefficient of centralized water treatment k
α_t^{gas}	Natural gas price forecast in time period t
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

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

$c_{t,p}$	Salt concentration in fracturing tanks on wellpad p in time period t
$c^{i}_{t,p}$	Salt concentration of the inlets flows in fracturing tanks on wellpad p in time period t
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
$f^{well}_{t,p,w}$	Flowrate of produce water on well w wellpad p in time period t
$f^{pad}_{t,p}$	Flowrate of produce water on wellpad p in time period t
$f^{pre,in}_{t,p}$	Onsite pretreatment inflow in wellpad p in time period t
$f^{source}_{t,p,f}$	Flowrate of freshwater from natural source f to wellpad p in time period t
$f^{on,fwt}_{t,p}$	Flowrate of desalinated water from onsite treatment to freshwater tanks in wellpad p in time period t
$f^{pad,fwt}_{t,pp,p}$	Flowrate of desalinated water from wellpad pp to freshwater tanks in wellpad p in time period t

$f_{t,p}^{on,des}$	Flowrate of freshwater used in hydraulic fracturing in wellpad p in time period t
$f_{t,p}^{imp}$	Flowrate of impaired water used in hydraulic fracturing in wellpad p in time period t
$f_{t,p}^{dem}$	Flowrate of water demand in wellpad p in time period t
$f_{t,p}^{pre,out}$	Onsite pretreatment outflow in wellpad p in time period t
$f_{t,p}^{on,slud}$	Slud flowrate after onsite desalination process in wellpad p in time period t
$f_{t,p}^{on,in}$	Onsite desalination inflow in wellpad p in time period t
$f_{t,p}^{on,out}$	Onsite desalination outflow in wellpad p in time period t
$f_{t,p,d}^{on,brine}$	Brine flowrate after onsite desalination process in wellpad p in time period t
$f_{t,p}^{on,fresh}$	Flowrate of desalinated water from onsite treatment on wellpad p in time period t sent to discharge
$f_{t,k}^{cwt,in}$	Inlet flow in centralized water treatment k in time period t
$f_{t,k}^{cwt,out}$	Outlet flow in centralized water treatment k in time period t
$f_{t,p,k}^{cwt,fwt}$	Desalinated water from centralized water treatment k to freshwater tank on wellpad p in time period t
$f_{t,k}^{cwt,des}$	Desalinated water from centralized water treatment k to discharge in time period t
$f_{t,p,s}^{i}$	Outlet flow in tank s in wellpad p in time period t
$f_{t,p,s}^{o}$	Inelt flow in tank s in wellpad p in time period t

R^{gas}	Total gas revenue
$st_{t,p,s}$	Level of water in tank type s on wellpad p in time period t
$y^{fb}_{t,p,w}$	Indicates when the water starts to come out on well w on wellpad p in time period t

REFERENCES

1. U.S. Energy Information Administratio. International Energy Outlook 2016. http://www.eia.gov/outlooks. Published 2016. Accessed March 12, 2018.
2. Gao J, You F. Design and optimization of shale gas energy systems: Overview, research challenges, and future directions. *Comput Chem Eng*. 2017;106:699-718.
3. U.S. Environmental Portection Agency. *Technical Development Document For Effluent Limitations Guidelines and Standars for the Oil and Gas Extraction Point Source Category*. Washington, DC; 2016.
4. Holditch SA. Getting the Gas Out of the Ground. *Chem Eng Prog*. 2012.
5. Mimouni A, Kuzmyak N, Oort E van, Sharma M, Katz L. Compatibility of hydraulic fracturing additives with high salt concentrations for flowback water reuse. In: *World Environmental and Water Resources Congress 2015*. ; 2015:496-509.
6. Paktinat J, Neil BO, Tulissi M, Service TW. Case Studies : Improved Performance of High Brine Friction Reducers in Fracturing Shale Reserviors. *SPE Int*. 2011.
7. Ruyle B, Fragachan FE. Quantifiable Costs Savings by Using 100 % Raw Produced Water. . *SPE Int*. 2015.
8. Yang L, Grossmann IE, Manno J. Optimization models for shale gas water management. *AIChE J*. 2014;60(10):3490-3501.
9. Yang L, Grossmann IE, Mauter MS, Dilmore RM. Investment optimization model

for freshwater acquisition and wastewater handling in shale gas production. *AIChE J*. 2015;61(6):1770-1782.

10. Bartholomew T V, Mauter MS. Multiobjective Optimization Model for Minimizing Cost and Environmental Impact in Shale Gas Water and Wastewater Management. *ACS Sustain Chem Eng*. 2016;4(7):3728-3735.
11. Gao J, You F. Optimal Design and Operations of Supply Chain Networks for Water Management in Shale Gas Production : MILFP Model and Algorithms for the Water-Energy Nexus. *AIChE J*. 2015;61(4).
12. Gao J, You F. Shale Gas Supply Chain Design and Operations toward Better Economic and Life Cycle Environmental Performance: MINLP Model and Global Optimization Algorithm. *ACS Sustain Chem Eng*. 2015;3(7):1282-1291.
13. Guerra OJ, Calderón AJ, Papageorgiou LG, Siirola JJ, Reklaitis G V. An optimization framework for the integration of water management and shale gas supply chain design. *Comput Chem Eng*. 2016;92:230-255.
14. Lira-Barragán LF, Ponce-Ortega JM, Guillén-Gosálbez G, El-Halwagi MM. Optimal Water Management under Uncertainty for Shale Gas Production. *Ind Eng Chem Res*. 2016;55(5):1322-1335.
15. Lira-Barragán LF, Ponce-Ortega JM, Serna-González M, El-Halwagi MM. Optimal Reuse of Flowback Wastewater in Hydraulic Fracturing Including Seasonal and Environmental Constraints. *AIChE J*. 2016;62(5).
16. Drouven MG, Grossmann IE. Optimization models for impaired water management in active shale gas development areas. *J Pet Sci Eng*. 2017;156:983-995.
17. Zore Ž, Čuček L, Kravanja Z. Syntheses of sustainable supply networks with a new composite criterion – Sustainability profit. *Comput Chem Eng*. 2017;102:139-155.

18. Carrero-Parreño A, Onishi VC, Salcedo-Díaz R, Ruiz-Femenia R, Fraga ES, Caballero JA, Reyes-labarta JA. Optimal Pretreatment System of Flowback Water from Shale Gas Production. *Ind Eng Chem Res*. 2017;56(15):4386-4398.

19. Carrero-Parreño A, Onishi VC, Ruiz-Femenia R, Salcedo-Díaz R, Caballero JA, Reyes-labarta JA. Multistage Membrane Distillation for the Treatment of Shale Gas Flowback Water: Multi-Objective Optimization under Uncertainty. *Comput Aided Chem Eng*. 2017;40:571-576.

20. Onishi VC, Carrero-Parreño A, Reyes-Labarta JA, Ruiz-Femenia R, Salcedo-Díaz R, Fraga ES, Caballero JA. Shale gas flowback water desalination: Single vs multiple-effect evaporation with vapor recompression cycle and thermal integration. *Desalination*. 2017;404(C):230-248.

21. Onishi VC, Carrero-Parreño A, Reyes-Labarta JA, Fraga ES, Caballero JA. Desalination of shale gas produced water: A rigorous design approach for zero-liquid discharge evaporation systems. *J Clean Prod*. 2017;140:1399-1414.

22. Delft University of Technology. The Model of the Eco-costs/Value Ratio (EVR). http://www.ecocostsvalue.com. Published 2017. Accessed December 1, 2017.

23. Garth P. McCormick. Mathematical programming computability of global solutions to factorable nonconvex programs: Part i - convex underestimating problems. *Math Program*. 1976;10(1):147-175.

24. Rosenthal RE. GAMS — A User 's Guide. *GAMS Doc 246*. 2016;(January):1-316.

25. Gurobi Optimization I. Gurobi Optimizer Reference Manual. http://www.gurobi.com. Published 2016.

26. Duran MA, Grossmann IE. An outer-approximation algorithm for a class of mixed-integer nonlinear programs. *Math Program*. 1986;36:307-339.

27. Drud A. CONOPT: A GRG code for large sparse dynamic nonlinear optimization

problems. *Math Program*. 1985;31(2):153-191.

28. United States Department of Labor. Usual Weekly Earnings of Wage and Salary Workers. Bureau of Labor Statistics. https://www.bls.gov/news.release/wkyeng.toc.htm. Accessed March 12, 2018.

29. Petroleum Services Association of Canada. How many jobs does a single drilling rig create and where are they? Alberta Oil - The Business of Energy. https://www.albertaoilmagazine.com/2015/05/drilling-rig-jobs/. Published 2015. Accessed March 12, 2018.

30. Urban Institute & Brookings Institution. Tax Policy Center. http://www.taxpolicycenter.org/taxvox. Accessed March 12, 2018.

APPENDIX A

The parameters used in this work are listened in the following tables.

Table A.1. Costs coefficient

Parameter	Value	Units	Ref
Drilling cost (α^{drill})	270,000	\$	12
Production cost (α^{prod})	0.014	$\$/m^3$	12
Disposal cost (α_d^{dis})	90 - 120	$\$/m^3$	9
Truck cost (α^{truck})	0.15	$\$/km/m^3$	9
Storage cost (α_s^{sto})	70	\$/week/tank	*
Impoundment cost (α^{im})	3.86	$\$/m^3$	8
Pretreatment cost ($\alpha^{reuse}, \alpha^{treat}$)	0.8 - 2	$\$/m^3$	18
Desalination cost (α_n^{ondes})	6 - 15	$\$/m^3$	20,19
Demobilize, mobilize and clean out cost (β_n^{ondes})	2,000	\$/week	*
Centralized water treatment (α_k^{cwt})	42 - 84	$\$/m^3$	9
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	$\$/m^3$	8
Moving crew cost (α^{crew})	83,000	\$	*

*****Provided by a company

Table A.2. Model parameters

Parameter	Value	Units	Ref
CST_s	60	m^3	*
$C_{t,p,w}^{well}$	3,000 - 200,000	ppm	[3]
C^{con}	300	$g\ kg^{-1}$	[20]
$F_{t,p,w}^{well}$	2,400 – 9,300	$m^3\ week^{-1}$	[3]
$F_{t,p,w}^{gas}$	$2.8\ 10^6 - 0.6\ 10^6$	$m^3\ week^{-1}$	[3]
$F_n^{on,UP}$	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	$m^3\ week^{-1}$	[3]
τ_w	1-5	weeks	[3]

***Provided by a shale gas company**

Table A.3. Eco-cost coefficients [22]

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 A.4. Social coefficients

Parameter	Value	Units	Ref
N^{jobs}	145	-	29
S^{Gross}	857	\$ $week^{-1}$	28
S^{Net}	685	\$ $week^{-1}$	28,30
$C^{UNE,State}$	125	\$ $week^{-1}$	17
$C^{EMP,State}$	12.5	\$ $week^{-1}$	17
$C^{company}$	6.5	\$ $week^{-1}$	17