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ORIGINAL PAPER

# Optimal design of water networks for shale gas hydraulic fracturing including economic and environmental criteria

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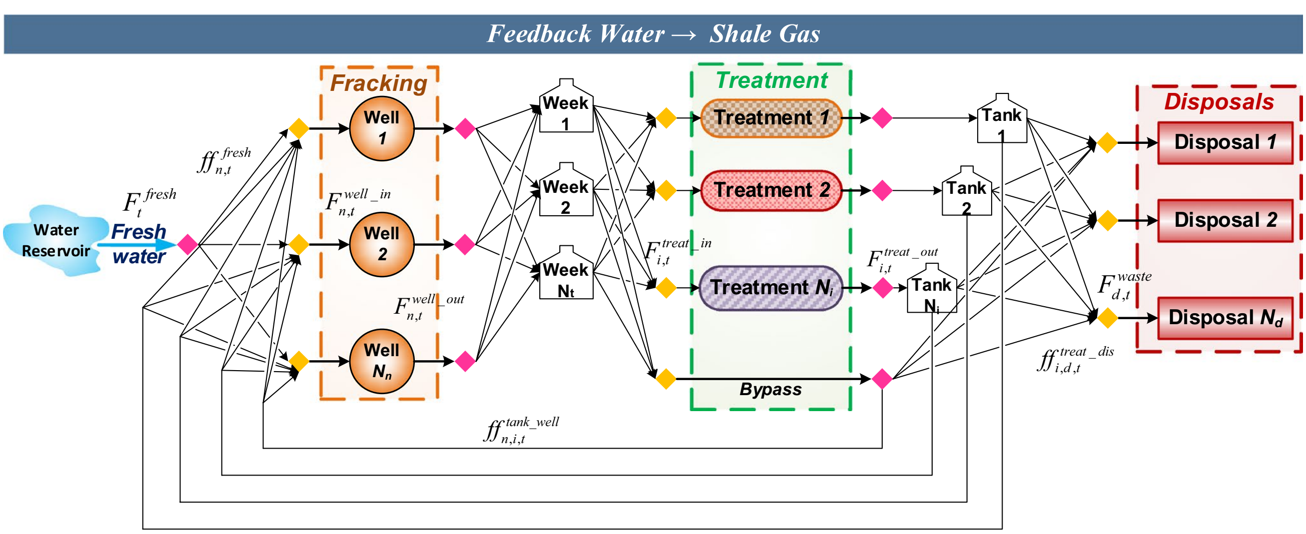
## Abstract

This work proposes an optimization approach for designing efficient water networks for the shale gas production through the recycle and reuse of wastewater streams reducing the freshwater consumption and effluents considering economic and environmental goals. The economic objective function aims to minimize the total annual cost for the water network including the costs associated with storage, treatment and disposal (capital cost) as well as freshwater cost, treatment cost and transportation costs. The environmental objective is addressed to deal with the minimization of the environmental impact associated with the discharged concentration of total dissolved solids in the wastewater streams and the freshwater consumption through an environmental function that represents the benefit for removing pollutants using the eco-indicator 99 methodology. The methodology requires a given scheduling for the completion phases of the target wells to be properly implemented by the available hydraulic fracturing crews during a time horizon. The model formulation is configured to determine the optimal sizes for the equipment involved by the project, particularly the sizes for storage and treatment units are quantified by the optimization process. A case study is solved to evaluate the effectiveness of the proposed optimization approach.


### Graphical abstract




**Keywords** Shale gas · Optimization · Hydraulic fracturing · Recycle and reuse water networks · Sustainable systems

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**List of symbols**

| | |
|---|---|
| $AvailV_t^{fresh\_max}$ | Availability of freshwater in the reservoirs ($m^3/s$) |
| $CapCost^{storage}$ | Capital cost for the installation of tanks in the storage system (US$/y) |
| $CapCost^{tank}$ | Capital cost for the installation of tanks of the flowback recovery system ($US/y) |
| $CapCost^{treat}$ | Capital cost for the installation of treatment system ($US/y) |
| $CapCost^{waste}$ | Capital cost for the piping and pumping system to send the final disposal ($US/y) |
| $Cost^{fresh}$ | Cost of the freshwater considering the price for industrial use ($US/y) |
| $Cost^{op\_treat}$ | Cost associated with the operation of the treatment units that involves the acquisition of chemical, use of external energy services, etc. ($US/y) |
| $Cost^{trans\_fb}$ | Cost for transporting the flowback fluid to the interception water network, mainly defined for piping and pumping costs ($US/y) |
| $Cost^{trans\_fresh}$ | Transportation cost to send freshwater from the reservoirs to the water network feed ($US/y) |
| $Cost^{trans\_storage\_treat}$ | Transportation cost to send the flowback fluid from the recovery storage system to the treatments units ($US/y) |
| $Cost^{trans\_tank\_dis}$ | Transportation cost to send the treated flowrate from the treatment units to the final disposals ($US/y) |
| $Cost^{trans\_tank\_well}$ | Transportation cost to recycle the treated flowrate from the storage tanks through the feed of the water network ($US/y) |
| $C_{c,t}^{bypass}$ | Concentration of total dissolved solids in the bypass flowrate (ppm) |
| $C_c^{fresh}$ | Concentration of total dissolved solids in the feeding of the freshwater in the water network (ppm) |
| $C_{c,j}^{storage}$ | Concentration of total dissolved solids at the storage tanks before the treatment system (ppm) |
| $C_{c,i,t}^{treat\_in}$ | Concentration of total dissolved solids that enters to the treatment system (ppm) |
| $C_{c,i}^{treat\_max}$ | Maximum concentration of total dissolved solids to be processed by each treatment technology (ppm) |
| $C_{c,i}^{treat\_out}$ | Concentration of total dissolved solids from the treatment units to be disposed (ppm) |
| $C_{c,d,t}^{waste}$ | Concentration of total dissolved solids in the wastewater effluents to be disposed (ppm) |
| $C_c^{waste\_max}$ | Maximum concentration limit of total dissolved solids in the effluents to be discharged to the disposals (ppm) |
| $C_{c,n,t}^{well\_in}$ | Concentration of total dissolved solids that enter to the wells as fracturing fluid (ppm) |
| $C_c^{well\_max}$ | Maximum concentration limit of total dissolved solid that is permitted as feed to the shale gas wells (ppm) |
| $IMPIN_{p,t}$ | Environmental damage that can be produce if the effluents can be discharge without treatment, eco-points |
| $IMPOUT_{p,t}$ | Environmental damage that can be produced by the discharge of effluents with treatment |
| $IMPTOL$ | Total environmental damage for the implementation of the treatment system for the effluents |
| $ff_{n,t}^{bypass\_well}$ | Flowrate that is recycled from the derivation to the system feed ($m^3/s$) |
| $ff_{d,t}^{bypass\_dis}$ | Flowrate in the bypass that is sent to the disposals directly ($m^3/s$) |
| $ff_{n,t}^{fresh}$ | Flowrate of freshwater that enters to the wells ($m^3/s$) |
| $ff_{j,t}^{storage\_bypass}$ | Flowrate from the recovery tanks to the bypass ($m^3/s$) |
| $ff_{j,i,t}^{storage\_treat}$ | Flowrate from the recovery tanks to the treatment units ($m^3/s$) |
| $ff_{n,i,t}^{tank\_well}$ | Flowrate from the storage system to the wells as recycled fluid ($m^3/s$) |
| $ff_{i,d,t}^{tank\_dis}$ | Flowrate from the storage system to the disposal alternatives ($m^3/s$) |
| $ff_{n,j,t}^{well\_storage}$ | Flowrate from the wells to the storage system ($m^3/s$) |
| $FC^{storage}$ | Fixed cost to install the storage system ($US/y) |
| $FC_i^{treat}$ | Fixed cost to install the treatment system ($US/y) |
| $F_{d,t}^{waste}$ | Total flowrate that is discharged to the final disposals ($m^3/s$) |
| $F_{n,t}^{well\_in}$ | Total flowrate that enters to the wells as fracturing fluid ($m^3/s$) |
| $F_{i,t}^{treat\_in}$ | Total flowrate that enters to the treatment system ($m^3/s$) |

$F_{i,t}^{tank\_out}$ Total flowrate that leaves each tank in the storage system (m$^3$/s)

$F_{j,t}^{storage\_in}$ Total flowrate that enters to each tank in the storage system (m$^3$/s)

$F_{j,t}^{storage\_out}$ Total flowrate that leaves each tank in the storage system (m$^3$/s)

$FC^{tank}$ Fixed cost to install tanks in the recovery system (m$^3$/s)

$FC^{waste}$ Fixed cost for sending the effluents to the final disposals (m$^3$/s)

$F_{i}^{treat\_cap}$ Total flowrate that the treatment technologies can be processed (m$^3$/s)

$F_{i,t}^{treat\_in}$ Flowrate that is fed in the treatment units (m$^3$/s)

$F_{i}^{treat\_\max}$ Maximum flowrate limit for the treatment units (m$^3$/s)

$F_{i,t}^{treat\_out}$ Flowrate that leaves the treatment units (m$^3$/s)

$F_{j,t}^{storage\_in}$ Flowrate that enters to the recovery tanks during the shale gas exploitation (m$^3$/s)

$F_{j,t}^{storage\_out}$ Flowrate that leaves the recovery storage system (m$^3$/s)

$F_{n,t}^{well\_out}$ Total flowrate of flowback fluid that leaves each pit (m$^3$/s)

$F_{t}^{bypass}$ Total flowrate in the bypass stream (m$^3$/s)

$F_{t}^{fresh}$ Freshwater fed to the water network (m$^3$/s)

$H^{time}$ Time conversion factor, time of unit operation (s)

$k_F$ Annualization factor (y$^{-1}$)

$TAC$ Total annual cost ($US/y)

$TCC$ Total capital cost ($US/y)

$TOC$ Total operational cost ($US/y)

$TWR$ Total water requirements (m$^3$)

$UC^{fresh}$ Unit cost for freshwater ($US/m$^3$/s)

$UOC_{i}^{treat}$ Unit cost for treatment technology ($US/m$^3$/s)

$UTC_{n}^{fresh}$ Freshwater unit transportation cost ($US/m$^3$/s)

$UTC_{n,j}^{well\_storage}$ Unit transportation cost of flowrate from the wells to the recovery storage system ($US/m$^3$/s)

$UTC_{j,i}^{storage\_treat}$ Unit transportation cost of flowrate from the recovery system to treatment units ($US/m$^3$/s)

$UTC_{i,d}^{tank\_dis}$ Unit transportation cost of flowrate from the recovery storage system ($US/m$^3$/s)

$UTC_{n,i}^{tank\_well}$ Unit transportation cost of flowrate from the treated storage system recycled to the pit ($US/m$^3$/s)

$VC^{storage}$ Variable cost for storage units ($US/m$^3$)

$VC^{tank}$ Variable cost for tanks ($US/m$^3$)

$VC^{waste}$ Variable cost for discharging the effluents to the disposals ($US/m$^3$)

$VC_{i}^{treat}$ Variable cost for installing treatment units ($US/m$^3$)

$V_{d}^{waste\_cap}$ Volume of effluents that can be discharged to the final disposal alternatives (m$^3$)

$V_{d}^{waste\_\max}$ Maximum volume that can be discharged to final disposal alternatives (m$^3$)

$V_{i}^{tank\_cap}$ Capacity of tanks in the storage system (m$^3$)

$V_{i}^{tank\_\max}$ Maximum capacity of tanks in the storage system (m$^3$)

$V_{i,t}^{tank}$ Volume of the tanks after the treatment unit in certain time period (m$^3$)

$V_{j}^{storage\_cap}$ Capacity of storage units (m$^3$)

$V_{j}^{storage\_initial}$ Capacity of storage units at the initial conditions (m$^3$)

$V_{j}^{storage\_\max}$ Maximum capacity of storage units (m$^3$)

$V_{j,t}^{storage}$ Capacity of storage units in certain time period (m$^3$)

$V_{j,t-1}^{storage}$ Volume of the storage units in a previous time period (m$^3$)

$y_{d}^{waste}$ Binary variable to decide the optimal final disposal

$y_{i}^{treat}$ Binary variable to decide the installation of treatment units

$y_{j}^{storage}$ Binary variable for the installation of tanks in the storage system

**Greek symbols**

$\alpha_{i}^{treat}$ Conversion factor for the flowrate in the treatment units

$\beta^{tank}$ Factor that represents the economies of scale for tanks

$\beta^{waste}$ Factor that represents the economies of scale in cost for discharge of effluents to a specific final disposal

$\beta^{storage}$ Factor that represents the economies of scale in cost for storage units

$\beta^{treat}$ Factor that represents the economies of scale in cost for treatment units

## Introduction

It is well known that the development of a country is strongly linked to the energy consumption; in other words, the countries with a higher level of progress demand more primary energy and as a country augments its development the energy consumption increases. In this context, natural gas offers an attractive alternative to satisfy the future energy demands owing to the recent discovery of new reserves (Melkoglu 2014). In addition, other advantages can be mentioned as some environmental benefits like the reduction in greenhouse emission, as well as the increase in efficiency in the processes that are operated with this energy alternative (Kuuskraa 2004). The importance of natural gas as fuel is widely recognized as well as its applications such as electricity production, transportation and chemical industries. The Energy Information Administration (EIA) has established that the USA has an amount of natural and shale gas reserves equivalent to meet domestic electricity demands for 575 years at current electricity generation levels and it is estimated that in 2035 shale gas is able to provide about half of the total natural gas supply in the USA (EIA 2015a, 2017). However, this information represents a great opportunity for the rest of countries with the largest shale gas reserves, particularly, the six countries with major reserves (China, Argentina, Algeria, U.S., Canada and Mexico) possess more than two-third of the technically recoverable shale gas resources around the world (EIA 2015b). Although only the USA and Canada have significant rates of shale gas production, it is foreseeable that the rest of the above-mentioned countries start the industrial production in a few years.

This resource involves some advantages in comparison with the rest of the fossil fuels, such as low carbon footprint, efficient energy resource, abundance of supplies, low price and the pipelines offering an easy way of transportation and control. Nevertheless, at the same time recent studies have focused on the environmental concerns due to the shale gas exploitation seeking to approximate processes to sustainability (see Fig. 1). In this regard, De Melo-Martín et al. (2014) analyzed the environmental and health problems associated with shale gas. Nicot and Scanlon (2012) investigated the environmental impact that the exploitation techniques produce for the large amounts of water and the use of toxic compounds, which are injected in the underground producing greater soil and water pollution. Annevelink et al. (2016) examined the environmental pollution related to the development of shale gas production. Zhang and Yang (2015) defined the damage for the practice of hydraulic fracturing during the operation of shale gas well in the USA. Whereas, Chang et al. (2014) and Zou (2015) evaluated the energy and water consumption related to the pollution generated by the hydraulic fracturing process. The huge volumes of water extracted from the freshwater reservoirs (groundwater and surface) to satisfy the requirements represent potential implications that should be analyzed (Best and Lowry 2014). Also, the inadequately treated wastewater streams and/or final disposal measures for hydraulic fracturing fluids and effluents represent a contamination source owing

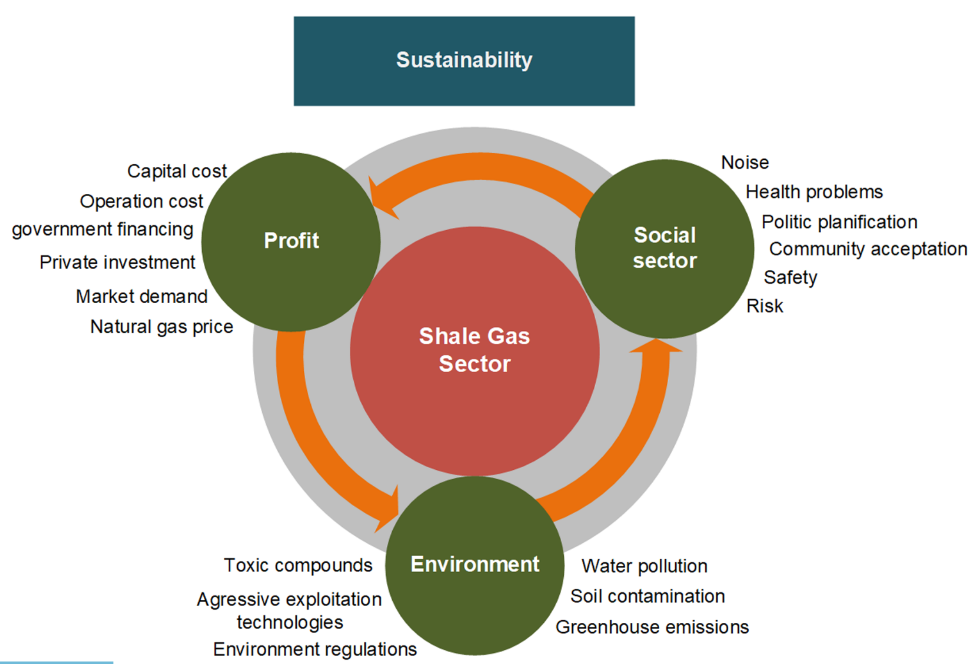


**Fig. 1** Sustainability in shale gas sector

to concentrated brine and other toxic compounds (Vengosh et al. 2014).

Moreover, in the literature can be found some attempts dealing with the environmental concerns associated with shale gas production with the purpose to quantify and mitigate their effects, which are related to the public perception of exploitation processes (Yu et al. 2018). For example, some authors have carried out life cycle assessments in shale gas operations. In this context, Tagliaferri et al. (2015) implemented a life cycle analysis for shale gas processes to determine the real damage, while Gao and You proposed several optimization approaches to design shale gas supply chains involving economic and environmental criteria, where it was included the water management in shale gas production (Gao and You 2015a), and involving the water–energy nexus (Gao and You 2015b). Whereas Gao and You (2017a) evaluated the environmental impact using the life cycle analysis quantifying the greenhouse emissions applying the game theory approach and Gao and You (2017b) carried out a study to analyze whether the modular manufacturing could be implemented in shale gas operation and design to have a sustainable process, as well Gao and You (2017c) presented a study to implement the application of economic and environmental life cycle optimization using robust algorithms (Gao and You 2018). Finally, Gao and You (2017d) examined the direction and challenges for this energy sector. In specific issues, Chang et al. (2015) included the comparison of greenhouse gas emissions and the water consumption for a specific case in China. In this sense, Nichols and Victor (2015) studied the environmental benefits obtained by the implementation of technologies for the capture and storage of $CO_2$ emissions, Jiang et al. (2013) proposed the application of ceramic membrane and ion exchange technologies to treat the produced water. Chen (2015) assessed the use of forward osmosis considering the membrane fouling and mitigation. Sophisticated technologies, as the use of innovative microbial capacitive distillation cells, also have shown significant advantages (Stoll et al. 2015). An attractive scheme was introduced by Racharaks et al. (2015) where the flowback water is used for microalgae cultivation to reduce the water and nutriment requirements. In spite of these advances, none of the previous works have implemented rigorous mathematical approaches to optimize the water management tasks involved in shale gas production.

Rahm et al. (2013) presented a couple of approaches for the optimal selection of treatment technologies for hazardous compounds removal from the flowback water, because the high concentration of total dissolved solids produces high salinity (Engelder et al. 2014), which represents an important challenge to generate wastewater streams with enough quality to be reused or disposed. In this sense, the optimization models to design efficient management systems for shale gas process have demonstrated the environmental and economic benefits of their employment (Yang et al. 2014). Grossmann et al. (2014) proposed a mathematical formulation for the optimal investment and planning in shale gas exploitation including drilling and water management. Tan and Barton (2015) evaluated a model incorporating the dynamic location of mobile plants to monetize shale gas. Yuan et al. (2015) analyzed some polices to promote the shale gas development based on technical and economic evaluations and Arredondo-Ramírez et al. (2016) examined a methodology for the optimal planning and the corresponding infrastructure development in shale gas production.

Few years ago, Kharaka et al. (2013) integrated the energy–water nexus evaluating the degradation of the groundwater in shale gas production which was one of the first works that includes the concept of nexus in the shale gas. Savacool (2014) investigated the technical, economic, environmental and social costs for the hydraulic fracturing as approach to the sustainability aspects, while Gao and You (2017b) proposed a robust approximation to generate sustainable operations for shale gas systems identifying the challenges and the future directions for this sector. In this sense, Al-Douri et al. (2017) presented a review about the monetization of shale gas sector including the primary intermediates and products that can be derived by hydrocarbon components in shale gas as well as the conversion technologies providing the statists, challenges, opportunities and insights. Recently, Al-Aboosi and El-Halwagi (2018) presented a study for analyzing the water–energy nexus in shale gas production, and Oke et al. (2018) proposed a mathematical model to optimize the use of energy and water in hydraulic fracturing through the recycle and reuse of fracturing water implementing membrane distillation.

However, most of the environmental concerns are related to water management in the shale gas exploitation. In this aspect, Clark et al. (2013) estimated the water consumed over the life cycle of conventional and shale gas production, accounting for the different stages of production and for flowback water reuse. Lira-Barragán et al. (2016) proposed a mathematical programming model to find the optimal flowback wastewater management system minimizing the total annual cost. Because large amounts of produced water generate high risks of spill and leaks to the surface and subsurface environment (Clark et al. 2013), the proper treatment for the flowback fluid has generated significant concerns due to the risks of contamination of water bodies and reservoirs (including surface water and groundwater) during the effluent disposal. In this context, it is important to distinguish among flowback and produced water; thus, once the completion phase is finished, the flowback water is obtained during a short time with a great rate and an increasing pollutant concentrations, whereas the produced water returns gradually to the surface with a great concentration and a low constant rate. Nonetheless, pervious reports have not incorporated the environmental assessment in conjunction with economic objectives and the water management in hydraulic fracturing tasks.

This paper proposes an optimization approach to design a water network for hydraulic fracturing operations related to shale gas employing a recycle and reuse strategy for water streams through an efficient treatment system considering simultaneously environmental and economic objectives. The environmental target is defined as the maximization of the pollutants removal, which is equivalent to minimize the environmental impact whereas the economic goal consists in the minimization of the total annual cost (*TAC*). The model determines the number of treatment technologies, storage/pits and disposals required in the solution as well as their optimal size in addition to the inner configuration, specifically for the flowrates and concentrations.

## Problem statement

The problem addressed in this paper can be described as follows (which is based on the superstructure shown in Fig. 2).

Given is a water reservoir (such as a lake or river) available to extract water in order to be employed in hydraulic fracturing operation as well as the unit cost and unit transportation costs (accounting for the distance among the locations for freshwater source and the wells). The methodology considers a set of well pads ($N=\{n \mid n=1, 2,\ldots, N_n\}$) ready to implement the completion process (hydraulic fracturing), which is carried out by a set of crews operating simultaneously (it is worth to mention that the available equipment determines the maximum number of wells that can be completed simultaneously). In this context, the scheduling to carry out the fracking process for each well pad, the water requirements for each step, the available freshwater in water reservoirs, the portion of the injected water that returns to the surface, the maximum number of wells that can be simultaneously completed, the environmental regulations for wastewater discharges, the maximum capacities for the storage and treatment units and the operation time for completion per well are given. Once the flowback fluid returns to the surface, it is collected through a set of storage/pits ($J=\{j \mid j=1, 2, \ldots, N_j\}$) installed on site of exploitation with the purpose of storing the flowback water prior to be treated. In this case, the produced water is stored according to the time period (in weeks) where it is collected (because the water quality decreases as a function of time, due to the contact with toxic chemicals into the extracted wells); for this reason, the scheme considers the possible existence of three pits (most of the flowback water is generated during the first weeks). In this way, it avoids the mixing of water streams with different qualities. The exponent, fixed and variable costs for the capital cost function, and the maximum volume for each storage unit are known. Also, there is given a set of treatment technologies ($I=\{i \mid i=1, 2, \ldots, N_i\}$) in order to treat the flowback water and satisfy the quality conditions for its reuse or to be disposed in a final disposal. Each treatment unit has an associated storage tank (second storage system) to collect the treated hydraulic fracturing fluid prior to be reused or disposed, and a bypass stream is also included (for the case where a portion of the fluid does not need treatment). The formulation requires a unit operating cost, fixed and variable costs (accounting the exponent in the economies of scale) for the capital cost function as well as the maximum capacity of the flowrate that can be treated for each treatment and storage unit. Finally, it

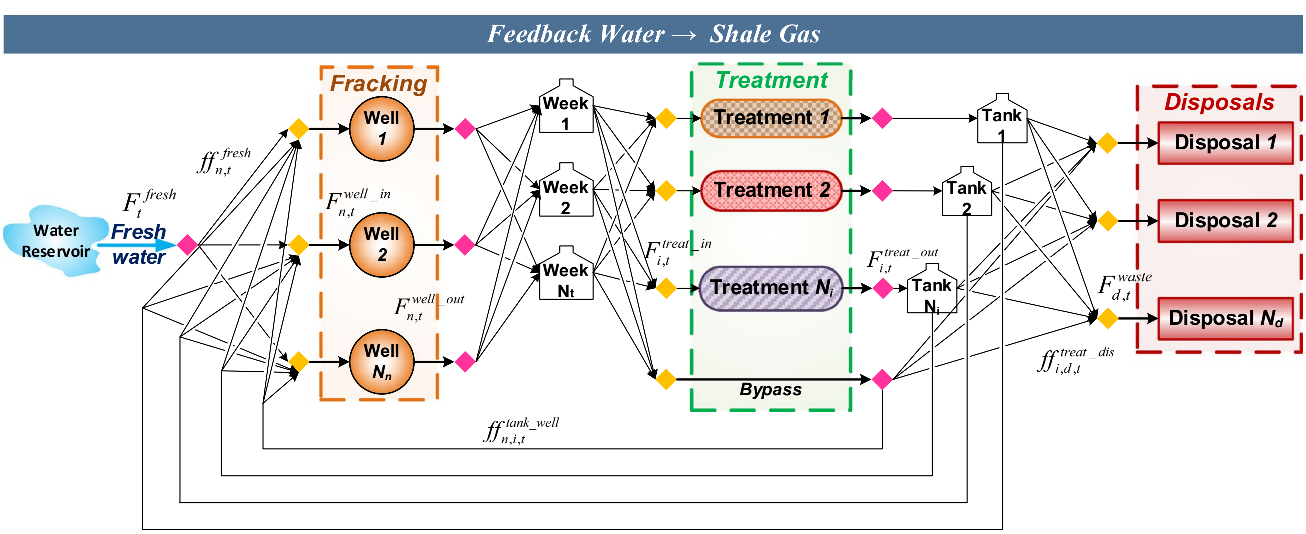


Fig. 2 Superstructure for the proposed water network

is given a set of disposals ($D=\{d \mid d=1, 2, \ldots, N_d\}$), where the treated flowback water can be disposed. Similarly, each disposal includes the parameters required in the capital cost function and a maximum volume. There is required the unit transportation cost for all the trajectories considered by the superstructure.

Then, the problem consists of determining the optimal configuration for the water management with the purpose of carrying out the completion step for all the target wells minimizing the total cost and at the same time maximizing the pollutant removal, this last point is equivalent to minimize the environmental impact. Thus, the optimization process is aimed to determine the number of treatment technologies, storage/pits (for the two storage systems) and disposals required in the solution as well as their optimal sizes in addition to the internal configuration with respect to flowrates and concentrations. The objective function consists of minimization of the total annual cost (*TAC*), which is composed by the total operating cost (*TOC*) and the total capital cost (*TCC*). The *TOC* includes the freshwater costs, the operating costs for treatment units and the transportation costs for all the considered routes, whereas the *TCC* considers the capital costs associated with the treatment units, storage/pits units and disposals.

## Model formulation

This paper proposes an optimization approach for a recycle and reuse water network in shale gas hydraulic fracturing operations in order to generate significant reductions for the freshwater consumption. Thus, the scheme includes a set of wells available to carry out the hydraulic fracturing, which requires important amounts of water. The water demands can be satisfied through freshwater sources or even with treated water (i.e., recycled water). Once the water is injected into the wells, the flowback water can be collected to be sent to a set of storage tanks; in this regard, the storage tanks are able to collect the flowback water according to different qualities for the flowback fluid, which depend strongly on the time period once the hydraulic fracturing is completed (i.e., the water properties are getting worse according to the week when is collected). This configuration is proposed with the purpose to avoid the mixing of water with drastically different conditions. At the exit of the first storage, it is placed a set of treatment technologies, and a bypass is also considered for the case that the water streams can satisfy the required quality to be disposed or reused in the wells. It should be noted that in this case the reused streams can be mixed with freshwater, and in this way the corresponding properties are modified. Then, there is a set of tanks to provide residence time to the water streams that can be reused (remember that the hydraulic fracturing operation for each well is previously scheduled) and finally it is considered the final disposal (see Fig. 2).

## Optimization model

The proposed optimization approach corresponds to the following mathematical formulation.

### Availability limitations for freshwater

It is well known that an important challenge for shale gas industry is the limitations in the water availability owing to this sector demands enormous amounts of water for the hydraulic fracturing process (see Myers 2012; Vidic et al. 2013). Then, this aspect can be modeled trough the following relationship:

$$F_t^{fresh} \leq \left( \frac{AvailV_t^{fresh\_\max}}{H^{time}} \right), \quad \forall t \tag{1}$$

where $F_t^{fresh}$ is the freshwater consumption over the time period $t$, $AvailV_t^{fresh\_\max}$ is the water availability over the time period $t$ and $H^{time}$ is a time conversion factor.

### Segregation of freshwater

According to the proposed scheme, the freshwater is divided and sent to each well $n$ during their completion phase:

$$F_t^{fresh} = \sum_n ff_{n,t}^{fresh}, \quad \forall t \tag{2}$$

### Water supply to wells

Additionally, the water requirements for hydraulic fracturing in each well $n$ ($F_{n,t}^{well\_in}$) are supplied by the freshwater source ($ff_{n,t}^{fresh}$) plus the water coming from the tanks located at the exit of the treatment ($ff_{n,i,t}^{tank\_well}$) and the bypass stream ($ff_{n,t}^{bypass\_well}$):

$$F_{n,t}^{well\_in} = ff_{n,t}^{fresh} + \sum_i ff_{n,i,t}^{tank\_well} + ff_{n,t}^{bypass\_well}, \quad \forall n, t \tag{3}$$

In order to determine the concentration entering each well ($C_{c,n,t}^{well\_in}$), it is necessary to multiply each term of the previous relationship by its concentration as follows:

$$F_{n,t}^{well\_in} C_{c,n,t}^{well\_in} = ff_{n,t}^{fresh} C_c^{fresh} + \sum_i ff_{n,i,t}^{tank\_well} C_{c,i}^{treat\_out} + ff_{n,t}^{bypass\_well} C_{c,t}^{bypass}, \quad \forall c, n, t \tag{4}$$

where $C_c^{fresh}$ represents the concentration of the freshwater, $C_{c,i}^{treat\_out}$ is the concentration leaving the treatment units, and finally $C_{c,t}^{bypass}$ is the concentration of the bypass stream. It should be noted that $C_{c,i}^{treat\_out}$ does not change with respect to the time (in this case, it is considered that the treatment technology $i$ always provides the same water quality).

### Flowback water

Several studies have pointed out that flowback water can be obtained once the completion phase has finished; however, most of this fluid can be collected only during the first weeks. Therefore, flowback water ($F_{n,t}^{well\_out}$) is sent to a set of storage tanks prior to be treated ($ff_{n,j,t}^{well\_storage}$):

$$F_{n,t}^{well\_out} = \sum_j ff_{n,j,t}^{well\_storage}, \quad \forall n, t \tag{5}$$

### Water inlet to storage units per week

It is well known that the pollutants concentration for the flowback water increases during the time (see Haluszczak et al. 2013; Marcon et al. 2017); thus, the water captured during the first week is cleaner with respect to the second week and subsequently the produced water in the second week is collected at better conditions than the third week (notice that there is a difference among the flowback and produced water with respect to the quality and the proposed methodology is aimed to deal with flowback water owing to the produced water contains gas and oil). In other words, the cleanest water is collected during the first week (after the completion) and the worst quality water is obtained in the third week. In this regard, the proposed configuration considers the possible existence of a set of tanks (and each one of them is employed for each week); however, it is not allowed the mixing of water streams with different qualities. For this reason, the scheme is able to save the flowback water according to the period when it has been gathered. Then, in the first tank $j = 1$ (called "Week 1" in the proposed superstructure) only flowback water is fed during the first week $t = fbw1$ (once the hydraulic fracturing process has finished):

$$F_{j,t}^{storage\_in} = \sum_n ff_{n,j,t}^{well\_storage}, \quad \forall j = 1, t = fbw1 \tag{6}$$

Similarly, for the second and third weeks,

$$F_{j,t}^{storage\_in} = \sum_n ff_{n,j,t}^{well\_storage}, \quad \forall j = 2, t = fbw2 \tag{7}$$

$$F_{j,t}^{storage\_in} = \sum_n ff_{n,j,t}^{well\_storage}, \quad \forall j = 3, t = fbw3 \tag{8}$$

### Water outlet from storage units

The water streams leaving the impoundments or pits ($F_{j,t}^{storage\_out}$) are segregated to be sent to all the treatment technologies ($ff_{j,i,t}^{storage\_treat}$) or to the bypass stream ($ff_{j,t}^{storage\_bypass}$):

$$F_{j,t}^{storage\_out} = \sum_i ff_{j,i,t}^{storage\_treat} + ff_{j,t}^{storage\_bypass}, \quad \forall j, t \tag{9}$$

### Water inlet to treatment units

The proposed superstructure includes an interception network composed by a set of proven treatment technologies to process the flowback water, which have been previously reported and recognized to efficiently process this type of streams. For each of the potential treatment units, the methodology requires the unit capital and operating costs, volumetric efficiencies, maximum inlet and outlet concentrations. Additionally, the optimization process selects the required technologies and determines their optimal size. The balance for the mixer at the inlet of each treatment unit states that the inlet flowrate for the technology $i$ ($F_{i,t}^{treat\_in}$) is supplied by the water streams leaving the storage tanks ($ff_{j,i,t}^{storage\_treat}$):

$$F_{i,t}^{treat\_in} = \sum_j ff_{j,i,t}^{storage\_treat}, \quad \forall i, t \tag{10}$$

The following component balance is employed to calculate the concentration entering to each treatment unit ($C_{c,i,t}^{treat\_in}$):

$$F_{i,t}^{treat\_in} C_{c,i,t}^{treat\_in} = \sum_j ff_{j,i,t}^{storage\_treat} C_{c,j}^{storage}, \quad \forall c, i, t \tag{11}$$

where $C_{c,j}^{storage}$ represents the concentration at the storage tanks placed before the treatment (it should be noticed that these concentrations are known).

In the same way, there can be determined the flowrates ($F_t^{bypass}$) and concentrations ($C_{c,t}^{bypass}$) for the bypass stream:

$$F_t^{bypass} = \sum_j ff_{j,t}^{storage\_bypass}, \quad \forall t \tag{12}$$

$$F_t^{bypass} C_{c,t}^{bypass} = \sum_j ff_{j,t}^{storage\_bypass} C_{c,j}^{storage}, \quad \forall c, t \tag{13}$$

### Water outlet from tanks belonging to treatment units

As can be seen in the proposed superstructure, the model considers a tank per treatment unit to store the fluid. Notice that Tank 1 stores all the water coming from Treatment 1, Tank 2 only receives fluid from Treatment 2 and the same sequence is employed for all the treatment technologies considered. It should be noted that the bypass stream does not require a tank to store the fluid. Whereas the outlet streams for these tanks ($F_{i,t}^{tank\_out}$) are split and sent to wells in order to be reused ($ff_{n,i,t}^{tank\_well}$) and to the waste disposals ($ff_{i,d,t}^{tank\_dis}$):

$$F_{i,t}^{tank\_out} = \sum_n ff_{n,i,t}^{tank\_well} + \sum_d ff_{i,d,t}^{tank\_dis}, \quad \forall i, t \tag{14}$$

Similarly, the bypass stream is sent to the same destinations:

$$F_t^{bypass} = \sum_n ff_{n,t}^{bypass\_well} + \sum_d ff_{d,t}^{bypass\_dis}, \quad \forall t \tag{15}$$

#### Water balance for waste disposal and discharge

The wastewater streams generated by the project ($F_{d,t}^{waste}$) are coming from the tanks located after the treatment ($ff_{i,d,t}^{tank\_dis}$). Also, the bypass stream is able to send wastewater to be disposed ($ff_{d,t}^{bypass\_dis}$):

$$F_{d,t}^{waste} = \sum_i ff_{i,d,t}^{tank\_dis} + ff_{d,t}^{bypass\_dis}, \quad \forall d, t \tag{16}$$

With the purpose to determine the concentration of pollutants at the final disposals ($C_{c,d,t}^{waste}$), it is included the component balance as follows:

$$F_{d,t}^{waste} C_{c,d,t}^{waste} = \sum_i ff_{i,d,t}^{tank\_dis} C_{c,i}^{treat\_out} + ff_{d,t}^{bypass\_dis} C_{c,t}^{bypass}, \quad \forall c, d, t \tag{17}$$

Previous relationships simulate the operation for all the mixers and splitters considered by the superstructure; nevertheless, the mathematical model must include mathematical relationships to model the operation for treatment units, storage tanks (prior and after of the treatment), equipment capacities, as well as the economic (i.e., the minimization of the total annual cost) and environmental (minimization of the environmental impact including the consumption of freshwater) objective functions. These expressions are incorporated as follows.

#### Balances in treatment units

Usually the operation of treatment technologies involves flowrate losses (considering outlet streams with respect to inlet streams), this aspect is modeled as follows:

$$F_{i,t}^{treat\_out} = \alpha_i^{treat} F_{i,t}^{treat\_in}, \quad \forall i, t \tag{18}$$

where $\alpha_i^{treat}$ is volumetric efficiency of the treatment technologies because some time of the total wastewater that the treatment units receive just a fraction can be treated for different reason, for example losses for transportation or low efficiencies in the processes, etc. While $F_{i,t}^{treat\_out}$ is the treated water flowrate from the treatment units and $F_{i,t}^{treat\_in}$ is the untreated water flowrate that requires treatment in the treatment units.

#### Balances in storage units

It is not allowed to mix streams with different values for pollutant concentrations for storage tanks (prior and after treatment) with the purpose to set their concentrations as given data. However, it is important to include these sets of tanks consist in saving the fluid to be employed during the optimal time periods where the water streams are required (in this aspect, the reused water also represents a backup resource for time periods with low freshwater availability). It should also be noticed that the mixing at the inlet for treatment, disposal and reuse (directly in wells) is allowed. This last consideration is useful in order to meet the pollutant restrictions included at the inlet of the key activities for the proposed water network (treatment, disposal and reuse) owing that the fluid streams with different qualities can be mixed among them to achieve a lower value than the maximum allowed concentration in each task (even in the reuse of freshwater is able to be employed).

In this regard, the accumulation balances for the storage pits state that the volume in the pit $j$ at the time $t$ ($V_{j,t}^{storage}$) is equal to the one at the end of the previous time period ($V_{j,t-1}^{storage}$), plus the difference of the inlet ($F_{j,t}^{storage\_in}$) and outlet ($F_{j,t}^{storage\_out}$) flowrates multiplied by a time conversion factor ($H^{time}$),

$$V_{j,t}^{storage} = V_j^{storage\_initial} + H^{time}\left(F_{j,t}^{storage\_in} - F_{j,t}^{storage\_out}\right), \quad \forall j, t = 1 \tag{19}$$

$$V_{j,t}^{storage} = V_{j,t-1}^{storage} + H^{time}\left(F_{j,t}^{storage\_in} - F_{j,t}^{storage\_out}\right), \quad \forall j, t > 1 \tag{20}$$

It should be noticed that at the beginning (first period) there is considered a known initial pit volume ($V_j^{storage\_initial}$). Also, the next relationship is required to guarantee the continuity of the cycles, so the initial volume is equal to the last volume:

$$V_{j,t}^{storage} = V_j^{storage\_initial}, \quad \forall j, t = t^{final} \tag{21}$$

#### Balances in tanks belonging to treatment units

The same type of balances is required to simulate the operation of the tanks located at the exit of treatment:

$$V_{i,t}^{tank} = V_i^{tank\_initial} + H^{time}\left(F_{i,t}^{treat\_out} - F_{i,t}^{tank\_out}\right), \quad \forall i, t = 1 \tag{22}$$

$$V_{i,t}^{tank} = V_{i,t-1}^{tank} + H^{time}\left(F_{i,t}^{treat\_out} - F_{i,t}^{tank\_out}\right), \quad \forall i, t > 1 \tag{23}$$

$$V_{i,t}^{tank} = V_i^{tank\_initial}, \quad \forall i, t = t^{final} \tag{24}$$

It is important to remark that the typical storage units employed in shale gas industry correspond to storage pits, impoundments or even above ground storage tanks can be used.

### Capacity and existence of treatment units

The proposed methodology is aimed to determine the capacity and the possible existence of each unit (i.e., treatment technologies including tanks and final disposals) required in the optimal solution. Then, for the treatment units the following couple of relationships select whether each technology is needed or not (the existence of the treatment units is modeled through the binary variable $y_i^{treat}$); in addition, the operational capacity for each treatment is represented by $F_i^{treat\_cap}$:

$$F_i^{treat\_cap} \geq F_{i,t}^{treat\_in}, \quad \forall i, t \tag{25}$$

$$F_i^{treat\_cap} \leq F_i^{treat\_\max} y_i^{treat}, \quad \forall i \tag{26}$$

where $F_i^{treat\_\max}$ represents an upper limit for the operational capacity associated with the unit $i$ (this information can be provided by sellers of treatment technologies). It should be noted that the optimal capacity ($F_i^{treat\_cap}$) must be used in the cost functions related to the capital costs for the treatment units.

### Capacity and existence of storage units

Similarly, for the storage/pits units, the following relationships determine the operational capacity and the existence of the storage units:

$$V_j^{storage\_cap} \geq V_{j,t}^{storage}, \quad \forall j, t \tag{27}$$

$$V_j^{storage\_cap} \leq V_j^{storage\_\max} y_j^{storage}, \quad \forall j \tag{28}$$

where $V_j^{storage\_cap}$ denotes the optimal size for the storage unit, $V_j^{storage\_\max}$ represents the maximum allowed capacity for the pit and $y_j^{storage}$ is a binary variable employed to model the existence of the storage/pits unit.

### Capacity and existence of tanks belonging to treatment units

In analogy to previous relationships, the following expressions are added to model the tanks located at the exit of the treatment:

$$V_i^{tank\_cap} \geq V_{i,t}^{tank}, \quad \forall i, t \tag{29}$$

$$V_i^{tank\_cap} \leq V_i^{tank\_\max} y_i^{treat}, \quad \forall i \tag{30}$$

### Capacity and existence of disposals

Finally, the operational capacity for the final disposal $d$ ($V_d^{waste\_cap}$) is computed by the sum of all the flowrates disposed by the project ($F_{d,t}^{waste}$) and considering the time conversion factor ($H^{time}$) as follows:

$$V_d^{waste\_cap} = H^{time} \sum_t F_{d,t}^{waste}, \quad \forall d \tag{31}$$

$$V_d^{waste\_cap} \leq V_d^{waste\_\max} y_d^{waste}, \quad \forall d \tag{32}$$

However, the last equation is incorporated to avoid that the optimal size (determined by the optimization process) exceeds the maximum capacity for each disposal ($V_d^{waste\_\max}$). The existence of each disposal is modeled through the binary variable $y_d^{waste}$. Thus, the implementation of the proposed methodology can determine the number of units (treatment technologies, storages/pits and disposals) required in the optimal solution as well as their capacities.

### Upper limits for concentrations

The following constraints are needed to ensure that water streams are in adequate conditions to be processed for hydraulic fracturing, to be treated, as well as to be disposed. These constraints are modeled as follows:

$$C_{c,n,t}^{well\_in} \leq C_c^{well\_\max}, \quad \forall c, n, t \tag{33}$$

$$C_{c,i,t}^{treat\_in} \leq C_{c,i}^{treat\_\max}, \quad \forall c, i, t \tag{34}$$

$$C_{c,d,t}^{waste} \leq C_c^{waste\_\max}, \quad \forall c, d, t \tag{35}$$

### Total water used

An important aspect to be quantified in the proposed project is the total freshwater required to complete all the target wells (this concern can be considered as an environmental objective function); this is determined as follows:

$$TWR = H^{time} \sum_t F_t^{fresh} \tag{36}$$

#### Operating costs

The operating costs considered in this project correspond to the freshwater cost, operating costs for treatment units and transportation costs (including all the trajectories), which are described in details as follows.

#### Freshwater cost

The freshwater cost ($Cost^{fresh}$) is determined by multiplying the sum of the water required during all periods ($F_t^{fresh}$) with the unit cost for the freshwater ($UC^{fresh}$) and including the time conversion factor ($H^{time}$):

$$Cost^{fresh} = H^{time} UC^{fresh} \sum_t F_t^{fresh} \tag{37}$$

#### Operating costs for treatment units

The operation of treatment units involves the acquisition of chemicals, use of external energy utilities (i.e., electricity or steam) and workers. These costs require to consider the efficiency for the operation of the treatment technologies, which are included in the unit cost $UOC_i^{treat}$; then, to obtain operating costs for treatment units ($Cost^{op\_treat}$), the unit cost is multiplied by the flowrate entering each treatment unit in all the periods as follows:

$$Cost^{op\_treat} = H^{time} \sum_i \sum_t UOC_i^{treat} F_{i,t}^{treat\_in} \tag{38}$$

#### Freshwater transportation cost

Similarly, the freshwater transportation cost ($Cost^{trans\_fresh}$) is determined as follows:

$$Cost^{trans\_fresh} = H^{time} \sum_n \sum_t UTC_n^{fresh} ff_{n,t}^{fresh} \tag{39}$$

where $UTC_n^{fresh}$ represents the unit transportation cost for freshwater from its source (lake or river) to shale play (well pad). It should be noticed that the unit costs to transport the freshwater are different considering the geographical distance between the fresh sources with respect to each pad. It is worth to mention that for some existing shale plays the freshwater resource is available at significant distances from the well pad and even in some relevant cases like Marcellus shale region, the freshwater transportation is significant (several times) higher than freshwater cost.

#### Flowback water transportation cost

The flowback water produced at wells is collected and transported to the first storage (prior to treatment); in this order, the cost associated with this transportation route ($Cost^{trans\_fb}$) is considered through the next relationship:

$$Cost^{trans\_fb} = H^{time} \sum_n \sum_j \sum_t UTC_{n,j}^{well\_storage} ff_{n,j,t}^{well\_storage} \tag{40}$$

where $UTC_{n,j}^{well\_storage}$ is the unit transportation cost for the flowback water in the path generated by the well $n$ and the storage unit $j$ (which are called Week 1, Week 2 and Week 3). Notice that this cost can fluctuate according to each trajectory.

#### Transportation cost for the stored water to treatment

Once time residence is provided by the set of storage units, the produced water is sent to a set of treatment units; consequently, a new transportation process is needed, which generates the following cost ($Cost^{trans\_storage\_treat}$):

$$Cost^{trans\_storage\_treat} = H^{time} \sum_j \sum_i \sum_t UTC_{j,i}^{storage\_treat} ff_{j,i,t}^{storage\_treat} \tag{41}$$

where $UTC_{j,i}^{storage\_treat}$ is the unit transportation cost from the storage pit $j$ to the treatment unit $i$.

#### Transportation cost for the treated water to disposals

The flowrate leaving the set of tanks belonging to the second storage can be sent to the final disposals, and the transportation cost associated with this process ($Cost^{trans\_tank\_dis}$) is incorporated through the following relationship:

$$Cost^{trans\_tank\_dis} = H^{time} \sum_i \sum_d \sum_t UTC_{i,d}^{tank\_dis} ff_{i,d,t}^{tank\_dis} \tag{42}$$

where $UTC_{i,d}^{tank\_dis}$ is the unit transportation cost from the tank $i$ to the disposal $d$. It is worth to mention that in some existing shale regions, like Marcellus shale play, the distances between the well pads and the final disposals are considerable, and as a consequence the cost to transport the wastewater streams represents an important concern in shale gas industry (remember that similar cases occur for the transportation cost for freshwater).

#### Transportation cost for reused water to well

The water streams leaving the set of tanks also can be sent to the wells (in order to be reused) and the generated transportation cost ($Cost^{trans\_tank\_well}$) is accounted as follows:

$$Cost^{trans\_tank\_well} = H^{time} \sum_{n} \sum_{i} \sum_{t} UTC_{n,i}^{tank\_well} ff_{n,i,t}^{tank\_well} \quad (43)$$

where $UTC_{n,i}^{tank\_well}$ is the unit transportation cost for the reused water from the tank $i$ to the well $n$. The unit transportation costs depend of each trajectory according to geographical locations.

#### Total operating cost

Finally, the total operating cost ($TOC$) for the project is calculated by the sum of all operating costs previously described:

$$\begin{aligned} TOC = & Cost^{fresh} + Cost^{op\_treat} + Cost^{trans\_fresh} \\ & + Cost^{trans\_fb} + Cost^{trans\_storage\_treat} \\ & + Cost^{trans\_tank\_dis} + Cost^{trans\_tank\_well} \end{aligned} \quad (44)$$

### Capital costs

The acquisition of the treatment and storage units as well as the creation of final disposals generates capital costs, which are accounted for the economic objective function.

#### Capital cost for treatment units

The capital cost function associated with treatment technologies includes fixed ($FC_i^{treat}$) and variable ($VC_i^{treat}$) charges; the later term depends on the flowrate to be processed as follows:

$$CapCost^{treat} = k_F \sum_{i} \left[ FC_i^{treat} y_i^{treat} + VC_i^{treat} \left( F_i^{treat\_cap} \right)^{\beta^{treat}} \right] \quad (45)$$

where $k_F$ is a factor used to annualize the investment, whereas $\beta^{treat}$ represents the exponent associated with the economies of scale for the treatment units. In this context, $k_F$ depends on the useful life of the plant and the interest rate. On this way, this factor becomes the total investment into annualized capital costs.

#### Capital cost for storage units and disposals

Similar capital cost functions are included for the storage units (remember that the proposed scheme has considered two sets of storage units) and disposals:

$$CapCost^{storage} = k_F \sum_{j} \left[ FC^{storage} y_j^{storage} + VC^{storage} \left( V_j^{storage\_cap} \right)^{\beta^{storage}} \right] \quad (46)$$

$$CapCost^{tank} = k_F \sum_{i} \left[ FC^{tank} y_i^{treat} + VC^{tank} \left( V_i^{tank\_cap} \right)^{\beta^{tank}} \right] \quad (47)$$

$$CapCost^{waste} = k_F \sum_{d} \left[ FC^{waste} y_d^{waste} + VC^{waste} \left( V_d^{waste\_cap} \right)^{\beta^{waste}} \right] \quad (48)$$

It should be noted that the previous four equations include the exponents ($\beta$), which are required to consider the economies of scale in the capital costs; however, at the same time this term incorporates nonlinearities in the model formulation (this aspect represents the only nonlinear terms included by the whole proposed mathematical model).

#### Total capital cost

Thus, the total capital cost ($TCC$) is composed by the capital costs for treatment, storage and tank units, as well as final disposals:

$$TCC = CapCost^{treat} + CapCost^{storage} + CapCost^{tank} + CapCost^{waste} \quad (49)$$

#### Total annual cost

Finally, the total annual cost ($TAC$) is constituted by the sum of $TOC$ and $TCC$:

$$Min \;\; TAC = TOC + TCC \quad (50)$$

## Environmental analysis

In this work, the environmental objective is addressed as the environmental benefit obtained by the implementation of the proposed project, specifically by the operation of the interception network in order to remove the toxic compounds contained in the flowback water. It is worth to mention that at the beginning of the shale gas industry the flowback water was discharged without adequate treatment (see Wang et al. 2014; Theodori et al. 2014; Estrada and Bhamidimarri 2016). However, the environmental regulations are becoming stricter and this situation leads to the implementation of treatment systems in shale gas industry. In this regard, the life cycle analysis (LCA) methodology is employed for determining the total environmental impact generated by the operation of this industry. Additionally, an important challenge in the shale gas sector is the generation of an adequate qualitative analysis for flowback water streams that represents an average study for this type of streams (it is well known that the composition of flowback water is significantly different even among adjacent wells). Nevertheless, once this drawback is overcome, the environmental impact can be quantified considering that each compound produces a different value for the environmental impact.

### Total environmental impact

The main goal of the treatment system is the removal of toxic compounds contained by the produced water streams. Then, the environmental objective consists of maximizing the total removal of pollutants in the treatment system (*IMPTOL*), which is estimated as the difference between the environmental impact produced for the flowback water with ($IMPIN_{p,t}$) and without ($IMPOUT_{p,t}$) treatment as follows:

$$Max\ \ IMPTOL = \sum_{p} \sum_{t} \left( IMPIN_{p,t} - IMPOUT_{p,t} \right) \quad (51)$$

Moreover, the environmental impact generated by the flowback water stream without treatment is calculated by the sum of individual unit impacts ($IMP_p$) times the pollutant concentration ($C^{wastep}_{c,d,t,p}$) and the disposed flowrate ($F^{waste}_{d,t}$) as follows:

$$IMPOUT_{p,t} = \sum_{c} \sum_{d} IMP_p C^{wastep}_{c,d,t,p} F^{waste}_{d,t}, \quad \forall p, t \quad (52)$$

Due to the variable composition of the flowback fluid that depends on the geological conditions in the reserves, the use of a global composition can be implemented. The use of the concentration of the total dissolved solids is the most popular in flowback fluid but other properties such as PH and turbidity can be used. The concentration of each compound in the total concentration ($C^{wastep}_{c,d,t,p}$) is estimated by multiplying the total concentration for the fraction of each chemical ($Xp_p$) in the fluid that enters to the treatment units:

$$C^{well\_in}_{c,i,t,p} = Xp_p C^{treat\_in}_{c,i,t}, \quad \forall c, i, t, p \quad (53)$$

and for the fluid that leaves the system:

$$C^{wastep}_{c,d,t,p} = Xp_p C^{waste}_{c,d,t}, \quad \forall c, d, t, p \quad (54)$$

The environmental impact for the initial conditions (before treatment) is defined as the total eco-points that can be produced by the toxic chemicals in the discharge stream as follows:

$$IMPIN_{p,t} = \sum_{c} \sum_{i} IMP_p C^{well\_in}_{c,i,t,p} F^{treat\_in}_{i,t}, \quad \forall p, t \quad (55)$$

The large amount of freshwater that is consumed for the shale gas exploitation processes has a specific impact for the extracted water from the reservoir, which is estimated as follows:

$$IFreshwater_t = IMP^{freshwater} F^{fresh}_t, \quad \forall t \quad (56)$$

In other words, the environmental objective function is strongly influenced by the efficiency of the treatment system and the variability between the operation of different technologies as well as the relationship with the selection of the final disposal.

## Results and discussion

The recent advances in drilling technologies and hydraulic fracturing processes have led to a growing interest for shale gas, which represents an attractive energy resource. However, this option involves important concerns. For example, the huge amounts of freshwater employed by hydraulic fracturing, and the final disposal for wastewater streams (which are discharged with high levels of pollution) represent a relevant challenge in order to avoid the contamination of superficial and underground water reservoirs. Besides, the environmental regulations for these streams are becoming stricter with the purpose to reduce the hazardous effluents; this task can be carried out through treatment systems with proved efficiency in this type of residual streams. In this regard, this work is aimed to deal with these challenges in shale gas industry. Then, the following case study is incorporated with the purpose to evaluate the capabilities of the proposed model formulation.

### Case study

The following case study is located in the northeastern of Mexico; in this zone, it is estimated an amount of technically recoverable shale reserves of 545 Tcf for natural gas. However, in Mexico the shale plays have not been exploited yet and as consequence there is more uncertainty in comparison with the documented shale plays in the USA. The investment, development and future production of this resource is led by PEMEX (Mexican governmental petroleum agency). Figure 3 shows the location for the potential shale reserves considered; however, this region presents critical conditions for the water scarcity and the study for the future implementation of hydraulic fracturing operations, where the freshwater resources are restricted, like in the proposed methodology, which represents a valuable tool to be taken into account. In this example, it considers the availability of three fracking crews to complete 20 wells during a time horizon of 52 weeks (a year). In this sense, Fig. 4 illustrates the well exploitation schedule according to a previous geographic and operation analysis where the first well pad has eight wells, the second is formed by seven wells, and finally the third is composed by five wells.

The hydraulic fracturing process requires a mixture of water, proppant materials and thickening agents to be pumped into the cracks of the fractures in the deep reserves

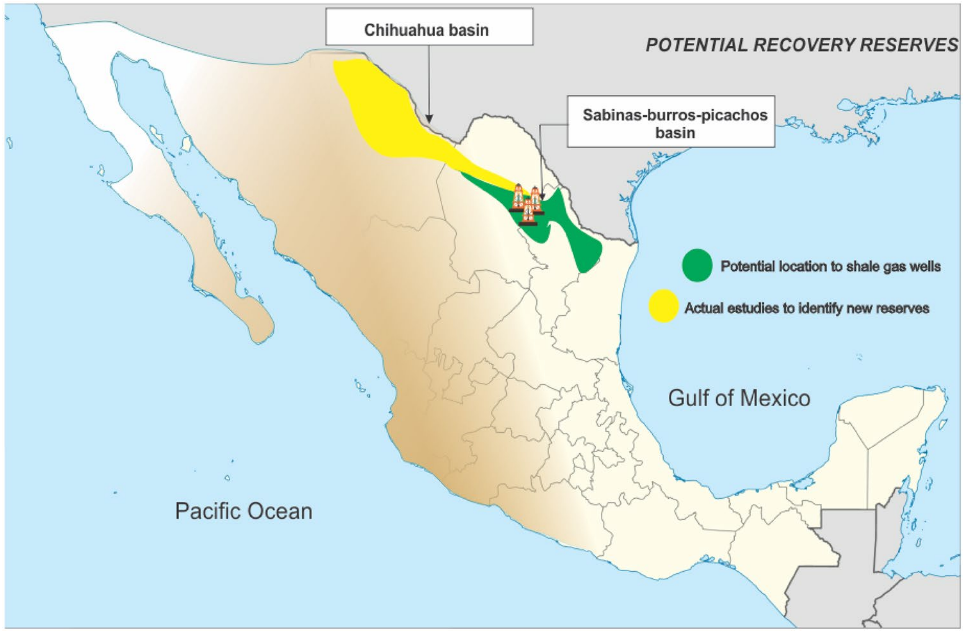


**Fig. 3** Location of the potential shale gas reserves according to studies by PEMEX

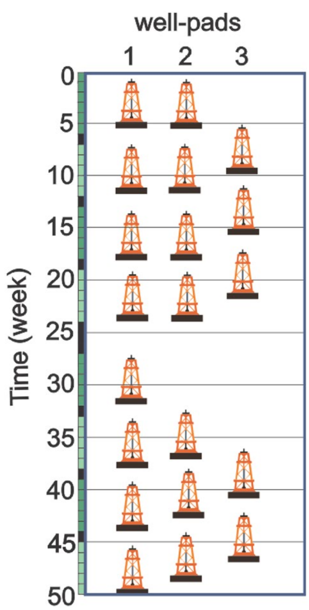


**Fig. 4** Schedule of exploitation for the shale gas pits

**Table 1** Environmental impact in eco-points for each component in the flowback fluid

| Compound | Individual environmental impact, E99/m$^3$ |
|---|---|
| Sodium | $3.23\times10^{-2}$ |
| Chloride | $1.14\times10^{-1}$ |
| Calcium | $1.02\times10^{-2}$ |
| Strontium | $1.73\times10^{-4}$ |
| Barium | $9.02\times10^{-4}$ |
| Sulfate | $2.33\times10^{-4}$ |
| Bromide | $6.79\times10^{-4}$ |

to release the trapped natural gas. However, depending on the geographical and geological conditions, the fracturing fluid must be prepared at different compositions. Typically, the consumption of water to be injected is estimated in 15,000 m$^3$ per well (this value is used by this work) and it is assumed that 35% of this amount returns to the surface (produced water) during the first three weeks after the completion phase; then, the flowback water is collected and sent to a storage system. Besides, the freshwater presents a TDS concentration of 500 ppm, whereas the concentrations of TDS for the produced water in the first, second and third week once the completion phase has finished are 75,000, 110,000 and 170,000 ppm, respectively. It should be noted that to obtain an adequately quantification for the environmental impact associated with wastewater streams, the composition of the flowback water streams based on TDS is not enough; consequently, there is requirement to know a wider chemical analysis. According to several studies, the average produced water is composed by 33% of sodium, 54% of chloride, 9% of calcium, 2.7% strontium, 0.6% of barium, 0.6% of bromide and finally 0.1% of sulfate (EPA 2011). Table 1 presents the individual environmental impact for each compound previously mentioned and defined by the life cycle analysis methodology.

On the other hand, the most common technologies employed in the treatment of produced water (with proven efficiency in shale gas industry) are forward osmosis, reverse osmosis, multi-effect flash, multi-effect distillation and

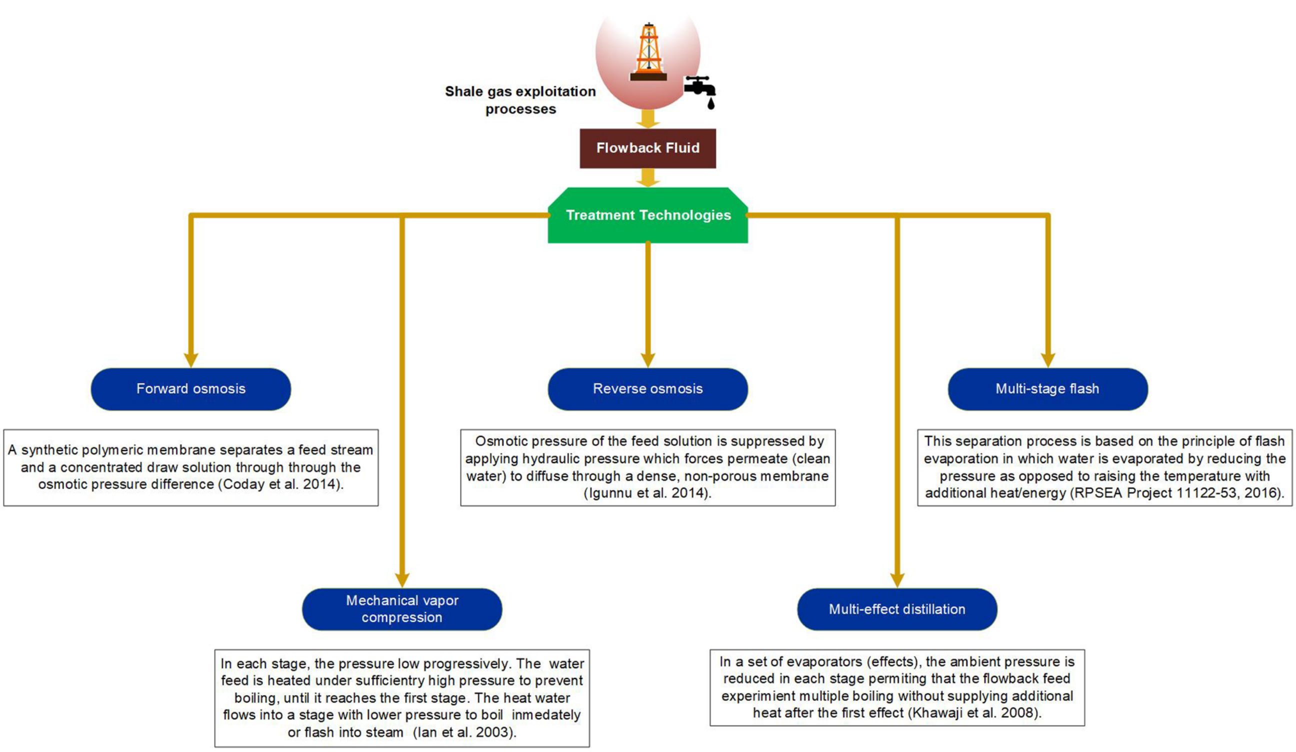


**Fig. 5** Treatment technologies for produced water

mechanic vapor compression. In this sense, Fig. 5 contains a brief description of the performance employed by each technology, whereas Table 2 presents the maximum TDS concentration at the inlet streams, maximum capacities and quality of outlet streams, as well as capital costs and operating cost for each of the abovementioned treatment units. It should be noted that forward osmosis has associated the most expensive costs (the capital cost is 5030 $/m^3$/d and the operation cost is 1.70 $/m^3$/d), and the capacity is really low but this unit involves the best recovery rates. Moreover, other important aspect is that after the processes some treated water can be recycled to wells to satisfy the consumption of water. But when the treated flowrate does not complete the regulations, some possibilities are considered in this work to dispose these streams to the environment as: additional treatment units, injection disposal wells, industrial use and discharging to a watershed; nevertheless, the limitation for effluents is fixed in 60,000 ppm of TDS when the final disposal corresponds to additional treatment units. While injection disposal in wells requires a maximum TDS value of 40,000 ppm with the purpose to mitigate the risks associated with the underground water reservoir contamination. In the industrial use case, the wastewater streams must not exceed a TDS concentration of 2000 ppm in order to avoid some operating problems such as brine incrustation in pipes and finally the environmental regulation to discharge the produced water over a watershed is of 800 ppm (EPA 2015).

Hence, all the previous information must be specified to implement the proposed methodology in the optimization software. In this context, the optimization approach

**Table 2** Summary of water treatment technologies (Coday et al. 2014; Arthur et al. 2005; Darwish et al. 2003; Drewes et al. 2009; El-Dessouky 2004; Ettouney et al. 2002; Igunnu and Chen 2014; Khawaji et al. 2008; McGinnis et al. 2013; Matz and Fisher 1981; Ophir and Lokiec 2004; Veza 1995; Wade 1993, 2001; Xu and Drewes 2006)

| | Technology | Maximum TDS concentration (mg/L) | Reference capacity (bpd)-(m$^3$/d) | Recovery rates | Capital cost (U$/m$^3$/d) | Operating cost ($/m$^3$) |
|---|---|---|---|---|---|---|
| 2 | Forward osmosis | 250,000 | 8 | 90% @ TDS 17,000 | 5030 | 1.70 |
| 4 | Reverse osmosis | 45,000 | 25,440 | 85% @ TDS 40,000 | 1905 | 1.38 |
| 3 | Multistage flash | 40,000 | 48,140 | 20% @ TDS 52,000 | 1830 | 1.45 |
| 5 | Multi-effect distillation | 100,000 | 48,140 | 35% @ TDS 58,000 | 2132 | 1.26 |
| 1 | Mechanical vapor compression | 200,000 | 5090 | 80% @ TDS 60,000 | 1510 | 2.83 |

corresponds to a MINLP (mixed-integer nonlinear programming) problem (It should be noted that the nonlinear terms appear in the capital cost functions, specifically in Eqs. 45–48.), and the proposed model was coded in GAMS® (General Algebraic Modeling System) using SBB solver (Brooke et al. 2018). This solver is based on the combination of the standard Branch and Bound (B&B) method for the mixed-integer linear programming part and some of the standard NLP solvers such as CONOPT, MINOS or SNOPT. The optimization problem involves 26,944 continuous variables, 14,568 constraints and 17 binary variables. While the CPU time depends on the analyzed scenario, therefore, an adequate interval is 2.5–15 s to obtain most solutions. Also, it is worth to mention that the optimization process was carried out with a processor Intel Core i7-3612QM at 2.10 GHz and 6 GB of RAM.

Furthermore, the multi-objective optimization problem considers two objectives that contradict each other (minimization of *TAC* vs. maximization of *IMPTOL*). It is important to clarify that *IMPTOL* represents an indirect measure of the pollutants removed by treatment technologies. It implies that when this objective is augmented, then the environmental impact decreases, but at the same time the *TAC* is increased (owing to the selection of more effective treatment units and typically these technologies are more expensive). In the contrary case, when the *TAC* is diminished, it generates a worst performance for *IMPTOL* (reducing its value) provoking a higher environmental impact. This phenomenon can be observed in Fig. 6, which shows the Pareto curve generated in this example. Notice that Point A (green point) represents the solution with the best performance for *TAC* (and at the same time the worst for *IMPTOL*). Whereas the opposite extreme solution is highlighted with Point C (red point), where *TAC* has the worst value but *IMPTOL* is significantly improved. Finally, the Pareto curve considers an intermediate solution with Point B (yellow point) in order to discuss a non-extreme solution. Also, notice that the freshwater consumption (this is a key criterion, which can play an important role in the selection of the final design) associated with each solution belonging to Pareto curve is presented in this Fig. 6. Table 3 contains the values of *TAC*, *IMPTOL*, *TWR* and the number of treatment, storage and disposal units required in solutions A, B and C. Therefore, each point of the Pareto curve (even the non-highlighted solutions) has involved different designs and configurations.

Additionally, the configuration for solution A is shown in Fig. 7. As it can be seen, this scheme requires two storage pits with the capacities of 2100 m$^3$ and 4950 m$^3$ to save the produced water leaving the well pads. The treatment system is composed by two forward osmosis units and a plant of mechanical vapor compression, while the second storage system requires three storage units with capacities of 670, 4950 and 700 m$^3$, respectively, and the final disposal selected is additional treatment. Figure 8 exhibits the optimal distribution for the water streams to properly operate in Point A. It should be noted that the freshwater is the main source to carry out the completion; nevertheless, in some

**Table 3** Results of the Pareto solution for the proposed case study

| Pareto solutions | A | C | B |
|---|---|---|---|
| TAC (US$/y) | $2.49\times10^6$ | $3.75\times10^6$ | $2.68\times10^6$ |
| IMPTOL (E99) | $6.65\times10^7$ | $1.02\times10^8$ | $9.60\times10^7$ |
| TWR (m$^3$/y) | $2.41\times10^5$ | $2.63\times10^5$ | $2.47\times10^5$ |
| Treatment units | 3 | 8 | 3 |
| Storage units | 2 | 3 | 1 |
| Final disposals | 1 | 2 | 1 |

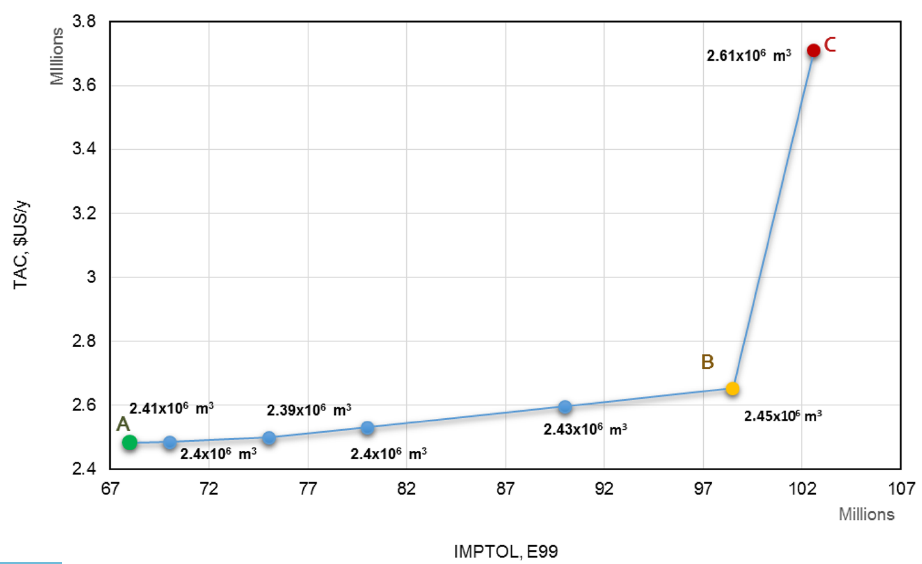


**Fig. 6** Pareto graph for the proposed optimization problem

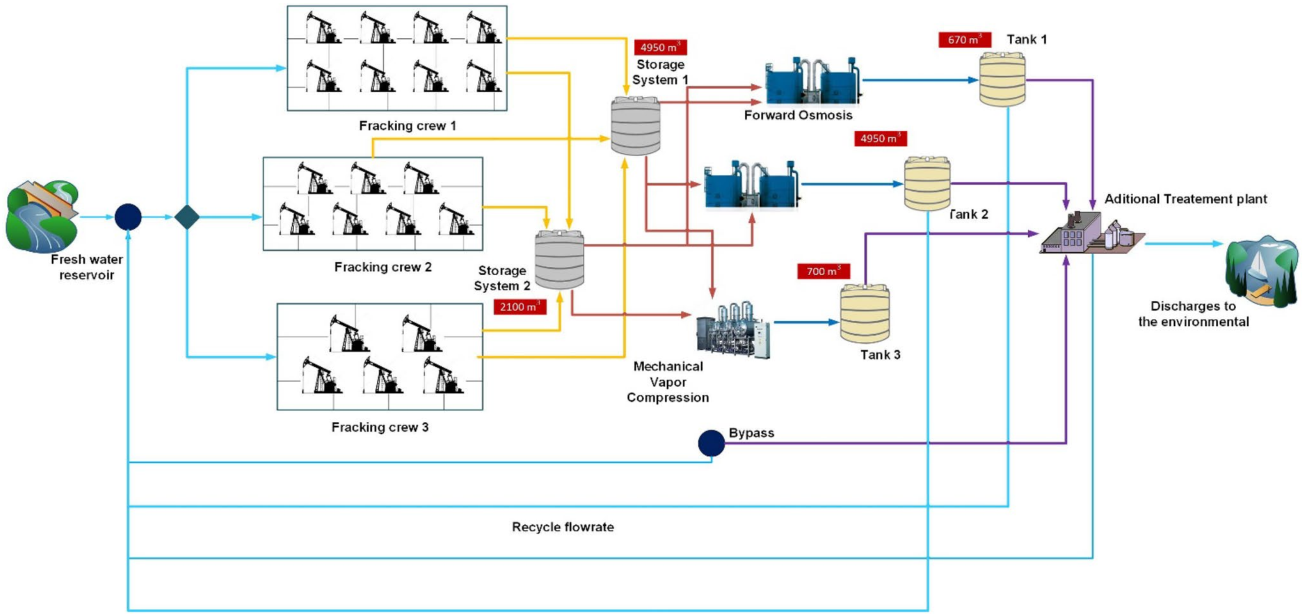


**Fig. 7** Configuration for solution A

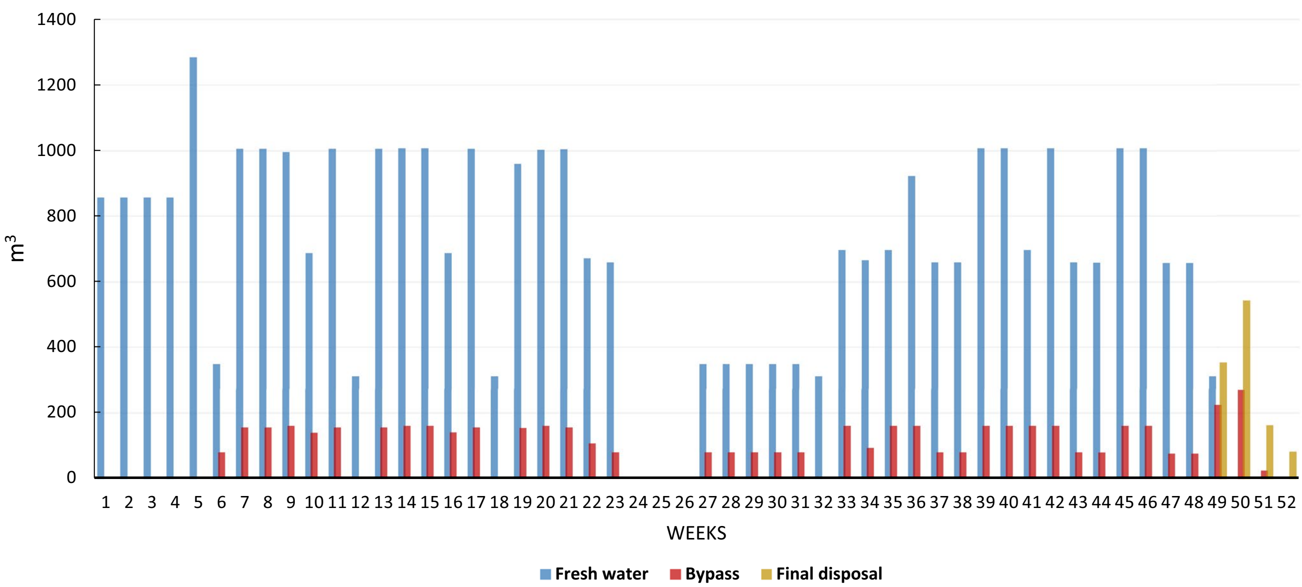


**Fig. 8** Water distribution in the water network for the solution A

periods (particularly in the middle of the year) the freshwater consumption is considerably reduced, because in these weeks the reused streams are employed in hydraulic fracturing processes. Another relevant event is that the wastewater streams are only disposed at the last weeks. Besides, Fig. 9 illustrates the optimal design for solution C, where *IMPTOL* is maximized (with the best environmental performance). Thus, more effective treatment technologies are selected; specifically, the interception network is constituted by forward osmosis, mechanical vapor compression, reverse osmosis and multi-effect distillation to improve, as much as possible, the quality of these water streams. In this way, the wastewater streams are able to be disposed in injection disposal wells (this option requires a strict environmental regulation) as well as in industrial uses. Figure 10 shows the water distribution for Point C, where it does not use the bypass stream with the purpose of prioritizing the pollutants removal and to increase the *IMPTOL* value. Finally, the optimal configuration and water streams distribution for Point B are shown in Figs. 11 and 12, respectively. In this regard, this

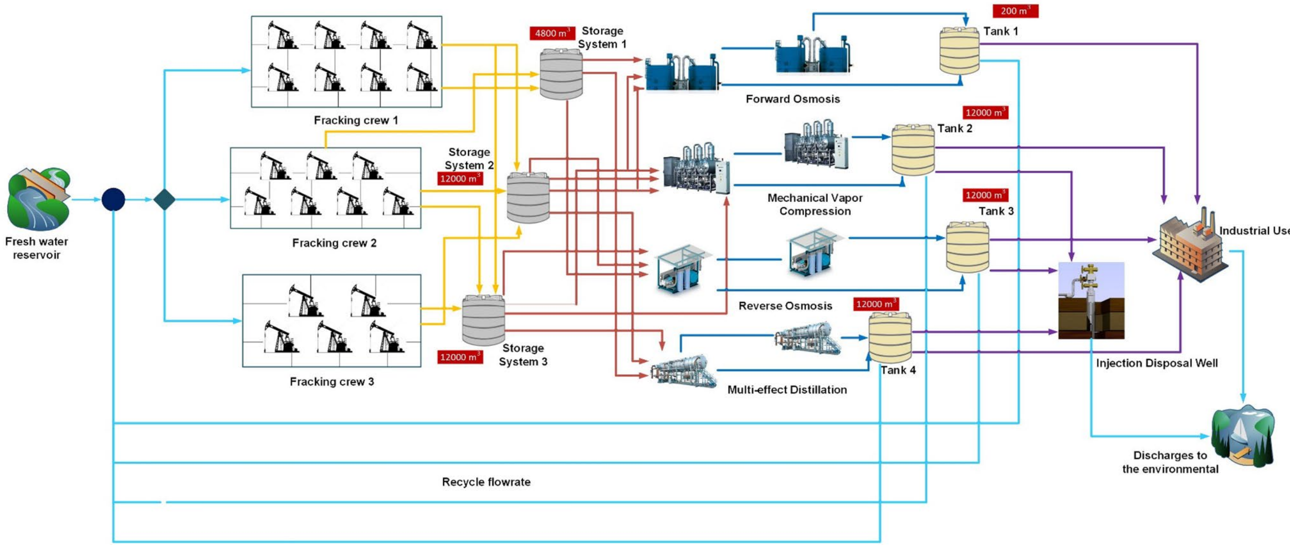


Fig. 9 Configuration for solution C

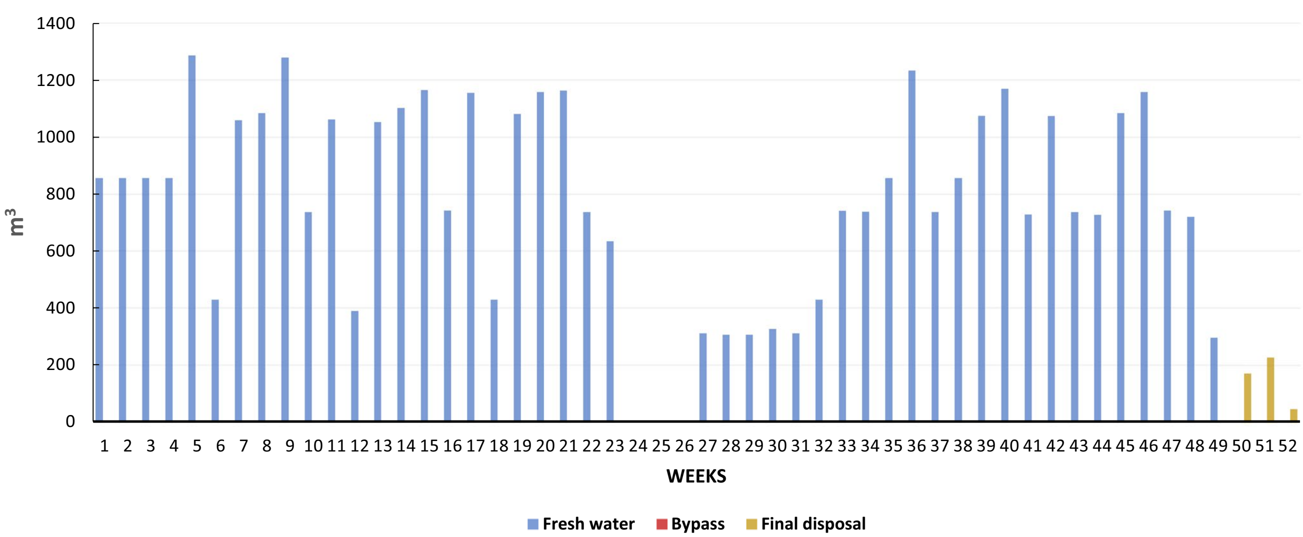


Fig. 10 Water distribution in the water network for the solution C

solution is analyzed to be considered an intermediate solution or breaking point because the *TAC* is reduced 40%, the *IMPTOL* is diminished 8.7% and *TWR* is 6.5% lower with respect to solution C; otherwise, when Point B is compared with Point A, the *TAC* augments 7.6%, whereas *IMPTOL* is increased 44.36%. In the optimal design for this case, only a storage pit is required (in the first storage system), two tanks (in the second storage system) and two treatment technologies (forward osmosis and mechanical vapor compression), and the final disposal selected is additional treatment. The water distribution seems similar to the first solution with minor differences.

As it can be seen in the three previously discussed solutions, there are important differences for the optimal configurations, the water network and for the objective functions, as well as for the total water requirements. For this reason, the Pareto curve is selected to show all the optimal solutions to the proposed methodology with the purpose to quickly visualize the main differences among them. It is worth mentioning that the selection of the final configuration must be taken by decision makers accounting for the most important aspects (such as total costs, environmental impact and freshwater consumption) and especially to the investors, government and society.

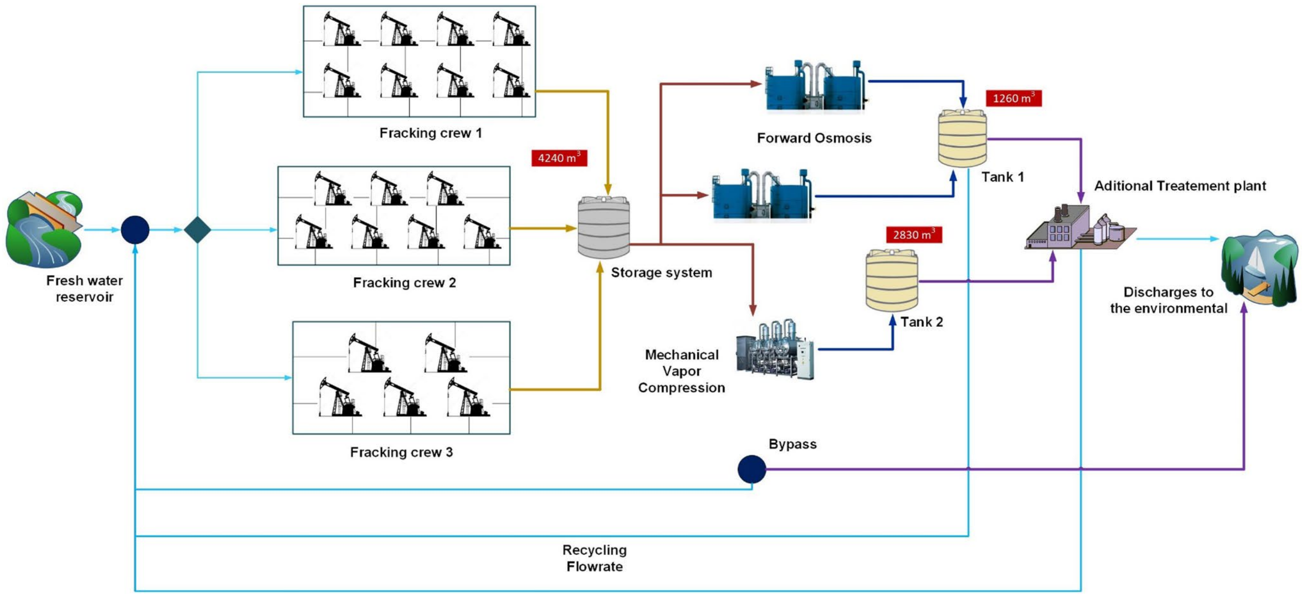


**Fig. 11** Configuration for solution B

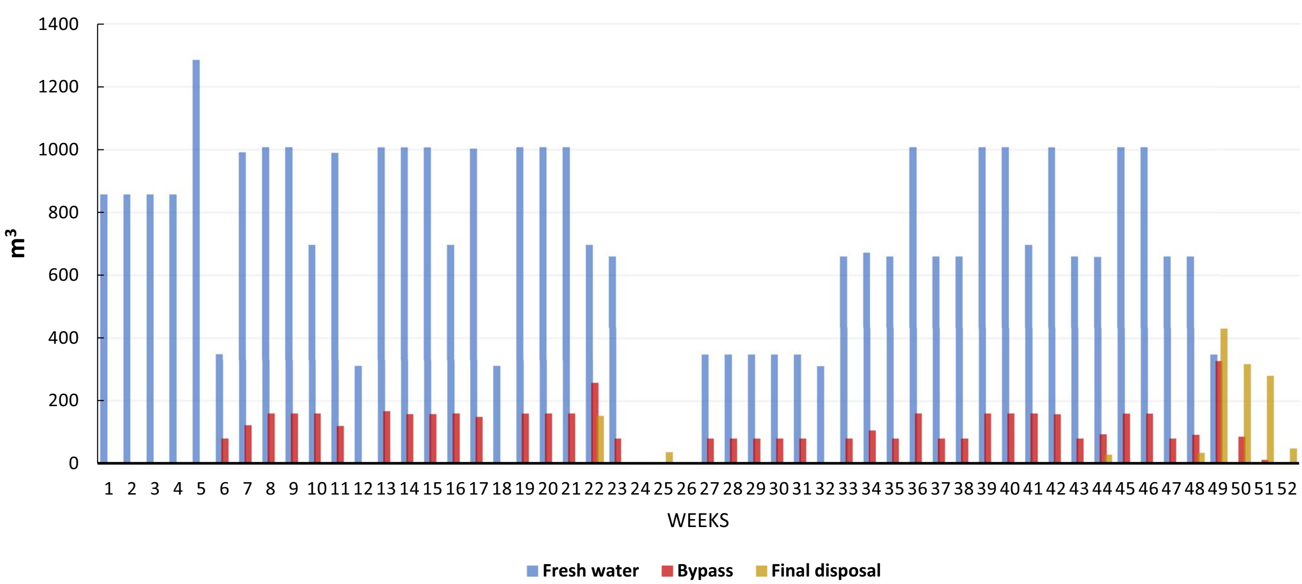


**Fig. 12** Water distribution in the water network for the solution B

## Conclusions

In this paper, a multi-objective optimization model is proposed to design water networks for the most important tasks in hydraulic fracturing. The solution of the proposed mixed-integer nonlinear programming problem is presented thought a Pareto set of optimal solutions, which show the tradeoffs between the economic and environmental objectives associated with shale gas exploitation. Specifically, the model formulation is aimed to minimize the total costs and simultaneously to maximize the removal of pollutants (this last effect minimizes the environmental impact). This approach is addressed to determine the freshwater requirements, amounts of flowback fluid collected and subsequently treated, reused and disposed, as well as the optimal capacities for storage and treatment units, including the selection of treatment technologies, quantify the flowrates for all the water streams considered by the superstructure and the selection of final disposals. Additionally, this work is useful to planning and scheduling the hydraulic fracturing operations dealing with challenges such as the freshwater availability due to the enormous water demand and the handling of wastewater disposal to avoid the polluted effluents that impact the environment causing contamination in underground and superficial water reservoirs and surrounding areas.

This paper also presented a case study to show the capabilities of the proposed approach. In this example, the most important differences in the optimal solutions were obtained when the economic or the environmental aspects are prioritized. In this sense, an intermediate solution was discussed with the purpose of highlighting the changes in the configuration involved in each case. In this type of methodologies (with two objectives that contradict each other), the Pareto curve is an attractive form to show the results due to the fact that it helps to identify the most important differences between the solutions. It is worth mentioning that the final design should be chosen by decision makers considering aspects, such as total costs, environmental impact and freshwater consumption, and especially to the investors, government and society. Finally, the proposed mathematical formulation is a general model and it can be applied to any case with the proper information.

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## Compliance with ethical standards

**Conflict of interest** The authors declare that there is no conflict of interests.

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