Environmental and Economic Water Management in Shale Gas Extraction.

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Abstract

This paper introduces a comprehensive study of the Life Cycle Impact Assessment (LCIA) of water management in shale gas exploitation. First, we present a comprehensive study of wastewater treatment in the shale gas extraction, including the most common technologies for the pretreatment and three different desalination technologies of recent interest: Single and Multiple-Effect Evaporation with Mechanical Vapor Recompression and Membrane Distillation. The analysis has been carried out through a generic Life Cycle Assessment (LCA) and the ReCiPe metric (at midpoint and endpoint levels), considering a wide range of environmental impacts. The results show that among these technologies Multiple-Effect Evaporation with Mechanical Vapor Recompression (MEE-MVR) is the most suitable technology for the wastewater treatment in shale gas extraction, taking into account its reduced environmental impact, the high water recovery compared to other alternatives as well as the lower cost of this technology. We also use a comprehensive water management model that includes previous results and discuss the main tradeoffs between optimal operation from the economic and environmental points of view.

Keywords: Life Cycle Assessment (LCA), Shale gas, Wastewater treatment, Thermal-based technology, Membrane distillation.

1. Introduction

Natural gas extracted from tight shale formations "shale gas" is playing an important role in satisfying the continuous increase in global energy demand. In the last year (2018) the primary energy consumption grew at a rate of 2.9% that is almost twice its 10 previous-year average growth, which was around 1.5% per year, and it was also the fastest since 2010 [1]. By fuel, energy consumption was driven by natural gas with a contribution greater than 40% of the increase. In 2018 natural gas consumption increased by 195 billion cubic meters (bcm), -a 5.3%- which is one of the fastest growths since 1984 [2].

In the year 2000, the contribution of shale gas to the natural gas production in the United States was close to 1%, in 2010 it was over 20%, and by 2035 it will be more than 46% of natural gas supply from shale gas [3]. According to a projection of the Energy Information Administration in 2050 the amount of natural gas produced from shale and tight oil formation will be over 75% of the total natural gas production in the United States [4]

The first extraction of shale gas was done in 1821 in Fredonia (New York). However, the horizontal drilling started in the 30s of the last century, and the first well was fractured in the United States in 1947. Since that time, the continuous advances in hydraulic fracturing and horizontal drilling technology have enhanced technically and economically the exploration of extensive shale gas formations in the United States [5–7], and they have significantly altered the global energy scenario for any foreseeable future [8,9]. Curiously, the public attention was focused on this issue only in 2007, when the «US Gas Committee» increased its estimations of unproven US gas reserves from 32.7 trillion cubic meters (tcm; 1tcm = 10^{12} m^3) to 47.7 tcm,- around 45% - [10]. The consequence of the increase in the supply of Natural Gas in the US produced a remarkable drop in the local natural gas prices. In the United States the average price between 2003 and 2008 was 242.2 \$ per thousand cubic meters (\$/Mm^3). It decreased to an average of 139.0 \$/Mm^3 in the period 2009-2011, and further decrease in the period 2012-2018 with an average value of 106.8 \$/Mm^3, with an even lower value in February 2012 of 86.9 \$/Mm^3.[2]. However, while in the United States the prices of natural gas decreased, in the rest of the world the prices have significantly increased. For example, in the OECD countries, the price increased from the 165.9 $/Mm^3 in 2003 to an average value of 614.4 $/Mm^3 in the period 2011-2014. Even though prices decreased to an average value of 309.4 $/Mm^3 in the period 2015-2018 (with a new important increment in 2018 -396 $/Mm^3-) the values are significantly larger than those in the United States [2].

Despite many countries having important reserves of shale gas, only the United States, Canada, China, and to a lesser extention Argentina and Australia, are currently producing shale gas at a commercial scale. Interestingly, the success of the «shale gas revolution» in the United States has not been replicated in other countries. Notwithstanding, in Europe for example, there is an important public and political opposition to hydraulic fracturing. Concerns on environmental impacts such as groundwater contamination, risk of earthquakes, greenhouse gas emissions, water consumption, or uncertainties about the correct management of water due to improper disposal of flowback and produced water, have led many countries to include moratoria subject to further research [11–13]. Despite the success in the United States, public opposition is growing, especially in Europe, and the debate is each time more polarized even though many times it is not based on scientific evidence.

Despite all its drawbacks, shale gas is considered an effective transition, in the short term, from fossil fuels to a future based on renewable energies by the substitution of coal-based energy [14]. Greenhouse gases (GHG) emissions in the production of electricity from shale gas are around 30-50% lower than those generated by coal [15,16]. However, from an environmental point of view, there is a growing concern that low gas prices increase the use of natural gas instead of developing the relatively more expensive renewables.

In the hydraulic fracturing, initially a vertical well is drilled and when the depth of the shale rocks is reached, the drilling turns in an angle to cover the layer in which the gas can be extracted. The horizontal drilling can be extended thousand of meters. Multiple wells can be drilled from a single surface pad, all of them with horizontal sections in such a way that a single wellpad can recover gas from around 1 km^2. Shale rocks have low permeability and consequently drilling alone is not enough to produce sufficient natural gas, so hydraulic fracturing is necessary [17]. In hydraulic fracturing, a fluid carrying a proppant and other compounds with different function are injected at high flow rates (up to 0.3 m^3 s^{-1}) and high pressures (480-640 bar) [18]. Wells are fracturing once after drilling in a set of stages (8-10 single fracturing stages per well).

One of the main environmental concerns of shalegas production is based on the large amount of water needed for the fracturing process. Production of shale gas involves around 7500 – 38000 m^3 of water per well. Within this amount, 90 % is required for the fracking process and the remaining 10 % is used for horizontal drilling activities [19]. A variable amount of water (between 10 % and 80 % of the injected fluid [20,21] is recovered in the first two weeks after beginning the process, which is known as "flowback water". However, the percentage of flowback water reported by other authors is quite different (between 8 – 15 % [22]) and values of 10 – 40 % [23], depending on the geology and the geomechanics of the formation. Thereafter, shale gas produced during the exploitation phase (~20 years) is accompanied by more water that is continuously recovered, known as "produced water" [24].

Thus, the physical and chemical properties of flowback water might vary significantly due to different factors such as the geology of shale formation, the interaction time between the fracking fluid and the rocks, and the input properties of the water used to fracture the well.

Flowback water is mainly composed of total dissolved solids (TDS), total organic carbon (TOC) and total suspended solids (TSS), among others [25,26]. Among all these contaminants, TDS (composed of salts, minerals and scaling ions with concentrations between 10,000 and 200,000 $mg \cdot L^{-1}$) separation is a difficult task due to the large amount of energy needed and the possible environmental impacts of high-salinity water disposal [23].

In addition to TDS, flowback water might also contain dissolved particles such as naturally occurring radioactive materials (NORMs) [27]. Within this group of NORMs, the most important are uranium, thorium, and radium, being the last most important because of its high solubility [28]. However, NORMs concentration in flowback water is lower than the content in other sectors, as in the medical and mining areas and, additionally, shale gas operations are the energy source with the lowest NORMs content [28]. As an example, in the case of Europe, data available up to now show that it has not been reported that any waste from hydraulic fracturing operations exceeds the restrictions allowed for radioactive materials in the UK [14]. For this reason, NORMs are not considered in the wastewater treatment of this paper. In any case, if these components were present, specific treatment should be also carried out [29].

Due to its physical and chemical properties, flowback water can be managed by different strategies, including disposal through Class II disposal wells, dispatch to other destinations such as a centralized water treatment facilities (CWT), or direct reuse in the drilling and fracturing operations of the well or subsequent wells.

Injection in Class II wells is the strategy most used in the USA. In fact, there are many places where local disposal is allowed, which makes the cost of water injection to be inexpensive. However, in other shale sites, there are no Class II wells and long distances must be traveled to inject the wastewater, which increases the cost [8]. It is not clear if, in Europe, injection in wells would be eventually an acceptable alternative for the disposal of flowback water [14]. For example, some reports refer to this decision as a possible solution in the UK. In addition, well injection has been correlated with seismic activity, whose contribution is significantly larger than hydraulic fracturing itself [30].

Nowadays, given the importance of water conservation, the best option is the direct reuse of the flowback water because it allows reducing freshwater consumption and the environmental problems associated with water management, such as transportation, disposal or treatment for its recovery. In any case, to guarantee adequate disposal to the environment and the final recovery of water, desalination post-treatment is receiving increased attention. Thus, [31] explored all the technical, economic and regulatory drivers that lead to the choice of desalination instead of injection disposal.

Effective desalination processes are needed in order to properly treat the high salinity of flowback water. Desalination processes include membrane-based technologies (such as reverse osmosis (RO) and forward osmosis (FO)) and thermal-based technologies, which comprise multistage flash (MSF) and single/multiple-effect evaporation (SEE/MEE) with/without thermal or mechanical vapor recompression (TVR/MVR). The most used technology in seawater desalination is RO, due to its economic performance. However, RO has the limitation of not being able to be used when TDS concentration is higher than ~40,000 – 45,000 mg/L [32]. Nevertheless, the critical point of FO is how to choose the right draw solution. Preferably, the desired draw solution has to be relatively cheap, must avoid fouling and have to be capable to provide sufficient high osmotic pressure to create a large flux across the membrane [33]. However, draw solutions have the disadvantage that they must be recovered in additional separation processes, which increase the cost of the process. Some of these limitations where solved combining FO and RO for shale water treatment [34]. Nevertheless, due to these limitations in the desalination of produced water, thermal desalination and membrane distillation are more attractive than membrane processes [31,35], and economically more efficient than membrane technologies. The objective of thermal desalination and membrane distillation is to recover treated water, reducing wastewater discharge and the corresponding water footprint.

In this sense, several studies have evaluated the carbon dioxide emissions of water management to estimate the environmental impacts of water and wastewater operations [36–39]. Just very few works have introduced other impact indicators in their studies, in addition to the global warming potential, such as fossil depletion, particulate matter formation, and human toxicity, among others [40–42]. Other studies have been focused on the design of shale gas supply chains for the optimal management of water [24,43–46].

At this point, it is important to remark that the main application of the previous environmental works was the estimation of greenhouse gas (GHG) emissions and the carbon footprint associated with the manufacture of shale gas [16,47,48]. However, none of these works has focused on studying the different alternatives for wastewater treatment and none of them shows a detailed and specific inventory of wastewater treatment. Therefore, in this paper we first address the life cycle impact assessment (LCIA) of three alternative desalination technologies for wastewater in shale gas extraction: Single-Effect Evaporation with Mechanical Vapor Recompression (SEE-MVR), Multiple-Effect Evaporation with Mechanical Vapor Recompression (MEE-MVR) and Membrane Distillation (MD). We analyze their corresponding LCIAs in order to compare their sustainability. This perspective also includes the analysis of the most common technologies for the initial pretreatment of this type of wastewater.

Furthermore, this work studies a wide range of environmental impacts, including the global warming potential, acidification potential, resource depletion, toxicities, etc. by using the ReCipe method [49] with different perspectives (mid and endpoint) from Ecoinvent database v.3.4.

In order to compare these new treatment alternatives, which might be promising for wastewater in the shale gas process, this paper is structured as follows: Section 2 introduces the life cycle assessment methodology and shows the alternatives studied for the wastewater treatment. In Section 3, we use the results of previous sections into a complete management model that takes into account the costs and environmental impacts of all activities related to water management in shale gas exploitation: Freshwater acquisition, transport to wellpads, freshwater storage, drilling, flowback water storage, wastewater pre-treatment(s), water reuse into the same wellpad to fracture other wells, transport of impaired water to other near wellpads (inter-wellpad recycling), on-site desalination, transport to Centralize Water Treatment Facilities and sludge and brine disposal. Finally, the conclusions and the list of references are provided at the end of the article.

2. Life Cycle Assessment Methodology

The Life Cycle Assessment (LCA) methodology is the most used technique to evaluate environmental impacts [50,51]. This method considers all the environmental characteristics and the potential impacts related to all phases of a product's life (that is, the supply of raw materials, the manufacturing of intermediates, and the final product, including storage, packaging, transportation, distribution, use and disposal of the product) [52]. Moreover, it helps to identify the activities with more negative environmental impacts and what damage categories are more relevant. This analysis allows defining the corresponding set of targets in order to develop more sustainable industrial processes and practices [52].

The LCA is implemented in four phases according to the standards [50,51]:

1. Goal and scope definition.
2. Life Cycle Inventory (LCI).
3. Life Cycle Impact Assessment (LCIA).
4. Interpretation.

The LCA begins with a clear explanation of the objective and scope of the study, which should be consistent with the purpose of the application. This phase considers the following points:

- The functional unit, which is essential to compare several alternatives.
- The system boundary.
- The political and/or technical decisions taken based on the results.

The LCI makes available all the information about the environmental contributions of all the inlet and outlet streams of the system.

In the LCIA phase, the classification of previous results into impact categories is carried out. Finally, all results are analyzed in the interpretation phase, drawing the conclusions and giving some recommendations.

ReCiPe 2008 method has been selected in this study for the impact assessment stage [49]. This methodology comprises eighteen impact subcategories at the midpoint level, and these midpoint subcategories are transformed and combined into three endpoint categories: ecosystem quality, human health, and resource depletion. **Figure 1** shows the relationships between LCI paramters, midpoint indicators and endpoint indicators according to RECIPE 2008..

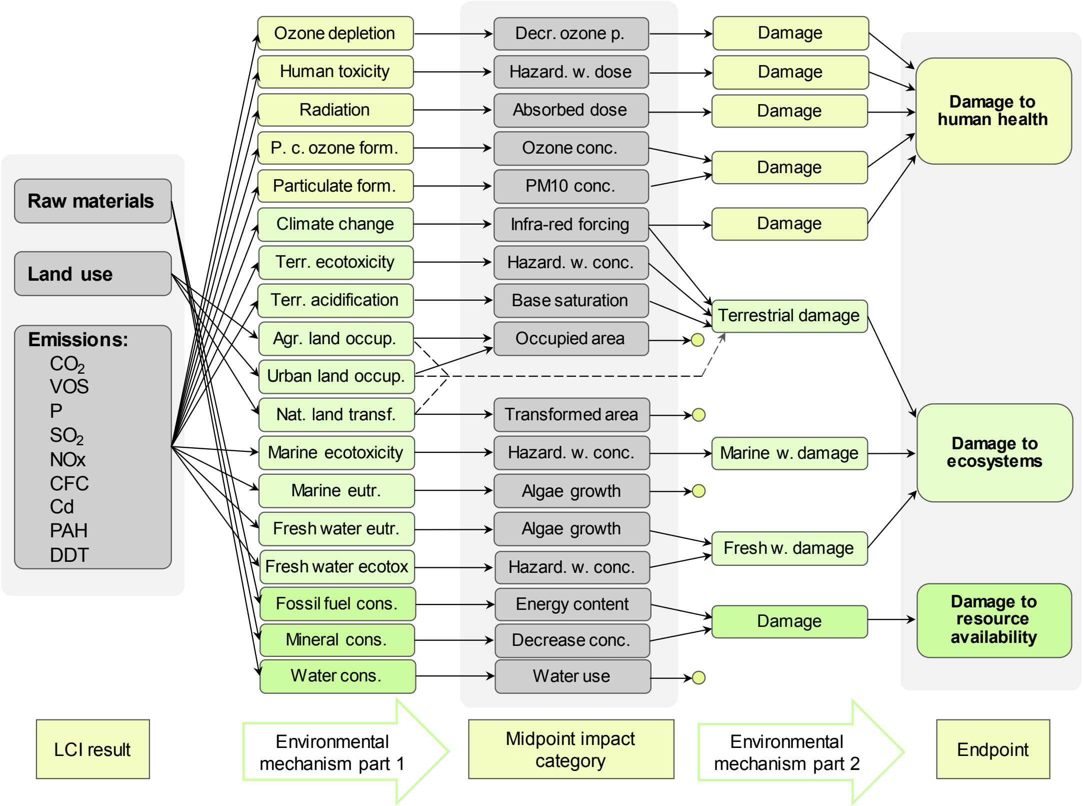

Figure 1. Relationship between LCI parameters (left), midpoint indicator (middle), and endpoint indicator (right) in ReCiPe 2008.

2.1. Modeling Assumption and System Boundary

The functional unit used in this work is the extraction of 1 m^3 of treated water for the comparison of wastewater treatment technologies, and 1dam^3 (1000 m^3) of produced gas for the complete managmement model. The system boundary for the wastewater treatment in shale gas extraction is shown in **Figure 2**. This includes freshwater consumption, the use of raw materials, energy and chemicals, wastewater treatment facilities and final disposals of waste material, such as the sludge and brine. The system boundary excludes the entire supply chain of shale gas extraction, processing, and distribution.

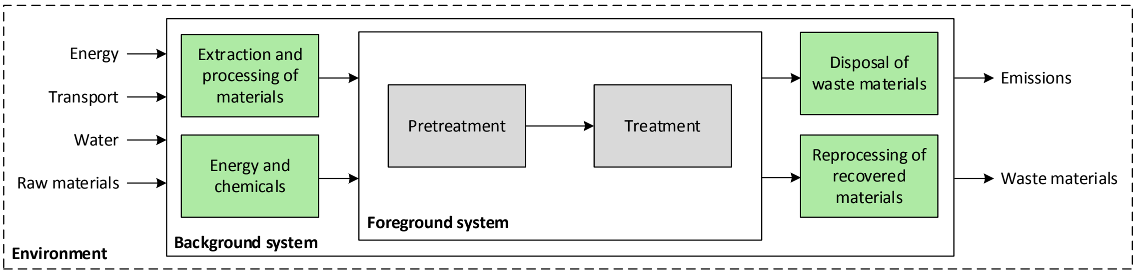

Figure 2. System boundary specific for wastewater treatment in shale gas extraction. Gray boxes correspond to the wastewater treatment and the green boxes identify the activities of the background system.

2.2. Wastewater Treatment

2.2.1. Initial Wastewater Pretreatment

A preliminary wastewater pretreatment has to be applied in order to prepare the wastewater for the selected desalination treatment or even for direct reuse on-site. There are some well-established treatment possibilities for the flowback water pretreatment, such as strainer filter, electrocoagulation, sedimentation, softening, etc.

The optimal pretreatment superstructure considered was obtained from the work by Carrero-Parreño et al. [53], where the optimal pretreatment arrangement is obtained depending on the input water properties and the desired destination of the wastewater. Our case study corresponds to the optimal pretreatment solution for a desalination treatment by membrane or thermal technologies in order to remove TDS content. Thus, the first stage of the pretreatment is a strainer filter, whose main objective is to eliminate large particles and sludge from flowback water. Secondly, the electrocoagulation stage eliminates many species that the strainer filter cannot remove, avoiding the use of additional chemicals such as coagulants ($Al_2(SO_4)_3$ or $FeCl_3$, among others). Then, the flocs formed are removed in a sedimentation tank and the resultant water is sent to a softener tank, where the lime-soda process is used to soften the water. This process removes Mg^{2+} and Ca^{2+} precipitated as calcium carbonate and magnesium hydroxide. After that, the wastewater is sent to the corresponding desalination process to remove the TDS content. In any case, especially working with membrane technology, an additional filtration might be needed for the membrane preservation by the use of ultrafiltration or cartridge filters. The sludge produced in the sedimentation tank and in the softening process is dispatched to a filter press, allowing filtered water returns to the beginning of the pretreatment plant to be further treated. The solid is handled as waste by an authorized manager.

The inventory data for the wastewater pretreatment system is given in **Table 1** and the inventory of potential emissions outputs is available in **Table 2**.

Table 1. Inventory data for the wastewater pretreatment. (Functional unit: m^3 treated water).

Parameter	Quantity	Units	Ecoinvent input
Pretreatment plant[*]			
Inlet flow	1.001	m^3/m^3 treated water	
Outlet flow	1.000	m^3/m^3 treated water	
Electrocoagulation			
Material – HDPE	$1.616 \cdot 10^{-4}$	kg/m^3 treated water	[GLO] market for polyethylene, high density
Electricity	4.336	kWh/m^3 treated water	[GB] market for electricity, high voltage
Sedimentation			
Electricity	$8.599 \cdot 10^{-3}$	kWh/m^3 treated water	[GB] market for electricity, high voltage
Steel	$8.799 \cdot 10^{-4}$	kg/m^3 treated water	[GLO] market for steel, chromium steel 18/8
HDPE	$5.799 \cdot 10^{-6}$	kg/m^3 treated water	[GLO] market for polyethylene, high density
Concrete	$9.999 \cdot 10^{-6}$	m^3/m^3 treated water	[RoW] concrete production, for civil engineering, with cement CEM II/B
Softening			
Material – Fiberglass	$4.483 \cdot 10^{-4}$	kg/m^3 treated water	[GLO] market for glass fiber reinforced plastic, polyamide, injection molded
Lime	0.199	kg/m^3 treated water	[GLO] market for lime
Soda	0.570	kg/m^3 treated water	[GLO] market for soda ash, light, crystalline, heptahydrate
Filter press			
Sludge inlet	1.218	kg/m^3 treated water	[RoW] drying, sewage sludge
Sludge outlet	0.616	kg/m^3 treated water	[GLO] market for sewage sludge, dried
Material – Polypropylene	$4.320 \cdot 10^{-5}$	kg/m^3 treated water	[GLO] market for polypropylene, granulate
Electricity	0.566	kWh/m^3 treated water	[GB] market for electricity, high voltage

[*] Source: Carrero-Parreño et al. [53]

Table 2. Inventory data for the potential emissions outputs of wastewater pretreatment.

Parameter	Quantity	Units
Pretreatment plant		
Emissions		
Sand (silica, quartz)	66.258	kg/m^3 treated water
Hydrochloric acid	1.469	kg/m^3 treated water
Petroleum distillate	0.367	kg/m^3 treated water
Isopropanol	0.367	kg/m^3 treated water
Potassium chloride	0.245	kg/m^3 treated water
Hydroxyethyl cellulose	0.245	kg/m^3 treated water
Ethylene glycol	0.184	kg/m^3 treated water
Sodium potassium hydroxide	$4.898 \cdot 10^{-2}$	kg/m^3 treated water
Ammonium persulfate	$4.898 \cdot 10^{-2}$	kg/m^3 treated water
Borate salts	$4.898 \cdot 10^{-2}$	kg/m^3 treated water
Citric acid	$1.837 \cdot 10^{-2}$	kg/m^3 treated water
Glutaraldehyde	$4.898 \cdot 10^{-3}$	kg/m^3 treated water
Formamide	$4.898 \cdot 10^{-3}$	kg/m^3 treated water
Diesel	9.304	kg/m^3 treated water
Polyacrylamide	0.556	kg/m^3 treated water
Sodium chloride	$5.831 \cdot 10^{-5}$	kg/m^3 treated water

2.2.2. Thermal-Based Technologies for the Wastewater Treatment

In this work, we have considered two thermal-based technologies of recent interest for the desalination process, based on the work by Onishi et al. [54], where a rigorous optimization model for the design of SEE/MEE systems that integrate MVR and heat recovery was introduced. The model was specially developed for the desalination of high-salinity produced water from the shale gas industry. The advantage of this technology relies on the improvement of energy efficiency, while a high freshwater recovery ratio is obtained and the brine disposal is reduced.

For the same ratio of recovery and water production, MEE-MVR arrangement seems to be the best desalination alternative for shale produced water. The main reason lies in the fact that it is less expensive and versatile than the SEE-MVR arrangement [54]. In this case, the optimal system is composed of two evaporation effects.

The inventory data for the thermal-based technologies are given in **Table 3**.

Table 3. Inventory data for thermal-based technologies. (Functional unit: m^3 treated water).

Parameter	Quantity	Units	Ecoinvent input
Single-Effect Evaporation with Mechanical Vapor Recompression (SEE-MVR)*			
Feed water	1.304	kg/s	
Nickel amount	$4.585\cdot10^{-3}$	kg/m^3 treated water	[GLO] market for nickel, 99.5%
Chromium steel amount	$5.047\cdot10^{-3}$	kg/m^3 treated water	[GLO] market for steel, chromium steel 18/8
Electricity	51.496	kWh/m^3 treated water	[GB] market for electricity, high voltage
Brine	93.064	kg/m^3 treated water	[RER] sodium chloride production, brine solution
Treated water	1.000	m^3/m^3 treated water	
Multiple-Effect Evaporation with Mechanical Vapor Recompression (MEE-MVR)*			
Feed water	1.304	kg/s	
Nickel amount	$3.212\cdot10^{-3}$	kg/m^3 treated water	[GLO] market for nickel, 99.5%
Chromium steel amount	$1.385\cdot10^{-3}$	kg/m^3 treated water	[GLO] market for steel, chromium steel 18/8
Electricity	29.188	kWh/m^3 treated water	[GB] market for electricity, high voltage
Brine	93.064	kg/m^3 treated water	[RER] sodium chloride production, brine solution
Treated water	1.000	m^3/m^3 treated water	

*Source: Onishi et al. [54]

2.2.3. Membrane Distillation Technology for the Wastewater Treatment

In this work, we have also considered a membrane-based technology from the work by Carrero-Parreño et al. [55] , where an optimization model for the optimal design of a multistage membrane distillation system is presented to recover treated water and brine near to the Zero-Liquid Discharge (ZLD) condition. An optimal membrane configuration including 3 stages is considered. The inventory data for the membrane distillation technology is given in **Table 4**.

Table 4. Inventory data for membrane distillation technology. (Functional unit: m^3 treated water).

Parameter	Quantity	Units	Ecoinvent input
Membrane technology*			
Feed water	2.985	m^3/m^3 treated water	
Electricity	8.310	kWh/m^3 treated water	[GB] market for electricity, high voltage
Cooling water	$1.204\cdot10^{5}$	kg/m^3 treated water	[Europe without Switzerland] market for tap water
Steam	$1.847\cdot10^{3}$	kg/m^3 treated water	[GLO] market for steam, in chemical industry
Membrane composition			
PTFE	$1.025\cdot10^{-3}$	kg/m^3 treated water	[GLO] market for polypropylene, granulate
PP	$1.377\cdot10^{-2}$	kg/m^3 treated water	[GLO] market for tetrafluoroethylene
Brine	607.433	kg/m^3 treated water	[RER] sodium chloride production, brine solution
Treated water	1.000	m^3/m^3 treated water	

*Source: Carrero-Parreño et al. (2017a)

2.4. Wastewater treatment results

The wastewater treatment process was modeled according to the data available in Ecoinvent database v.3.4 and ReCiPe 2008 characterization factors .

The environmental study was based on the LCA methodology, using ReCiPe Midpoint (H) and ReCiPe Endpoint (H, A) methods. These approaches allow the evaluation of several categories of environmental impact. Characterization factors at the midpoint level are focused on single environmental problems, while characterization factors at the endpoint level show the environmental impacts aggregated on three higher levels: human health, ecosystem quality and resource depletion [49]. Both approaches are complementary; the midpoint has a stronger relation to the environmental flows and has a lower uncertainty, while the endpoint shows an easier interpretation because it allows us to compare the indicators between them although it has a higher uncertainty [56].

In order to compare the total environmental impact of the three technologies that are studied, **Figure 3** illustrates the behavior of the treatment alternatives according to the production of 1 m^3 of treated water at the endpoint level, by using the hierarchical (H) perspective, based on the most usual policy principles, and the average (A) weighting. As can be seen, membrane technology has the highest environmental impact (in all damage categories). The total LCIA associated with the wastewater process reaches approximately 73.2 points/m^3 of treated water using membrane technology and this impact reaches approximately 6.0 points/m^3 treated water using MEE-MVR, which is around 91.8 % lower. This result is due to the use of steam needed as driving force in membrane distillation. From the environmental point of view, MEE-MVR has resulted to be the best alternative for the wastewater treatment in shale gas extraction because this technology uses less electricity than the SEE-MVR configuration (MEE-MVR has a total environmental impact 21.9 % lower than SEE-MVR technology).

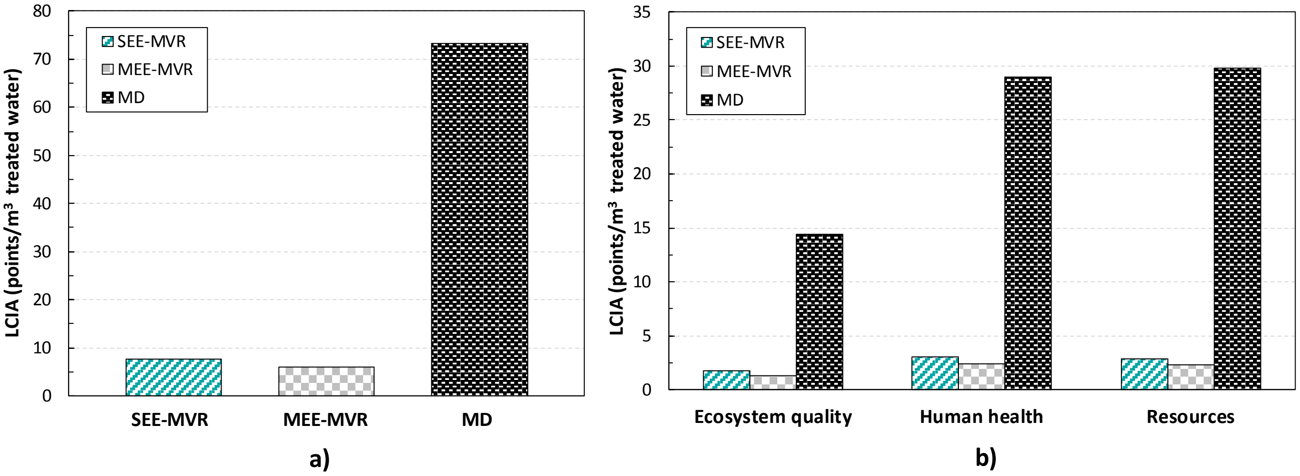

Figure 3. Comparison of the environmental impact of the three technologies. a) Total LCIA using ReCiPe Endpoint (H, A). b) LCIA of the main damage categories using ReCiPe Endpoint (H, A).

Additionally, in order to study the influence that each desalination technology has on the different subcategories **Figure 4** shows the contribution of each damage subcategory at the Endpoint (H, A) level in arbitrary units.

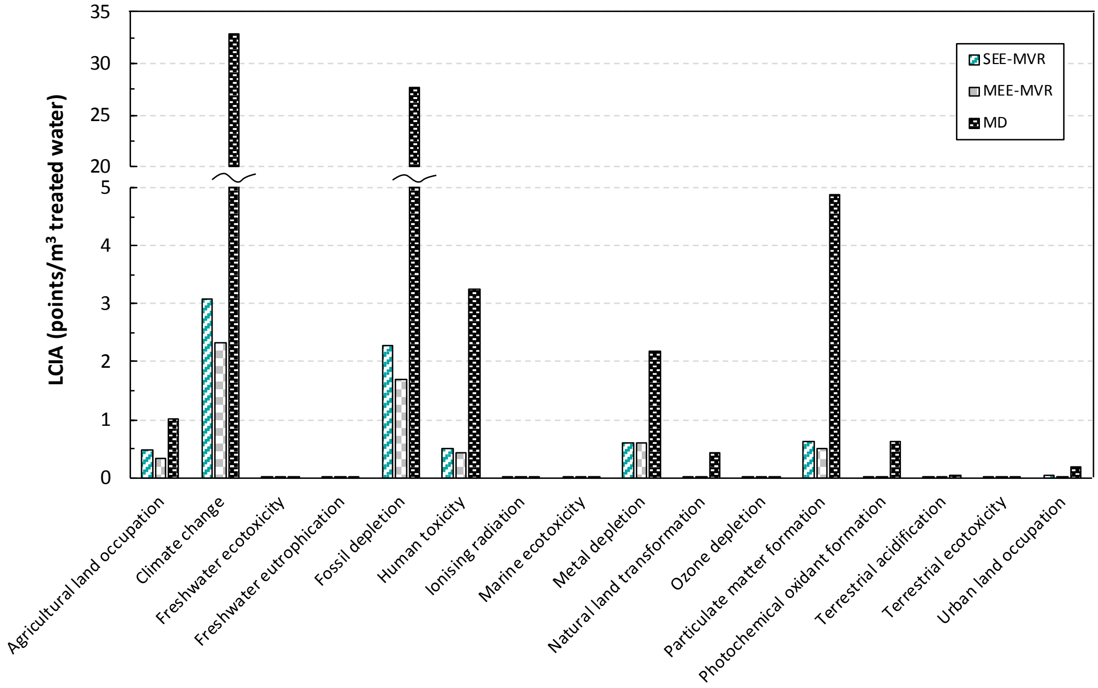

Figure 4. Comparison of the environmental impact subcategories using ReCiPe Endpoint (H, A).

As can be observed, the most affected damage subcategories by the wastewater treatment processes are climate change and fossil depletion due to the use of electricity and steam in the case of membrane distillation, and due to the use of electricity in the case of evaporation technologies. This result is in acconcordance with previous studies, whose their main focus was the estimation of GHG emissions associated with water management of shale gas process [36–39].

Although the rest of the subcategories are not really affected by wastewater treatments, the six more affected are shown in **Figure 5** in their corresponding units at the Midpoint (H) level. The remaining figures for the eighteen ReCiPe damage subcategories are available in the **Supplementary Material**. For all the cases, membrane distillation has the highest impacts compared to thermal desalination technologies and, among them, MEE-MVR has lower impacts in all categories.

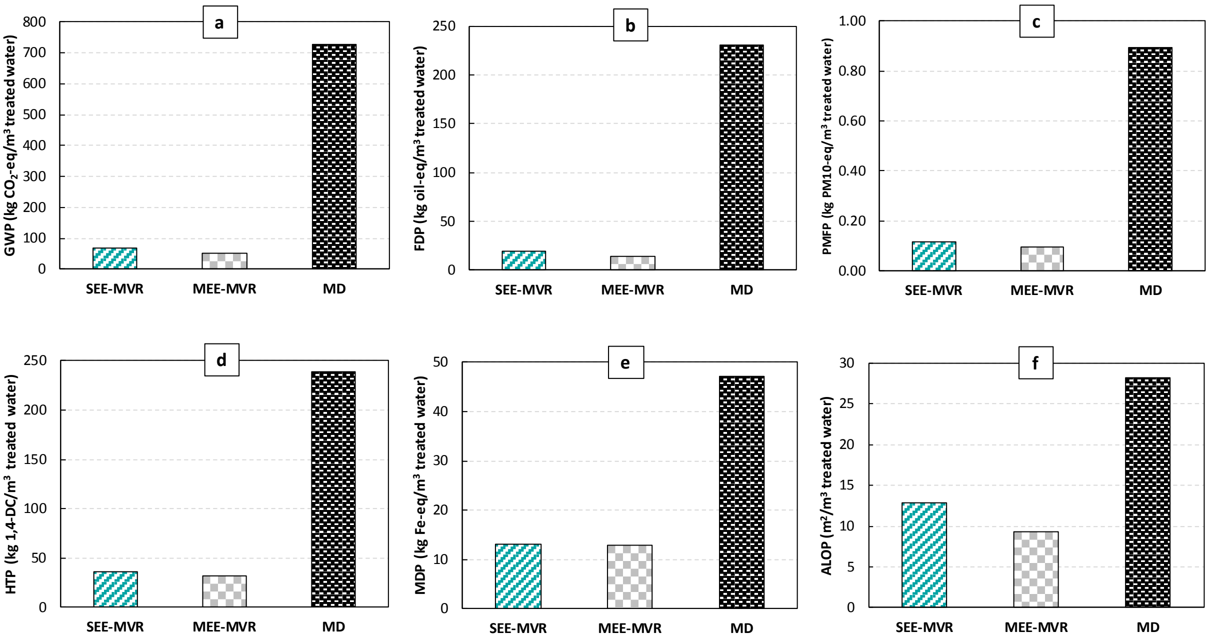

Figure 5. Environmental impact subcategories most affected by wastewater treatment: a) Global warming potential (GWP), b) Fossil depletion potential (FDP), c) Particulate matter formation potential (PMFP), d) Human toxicity potential (HTP), e) Metal depletion potential (MDP), and f) Agricultural land occupation potential (ALOP).

On the other hand, in order to evaluate the whole sustainability of the process, it is also interesting to compare the results obtained in our environmental study with other factors, such as the cost of each technology. In this sense, a comparison between the total impact and the cost of all the technologies (based on the works by Carrero-Parreño et al. [55] and Onishi et al. [54]) is shown in **Figure 6**.

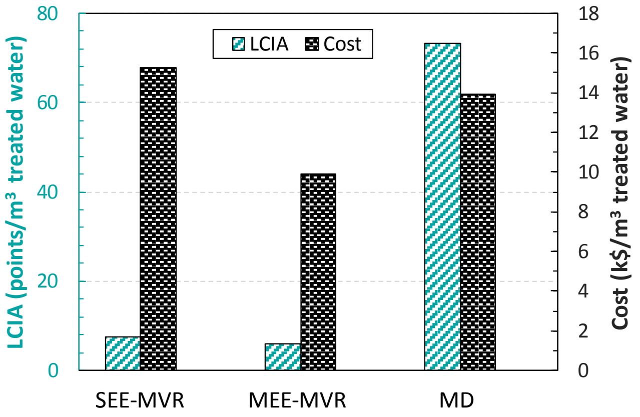

Figure 6. Comparison of the environmental impact subcategories.

The multiple-effect evaporation (MEE-MVR) system is around 35% less expensive than the SEE-MVR system, as was shown in the publication by Onishi et al. [54]. On the other hand, membrane distillation has a high cost due to the expensive cost of the steam used during the process. At the same time, MEE-MVR is the most environmentally friendly technology, which has a total environmental impact of around 91.8 % lower than membrane distillation.

Another important aspect to take into account is the amount of water recovered by each technology. In this way, a high rate of recovery should be obtained with the optimal configuration, at the same time that the brine removal should be near the zero liquid discharge (ZLD) strategy [54,55]. Thermal desalination technologies allow recovering approximately 76.7 % of water (regarding the inlet flow), while membrane distillation allows recovering approximately 33.5 % of water.

Due to the lower environmental impact, lower cost and higher water recovered, we can conclude that MEE-MVR is the most suitable technology for the wastewater treatment in shale gas extraction. For this reason, a more detailed study is presented for its optimal configuration. **Figure 7** illustrates the environmental contributions of all the stages of the MEE-MVR treatment.

Electricity used during the evaporation and the sedimentation stage is the factor that most influences the environmental impact, followed by brine discharge.

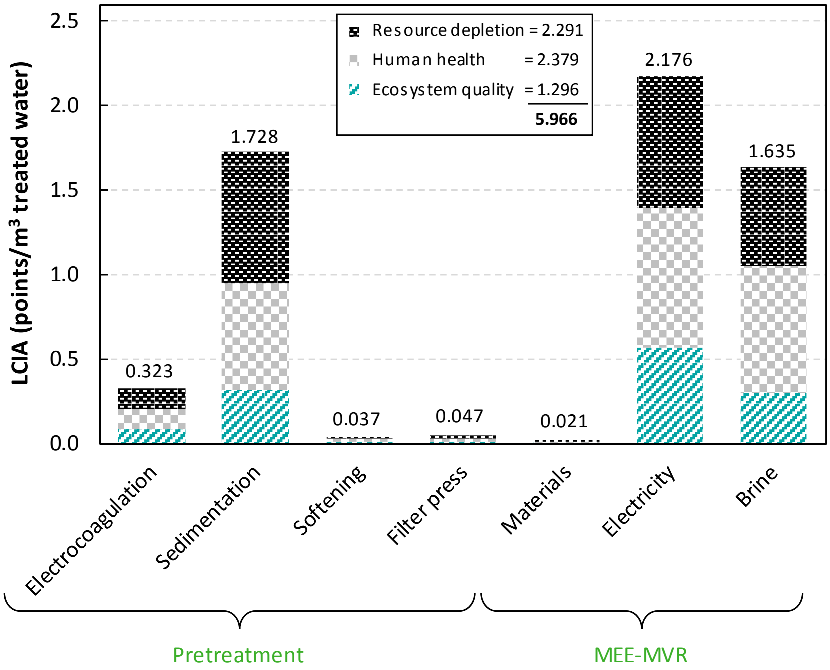

Figure 7. Environmental impact contributions of all the wastewater treatment stages in the optimal alternative (pretreatment + MEE-MVR) using ReCiPe Endpoint (H, A).

3. Economic vs LCA of the complete water management in shale gas exploitation.

In previous sections, we studied the pre-treatment and desalination stages related to flowback water in shale gas. However, to get a complete view of the relative importance of each one of the alternatives involved in shale gas exploitation, it is necessary to take into account the whole supply chain, and simultaneously consider the cost and environmental impacts of all the alternatives involved in shale gas water management. To that end, we adapted the model proposed by Carrero Parreño et al [57]. A brief description of the model capabilities is as follows:

A given company wants to fracture a set of wells distributed in different wellpads (typically a wellpad has between 6 and 20 wells) inside a period of time (i.e. one year). To that end, the company must decide, among a set of available freshwater sources, how much and when to acquire the water from each water source, and what quantity must be transported to each of the wellpads. The water is then stored in freshwater tanks until it is used to frack the different wells in each wellpad. The company must decide the optimal volume of each one of these tanks that will depend on the water availability and water demand in all the water-related activities. Once a well is fractured, there is a continuous flow of water (flowback water) that reaches the surface. This wastewater must be stored in appropriate tanks. Then this water can be sent to pre-treatment for posterior desalination in on-site facilities, It can be sent to a centralized water treatment facility, re-used in the fracture of other wells into the same wellpad, or sent to other wellpads of the same company with the objective of saving freshwater usage and reduce costs and environmental impacts.

The company should have data about the time to complete fracking operations, expected flow profile of flowback /produced water and gas release for each well as well as the gas prices. With that information, the company must decide the schedule of fracking activities in each wellpad and coordinate all water flows. A comprehensive description of the model is too large to be included here but a comprehensive description can be found in the **Supplementary Material**.

The following assumptions were made in the formulation of the model:

1. A fixed time period is discretized into weeks as time intervals.
2. Water transportation is only executed by trucks (the model can be easily extended to deal with transportation by pipes as well).
3. The volume of water used to fracture a well must be available when needed –this includes the possibility of storage in tanks, or a ‘just in time water availability’–, including water required in drilling, construction, and completion.
4. The amount of water needed to carry out all the operations, as well as the variation in flowback water with time after the wells are turned in operation is known a priory.
5. The well is turned in operation immediately after the drilled activities are finished.
6. The amount of gas that releases and its variation with time after the wells are turned in operation are known a priori.
7. Forecast of gas prices for the complete time period are known a priori.

Figure 8 shows graphically a superstructure that includes all the alternatives commented.

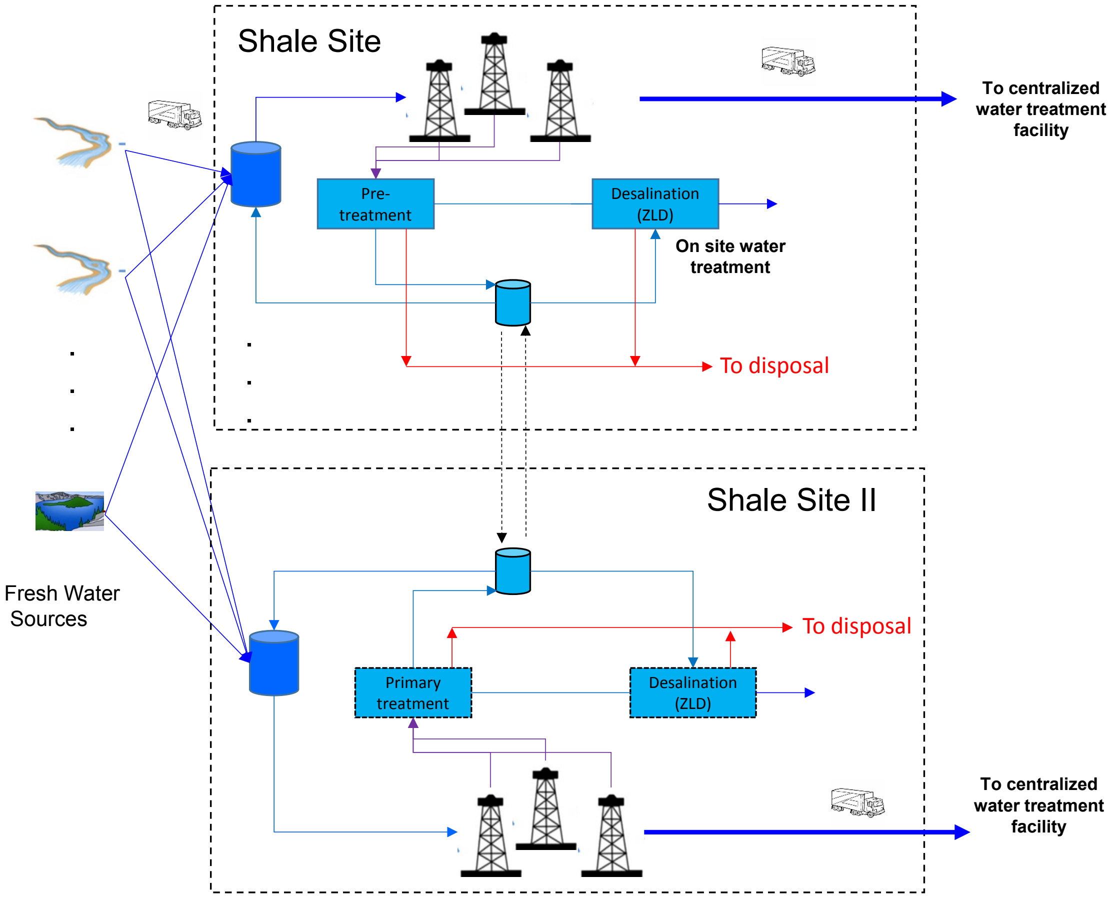

Figure 8. Superestructure of alternatives for the water management model. It includes different freshwater sources, a variable number of wells in each wellpad, freshwater tank(s), flowback water pre-treatment and desalination, waste water storage, inter and intra wellpad(s) recycling, centralized water treatment facilities and disposal sites.

For the environmental study, we follow the same approach as in the case of pre-treatment and desalination through the LCA methodology, using ReCiPe Midpoint (H) and ReCiPe Endpoint (H, A) methods. Data for LCIA inventory for water acquisition, freshwater and wastewater transport by trucks, etc. were obtained from the Ecoinvent database. v.3.4 and ReCiPe 2008 characterization factors. For the pre-treatment, we use the optimal configuration presented by Carrero-Parreño et al [53] and the impact factors obtained in previous sections. For the on-site desalination, we use the MEE-MVR configuration that has proved to be the best alternative from both the economic and environmental points of view. **Table** 5 shows the midpoint indicator for transport, water extraction, disposal, pre-treatment and treatment used in the LCA. In this case, all the impacts will be presented by dam^3 of produced gas.

Table 5 (a). ReCiPe Endpoint (H,A) indicator of ecosystem quality.

	Ecosystem quality									
	units	freshwater ecotoxicity	natural land transformation	marine ecotoxicity	climate change	terrestrial acidification	terrestrial ecotoxicity	agricultural land occupation	freshwater eutrophication	urban land occupation
Transport	points/T·km	$4.197\cdot10^{-7}$	$1.416\cdot10^{-4}$	$2.170\cdot10^{-7}$	$1.597\cdot10^{-3}$	$6.217\cdot10^{-6}$	$1.951\cdot10^{-5}$	$4.405\cdot10^{-5}$	$6.753\cdot10^{-7}$	$4.131\cdot10^{-4}$
Water extraction	points/kg	$4.876\cdot10^{-9}$	$7.197\cdot10^{-8}$	$9.823\cdot10^{-10}$	$3.247\cdot10^{-6}$	$1.049\cdot10^{-8}$	$2.851\cdot10^{-9}$	$7.656\cdot10^{-7}$	$1.785\cdot10^{-8}$	$8.810\cdot10^{-8}$
Disposal	points/kg	$6.248\cdot10^{-6}$	0.000	$2.532\cdot10^{-7}$	0.000	0.000	$1.374\cdot10^{-5}$	0.000	0.000	0.000
Pretreatment	points/kg	$7.045\cdot10^{-7}$	$4.649\cdot10^{-6}$	$1.490\cdot10^{-7}$	$3.104\cdot10^{-4}$	$9.500\cdot10^{-7}$	$3.357\cdot10^{-7}$	$8.978\cdot10^{-5}$	$7.351\cdot10^{-7}$	$8.831\cdot10^{-6}$
Treatment	points/kg	$5.748\cdot10^{-7}$	$9.257\cdot10^{-6}$	$1.249\cdot10^{-7}$	$4.390\cdot10^{-4}$	$1.646\cdot10^{-6}$	$5.473\cdot10^{-7}$	$1.892\cdot10^{-4}$	$1.441\cdot10^{-6}$	$1.462\cdot10^{-5}$

Table 5 (b). ReCiPe Endpoint (H,A) indicator of human health.

	Human health						
	units	photochemical oxidant formation	ozone depletion	particulate matter formation	ionizing radiation	climate change	human toxicity
Transport	points/T·km	$2.705\cdot10^{-5}$	$9.087\cdot10^{-7}$	$1.385\cdot10^{-3}$	$2.400\cdot10^{-6}$	$2.527\cdot10^{-3}$	$4.319\cdot10^{-4}$
Water extraction	points/kg	$2.687\cdot10^{-8}$	$7.558\cdot10^{-10}$	$1.507\cdot10^{-6}$	$3.010\cdot10^{-8}$	$5.137\cdot10^{-6}$	$1.698\cdot10^{-6}$
Disposal	points/kg	0.000	0.000	0.000	$1.580\cdot10^{-8}$	0.000	$5.524\cdot10^{-4}$
Pretreatment	points/kg	$6.333\cdot10^{-6}$	$3.377\cdot10^{-8}$	$2.002\cdot10^{-4}$	$3.445\cdot10^{-7}$	$4.911\cdot10^{-4}$	$7.862\cdot10^{-5}$
Treatment	points/kg	$5.911\cdot10^{-6}$	$6.604\cdot10^{-8}$	$2.283\cdot10^{-4}$	$9.430\cdot10^{-7}$	$6.945\cdot10^{-4}$	$2.670\cdot10^{-4}$

Table 5 (c) . ReCiPe Endpoint (H,A) indicator of resource depletion.

	Resource depletion		
	units	metal depletion	fossil depletion
Transport	points/T·km	$1.195\cdot10^{-4}$	$4.300\cdot10^{-3}$
Water extraction	points/kg	$1.902\cdot10^{-7}$	$6.173\cdot10^{-6}$
Disposal	points/kg	0.000	0.000
Pretreatment	points/kg	$3.707\cdot10^{-4}$	$5.397\cdot10^{-4}$
Treatment	points/kg	$1.664\cdot10^{-4}$	$8.621\cdot10^{-4}$

3.1. Case Study

The case study selected represents a possible typical situation for a shale company. Data are based on average values for the Marcellus basin. In this example, the company has to manage four wellpads separated from each other between 20 and 30 km. Therefore, the company considers that recycling water between the different wellpads could be a profitable strategy to reduce fresh water consumption. The company identified three possible freshwater sources placed between 25 and 65 km from the different wellpads. The four wellpads have 6, 8, 7 and 6 wells respectively, and the company wants to fracture all of them inside a period of 1 year. Based on their previous experience and knowledge of the basin characteristics, the company knows the water demand of each well, the expected variation with time of the flowback water, and the variation with time of gas release in each well. We assume that the company has a precise forecast of natural gas prices for the period considered.

The company is also interested in studying the possibility of installing on-site water treatment units in some (or all) wellpads or send the water to a centralized water treatment facility (CWT)

The problem requires a large amount of data, and therefore for the sake of clarity, we present all data needed in the case study in the **supplementary material.**

The resulting optimization model takes the form of a multi-objective mixed-integer linear programming problem (MO-MILP) in which we want to simultaneously maximize the profit and minimize the environmental impacts. In order to avoid the large dimensionality of dealing with all the mid-point categories, we focus our attention on the three end-point categories: Ecosystems Quality; Human Health; and Resources Depletion and the aggregated end-point. Initially, we consider a bi-objective optimization problem minimizing the aggregated end-point and maximizing the gross profit. Using the epsilon-constrained method [58,59] it is possible to generate the Pareto curve -shown in **Figure 9**-. If for each of the points in the Pareto surface we calculate the individual contribution of the three end-point environmental impacts we can see that they are correlated –**See Table 6**-. Therefore, just considering the aggregated end-point is enough to capture all the trade-offs between maximizing the profit and minimizing the environmental impact.

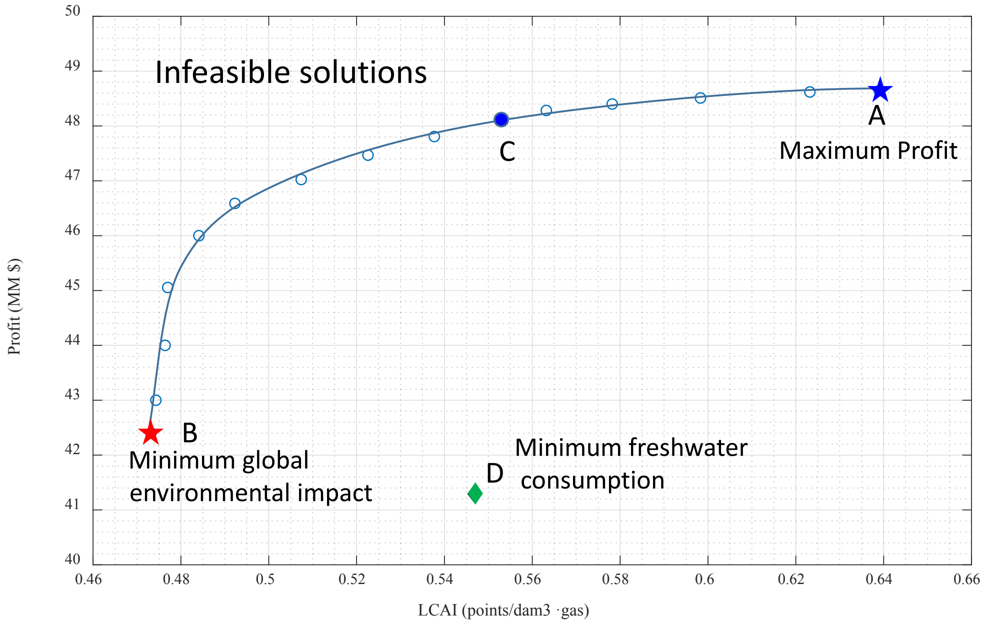

Figure 9. Pareto curve for the minimization of the global LCIA environmental impact and maximization of the gross profit. The point A is the maximum profit, B is the minimum global environmental impact. Point C is a point in which the profit decreases only a 1.06% while the environmental impact decreases in a 13.5%. Point D is the optimal solution when we minimize the freshwater consumption.

Table 6. Optimal points on the Pareto curve for the simultaneous maximization of profit and minimization of Agregated LCIA end point impact. Individual values of the three end-point categories (Ecosystem quality, Human Health and Resources Depletion) are also provided.

Profit (k$)	**Ecosystem Quality (points/dam^3)**	**Human Health (points/dam^3)**	**Resources Depletion (points/dam^3)**	**Aggregated end-point (points/dam^3)**	**FreshWater consumption (m^3)**
48643.0	0.1288	0.2522	0.2580	0.6390	178893.8
48620.0	0.1257	0.2459	0.2517	0.6232	178893.8
48510.7	0.1206	0.2360	0.2417	0.5983	178893.8
48400.1	0.1166	0.2282	0.2334	0.5782	167470.0
48282.6	0.1135	0.2222	0.2274	0.5632	167470.0
48129.5	0.1115	0.2182	0.2233	0.5529	164989.5
47807.7	0.1084	0.2122	0.2170	0.5377	157453.7
47468.1	0.1054	0.2063	0.2110	0.5226	155745.1
47024.1	0.1023	0.2003	0.2048	0.5074	149376.2
46588.4	0.0993	0.1944	0.1987	0.4923	146314.2
46000.0	0.0972	0.1913	0.1956	0.4841	144920.0
45055.0	0.0962	0.1883	0.1925	0.4770	141947.8
44000.0	0.0961	0.1881	0.1923	0.4764	141882.5
43000.0	0.0956	0.1873	0.1914	0.4743	141105.5

42404.0	0.0954	0.1870	0.1908	0.4732	139713.6

The **point A in Figure 9** corresponds to the maximum profit (MM$ 48.643) with an aggregated impact of 0.6390 points/dam^3·gas. **Point B in Figure 9** corresponds to the minimum environmental impact (0.4732 points/dam^3·gas) that is a reduction in environmental impact around 25.9%, with a gross profit of MM$ 42.404 that corresponds to a reduction in profit of around 12.8%. This result coincides with the intuition that indicates that when we operate at the optimal conditions, we can only reduce the environmental impacts by reducing the benefits (or, of course introducing some technological improvements). However, the most interesting part of the Pareto curve of **Figure 9** is that there is a relatively large zone in which we can considerably reduce the environmental impacts with a minimum reduction in the profit. For example, if we decide to operate in **point C in Figure 9** we can reduce the environmental impact by 13.5% with only 1.06% in the reduction of the gross profit.

Figure 10 shows the optimal schedules for **points A and B** in **Figure 9** (best economic and best environmental solutions). The schedule in the maximum profit solution tends to follow the gas prices to maximize the profit because the maximum gas production is just in the first weeks after the well is turned in operation. However it is worth to remark that gas prices forecasts have always some uncertainty. Therefore, good practice would be to operate, whenever possible, in a point in which the environmental impacts can be significantly reduced without scarifying too much the economic performance (e.g. **point C** in **Figure 9**)

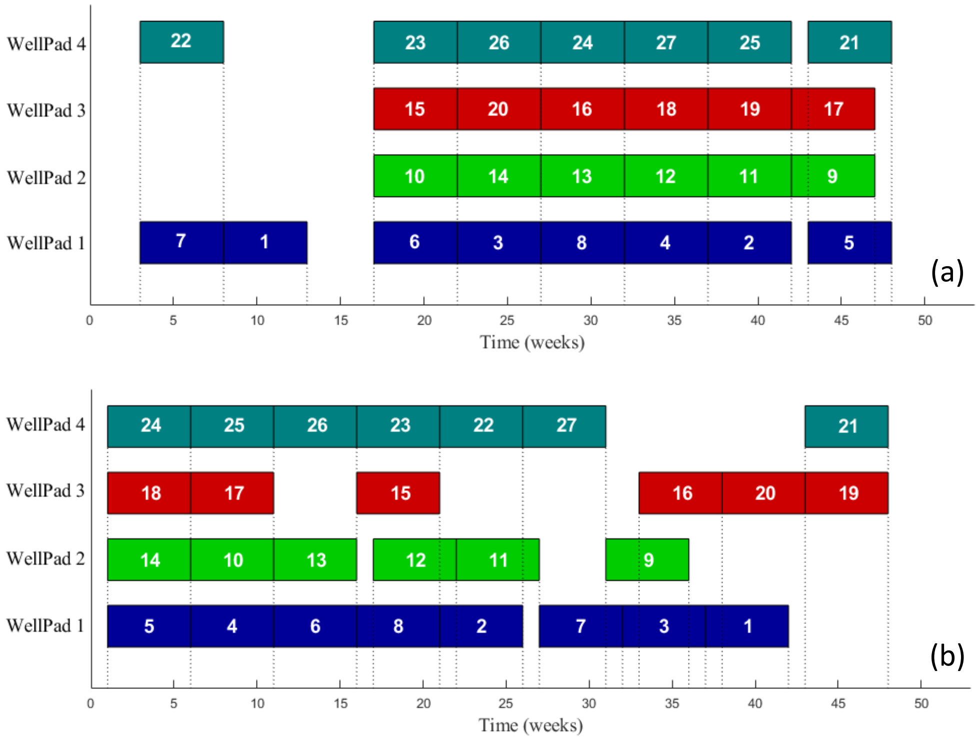

Figure 10. Gant Chart for the Optimal fracking schedule. (a) Maximum profit. (b) Minimum environmental impact. The number in each rectangle is the identification of individual wells in each wellpad.

In **Figure 11** we show a comparison of the main end-point and mid-point indicators for the best solution from the environmental point of view and economic point of view. The most important impacts are due to fossil fuel depletion, climate change, and to a lesser extension land occupation and particulate matter formation.

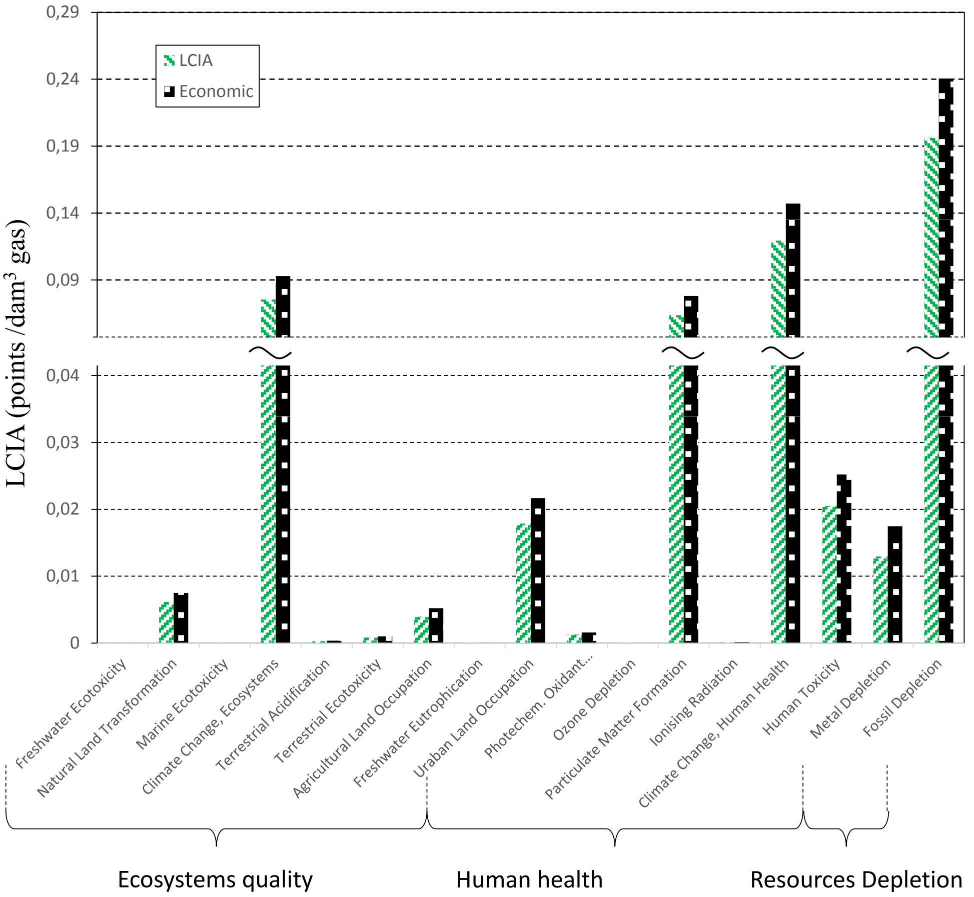

Figure 11. (a) Comparison of the environmental impact subcategories using ReCiPe Endpoint (H, A) for the optimal solution for the best economic and environmental solutions (points A and B in Figure 9).

Due to the large amount of data, a comprehensive summary of the results for the different scenarios (minimize the endpoint LCIA impact; maximize the profit and minimize freshwater consumption) can be found in the **supplementary material.**

One interesting result is that, although there is some correlation, minimizing the water footprint (e.g. minimizing freshwater consumption) it is not necessarily equivalent to minimize the global environmental impacts. **Point D** in **Figure 9** corresponds with the optimal solution when we minimize freshwater consumption. We get a very small reduction in freshwater consumption (%) compared with the best environmental alternative but at the price of significantly increasing the global environmental impacts. The reason is that the reduction in freshwater consumption is done by considerably increasing the water recycled between different wellpads (62 % more inter-wellpad recycling) which have an important impact on the transportation. Although the total water desalinated on-site is reduced (around 4%), it does not compensate for the increase in transport. Again the decision is case dependent and we have to decide which is the relative importance of the water footprint versus other impacts (e.g. climate change). Saving freshwater could be much more important in water-scarce zones. In any case, the final decision must be based on each case data and models like the one used in this work are a tool to take the informed decisions.

Conclusions

This paper studies the life cycle impact assessment of the wastewater treatment in the shale gas extraction, including the most common technologies for the pretreatment and three different desalination alternatives of recent interest, such as SEE-MVR, MEE-MVR and Membrane Distillation. Thus, the life cycle analyses developed in this work might be a valuable aspect to make the best decisions on environmental aspects related to the wastewater treatment for the water reuse in shale gas exploitation.

The best option to desalinate water is using a thermal-based technology. It is shown that multiple-effect evaporation with mechanical vapor recompression (MEE-MVR) is the best alternative. Membrane distillation has a higher environmental impact than thermal technologies, but it could be competitive in some circumstances. For example, at distant shale gas extraction sites, the power supply might be limited or even not available, which makes MEE-MVR alternative an impractical choice because it needs a constant power supply. However, the MD alternative works with industrial steam, which might be easily obtained from waste heat recovered from the shale gas operations.

Obviously, the best choice to treat shale wastewater from an environmental point of view is the direct reuse, which might be given in the wellpad itself or in other nearby wellpads.

Electricity and brine discharge are the factors that most influence the environmental impacts in the optimal configuration (pretreatment + MEE-MVR).

The optimal gas production, and therefore the drilling schedule, tends to follow the gas prices forecast to maximize the profit. However, the multi-objective optimization shows that it is possible to obtain important reductions in environmental impacts with small variations in the profit. If we take into account that in the gas prices forecast there is always some uncertainty a good practice would be to operate at a point in which we can reduce the environmental impacts without sacrificing too much the economic benefit.

Minimizing the water consumption it is not necessarily the best environmental alternative, even though there is a correlation between environmental impacts and freshwater consumption. It is possible that a reduction in the water footprint (i.e. freshwater consumption) be at the expense of increasing inter-wellpad recycling increasing the impacts related to transport and consequently increasing the impact of other environmental indicators. Of course the optimal trade-off is case dependent and the factors involved can only be treated through an optimization model that captures the most relevant factors in each case.

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Supplementary Material

Supporting Information contains:

- Comparison between thermal and membrane-based technologies for all the subcategories of impact using ReCiPe Midpoint (H)
- Waste Water Management:Comprehensive Mathematical Model Formulation.
- Case Study: Data and Results for the best environmental solution; best economic solution (maximum gross profit) and best solution for minimum freshwater consumption.

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Environmental and Economic Water Management in Shale Gas Extraction.

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Supplementary Information

This document contains the supplementary material for the article «*Environmental and Economic Water Management in Shale Gas Extraction*». The document is organized as follows:

S.1. Comparison between thermal and membrane-based technologies for all the subcategories of impact using ReCiPe Midpoint (H)

S.2. Waste Water Management: Mathematical model Formulation.

- Nomenclature
- Waste Water Management Model
- Model Parameter: typical values
- References

S3. Case Study Data and Results

- Case Study Data
- Results for the maximum profit optimization
- Results for the minimum total LCIA (endpoint)
- Results for the minimum fresh water consumption

S.1. Comparison between thermal and membrane-based technologies for all the subcategories of impact using ReCiPe Midpoint (H)

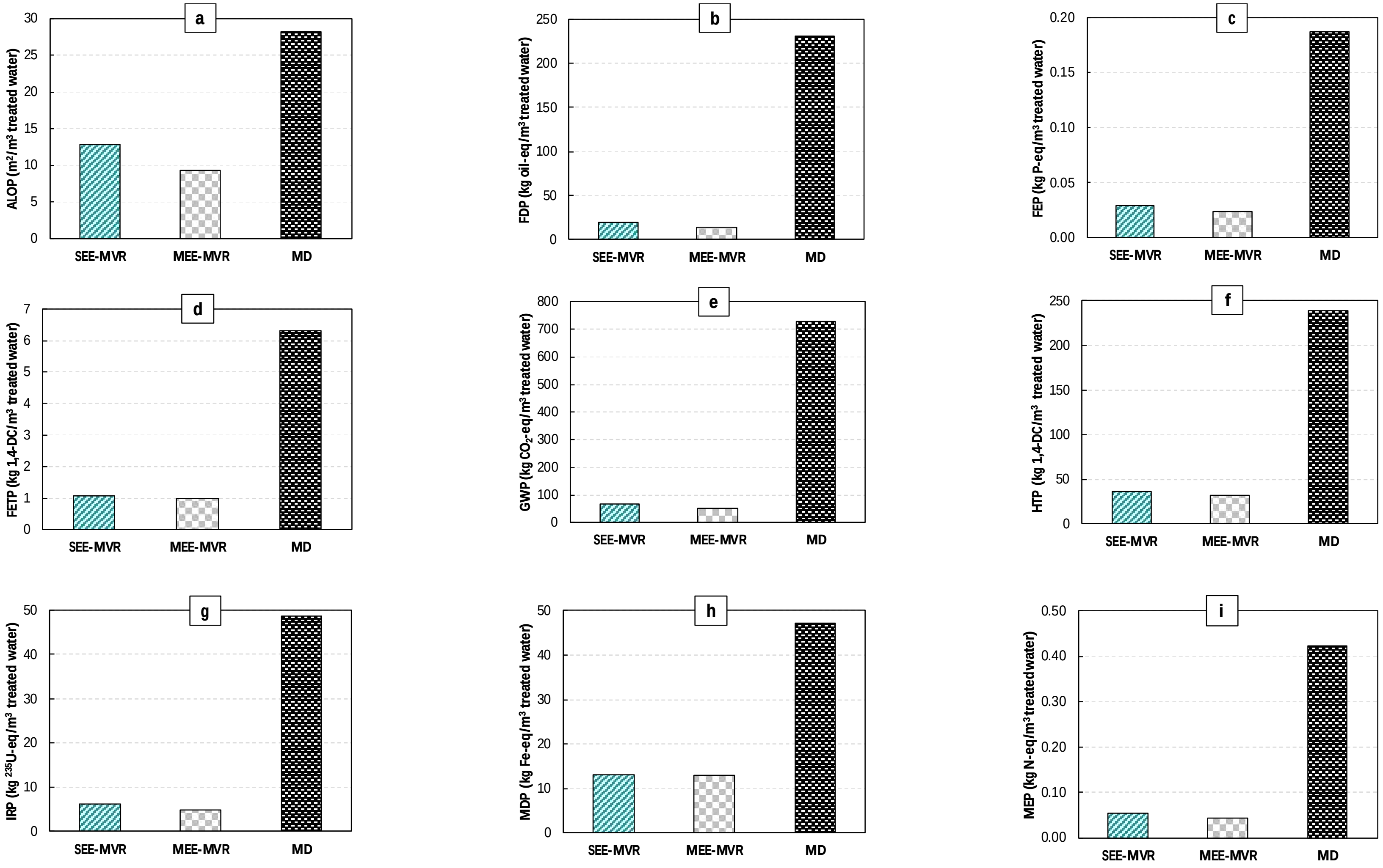

Figure S.1. Comparison between thermal and membrane-based technologies for all the subcategories of impact using ReCiPe Midpoint (H). a) Agricultural land occupation (ALOP), b) Fossil depletion (FDP), c) Freshwater eutrophication (FEP), d) Freshwater ecotoxicity (FETP), e) Global warming potential (GWP), f) Human toxicity (HTP), g) Ionizing radiation (IRP), h) Metal depletion (MDP), i) Marine eutrophication (MEP),

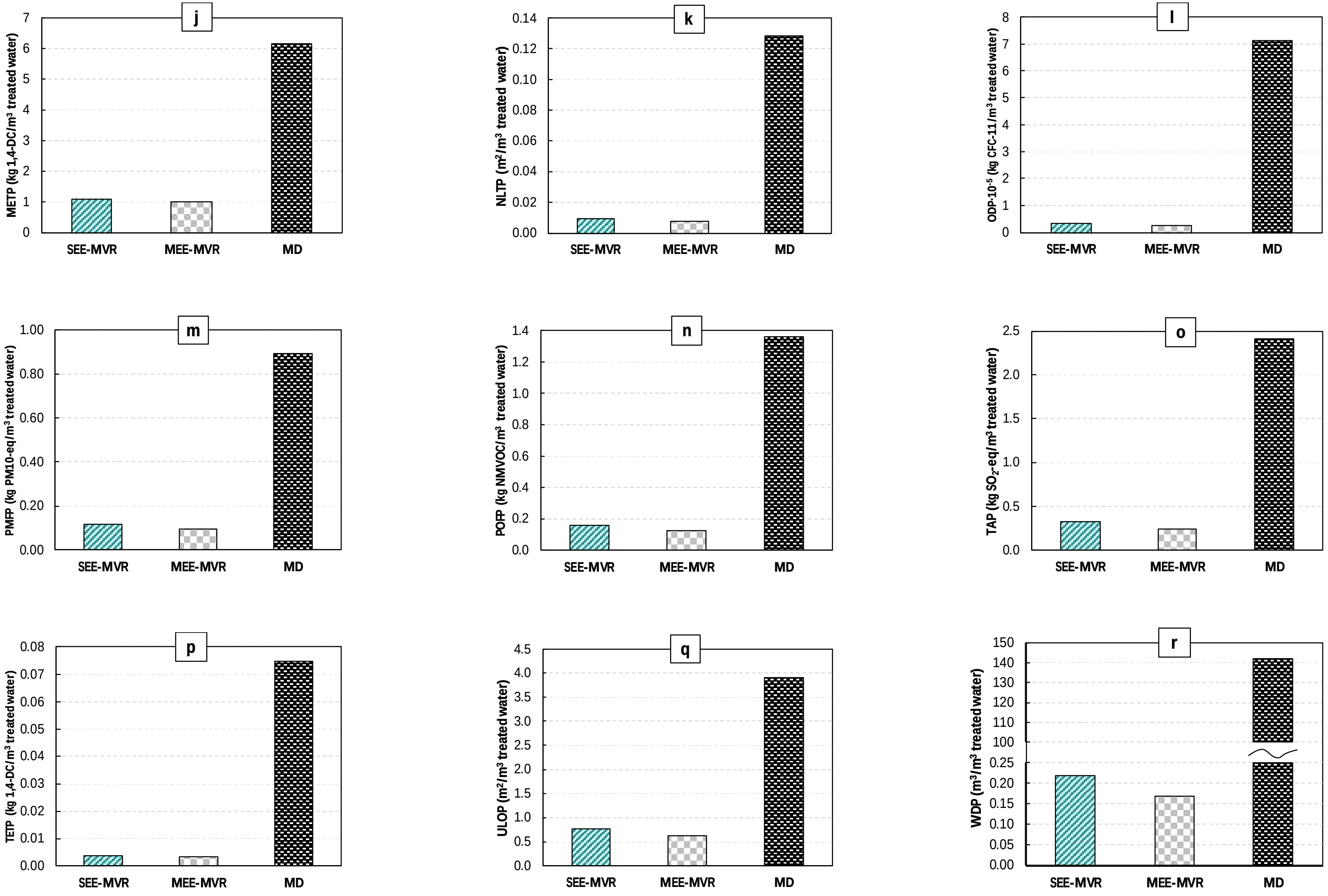

Figure S.1.(cont) Comparison between thermal and membrane-based technologies for all the subcategories of impact using ReCiPe Midpoint (H) j) Marine ecotoxicity (METP), k) Natural land transformation (NLTP), l) Ozone depletion (ODP), m) Particulate matter formation (PMFP), n) Photochemical oxidant formation (POFP), o) Terrestrial acidification (TAP), p) Terrestrial ecotoxicity (TETP), q) Urban land occupation (ULOP), and r) Water depletion (WDP).

S.2. Waste Water Management: Mathematical model Formulation

The shale gas water management mathematical model is based on the model proposed by Carrero-Parreño et al. [1] The equations that define this problem are detailed below:

NOMENCLATURE

Indexes

c	Fracturing crew
d	Disposal well
f	Source
k	Capacity
n	Onsite treatment
p	Wellpad
t	Time period
w	Well
wt	Treatment

Parameters

$D_{p,d}^{pad-dis}$	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*
$F_{n}^{on,LO}$	Minimum onsite capacity for treatment *wt*
$F_{n}^{on,UP}$	Maximum onsite capacity for treatment *wt*
$F_{k}^{cwt,UP}$	Maximum centralize water treatment capacity *k*
V_{s}^{UP}	Maximum storage volume of tank type *s*
WD_{w}	Water demand of well *w*
α_{k}^{cwt}	Cost coefficient of centralized water treatment *k*
α^{des}	Onsite treatment recovery factor
α_{d}^{dis}	Disposal coefficient cost coefficient for disposal *d*
α^{fr}	Friction reducer cost coefficient
α^{ft}	Fracturing tank cost coefficient
α^{fwt}	Fresh water tank cost coefficient
α_{p}^{on}	Onsite desalination cost coefficient on wellpad *p*
α^{pre}	Pretreatment recovery factor

α^{rec}	Centralized water treatment recovery factor
α^{reuse}	Pretreatment cost coefficient aiming its reuse
α_{f}^{source}	Freshwater cost coefficient in freshwater source *f*
α^{treat}	Pretreatment cost coefficient aiming its treatment
α^{truck}	Trucking cost coefficient
β^{ft}	Mobilize, demobilize and cleaning cost coefficient for storage tank
β_{p}^{on}	Maintenance cost coefficient for onsite treatment on wellpad *p*
τ_{w}	Time to fracture well *w*

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*
$y_{t,p,n}^{on}$	Indicates if onsite treatment *n* is used on wellpad *p* in time period *t*

Variables

$f_{t,p,k}^{cwt,in}$	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*
$f_{t,p}^{dem}$	Flowrate of water demand in wellpad *p* in time period *t*
$f_{t,p}^{fresh}$	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*
$f_{t,p,pp}^{imp,pad}$	Flowrate of impaired water from wellpad *p* to wellpad *pp* in time period *t*
$f_{t,p,d}^{on,brine}$	Brine flowrate after onsite desalination process in wellpad *p* in time period *t*
$f_{t,p}^{on,in}$	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*
$f_{t,p}^{on,slud}$	Sludge flowrate after onsite desalination process in wellpad *p* in time period *t*
$f_{t,p}^{pad}$	Flowrate of produce water on wellpad *p* in time period *t*
$f_{t,p}^{pre,in}$	Onsite pretreatment inflow in wellpad *p* in time period *t*
$f_{t,p}^{pre,out}$	Onsite pretreatment outflow in wellpad *p* in time period *t*
$f_{t,p,f}^{source}$	Flowrate of freshwater from natural source *f* to wellpad *p* in time period *t*
$f_{t,p,w}^{well}$	Flowrate of produce water on well *w* wellpad *p* in time period *t*
$st_{t,p,s}$	Level of water in tank type *s* on wellpad *p* in time period *t*
$y_{t,p,w}^{fb}$	Indicates when the water starts to come out on well *w* on wellpad *p* in time period *t*

WASTE WATER MANAGEMENT MODEL.

Assignment constraint

Eq. (S1) guarantees that at the time period each well is going to fracture,

$$\sum_{t \in T} y^{hf}_{t,p,w} = 1 \qquad \forall w \in RPW_p, p \in P \tag{S1}$$

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

Eq. (S2) ensures that there is no overlap in drilling operations between different wells,

$$\sum_{w \in RPW_p} \sum_{tt=t-\tau_w+1}^{t} y^{hf}_{tt,p,w} = 1 \qquad \forall t \in T, p \in P \tag{S2}$$

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

Shale water recovered

After fracturing a well, a portion of the freshwater injected returns to the wellhead,

$$y^{hf}_{t,p,w} = y^{fb}_{t+\tau_w,p,w} \qquad t \le T - \tau_w, \forall w \in RPW_p, p \in P \tag{S3}$$

where $y^{fb}_{t,p,w}$ represents the time period when the flowback water comes out. The binary variable $y^{fb}_{t,p,w}$ is treated as a continuous variable since its integrality is enforced by the Eq (S3)

The wastewater from each wellpad is calculated with **Eq. (S4)**,

$$f^{well}_{t,p,w} = \sum_{w \in RPW_p} \sum_{tt=0}^{tt \le t-1} F^{well}_{t-tt,p,w} \cdot y^{fb}_{tt+1,p,w} \qquad \forall t \in T, p \in P \tag{S4}$$

where $F^{well}_{t,p,w}$ are parameters that indicate flowback flowrate.

Eq. (S5) describes the mass balance of flowback water collected from the wells belonging to wellpad *p*,

$$f^{pad}_{t,p} = \sum_{w \in RPW_p} f^{well}_{t,p,w} \qquad \forall t \in T, p \in P \tag{S5}$$

Mass balance in storage tanks

The level of the fracturing tank in each time period ($st_{t-1,p,s}$) depends on water stored in the previous time period, the flowback water recovered after the hydraulic fracturing $\left(f_{t,p}^{pad} \right)$, the water sent to another wellpad to be reused ($f_{t,pp,p}^{imp,pad}$), the water sent to CWT ($f_{t,p,k}^{cwt,in}$) or onsite ($f_{t,p}^{onpre,in}$) treatment and the water sent to disposal ($f_{t,p,d}^{dis}$). The mass balance in the storage tank is described in **Eq. (S6).**

$$\begin{aligned} & st_{t-1,p,s} + f_{t,p}^{pad} + \sum_{\substack{pp \in P \\ pp \neq p}} f_{t,pp,p}^{imp,pad} = st_{t,p,s} + \sum_{\substack{pp \in P \\ pp \neq p}} f_{t,p,pp}^{imp,pad} \\ & + f_{t,p}^{onpre,in} + \sum_{k \in K} f_{t,p,k}^{cwt,in} + \sum_{d \in D} f_{t,p,d}^{dis} \qquad \forall t \in T, p \in P, s \in \{s1\} \end{aligned} \tag{S6}$$

The fresh water is also stored in portable tanks. The mass balance is detailed in **Eq. (S7)**.

$$st_{t-1,p,s} + \sum_{f \in F} f_{t,p,f}^{source} = st_{t,p,s} + f_{t,p}^{fresh} \qquad \forall t \in T, p \in P, s \in \{s2\} \tag{S7}$$

The volume of the tank (v_s) is calculated by **Eq. (S8)**,

$$st_{t,p,s} + \theta_{t,p,s} \le v_s \qquad \forall t \in T, p \in P, s \in S \tag{S8}$$

where $\theta_{t,p,s}$ represents the inlet water in the storage tank divided by the number of days in a week. This variable is introduced due to as the time horizon is discretized into weeks, the storage tank should handle the inlet water that comes from one day.

The volume of the tank is bounded by the maximum storage capacity allowed in a wellpad per week.

$$v_s \le V_s^{UP} \qquad \forall s \in S \tag{S9}$$

Water demand

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

$$f_{t,p}^{dem} = f_{t,p}^{fresh} + f_{t,p}^{imp} \qquad \forall t \in T, p \in P \tag{S10}$$

The amount of water demand per well is given by **Eq. (S11)**,

$$f_{t,p}^{dem} = \sum_{w \in RPW_p} f_{t,p,w}^{dem} \qquad \forall t \in T, p \in P \tag{S11}$$

Eq. (S12) indicates that the water when the well is going to be drilled, must be greater or equal than the well water demand (WD_w),

$$f_{t,p,w}^{dem} \geq WD_w \cdot \sum_{c \in C} y_{t,p,w,c}^{hf} \qquad \forall t \in T, w \in RPW_p, p \in P \tag{S12}$$

Onsite treatment

Onsite pretreatment mass balance is described in **Eq. (S13)**,

$$f_{t,p}^{pre,out} + f_{t,p}^{on,slud} = f_{t,p}^{pre,in} \qquad \forall t \in T, p \in P \tag{S13}$$

The recovery factor (α^{pre}) is used to model the relationship between the inlet and outlet streams.

$$f_{t,p}^{pre,out} = \alpha^{pre} \cdot f_{t,p}^{pre,in} \qquad \forall t \in T, p \in P \tag{S14}$$

The outlet pretreated water can be used as a fracturing fluid ($f_{t,p}^{imp}$) or/and can be sent to onsite desalination treatment ($f_{t,p}^{on,in}$),

$$f_{t,p}^{pre,out} = f_{t,p}^{imp} + f_{t,p}^{on,in} \qquad \forall t \in T, p \in P \tag{S15}$$

Mass balance around onsite desalination technology is given by **Eq. (S16)**,

$$f_{t,p}^{on,out} + f_{t,p}^{on,brine} = f_{t,p}^{on,in} \qquad \forall t \in T, p \in P \tag{S16}$$

Again, the relation between inlet and outlet mass flowrate in onsite desalination unit is addressed by using the recovery factor (α^{on}),

$$f_{t,p}^{on,out} = \alpha^{on} \cdot f_{t,p}^{on,in} \qquad \forall t \in T, p \in P \qquad \forall t \in T, p \in P \tag{S17}$$

The following equation **Eq. (S18)** represents the maximum and minimum capacity of the desalination treatment.

$$F^{on,LO} \cdot y_{t,p}^{on} \leq f_{t,p}^{on,in} \leq F^{on,UP} \cdot y_{t,p}^{on} \qquad \forall t \in T, p \in P \tag{S18}$$

Centralized water treatment

Eq. (S19) shows the connection between inlet and outlet streams, and **Eq. (S20)** limits the inlet water of CWT *k* with the maximum capacity allowed.

$$f_{t,k}^{cwt,out} = \alpha_k^{off} \cdot \sum_{p\in P} f_{t,p,k}^{cwt,in} \qquad \forall t \in T, k \in K \tag{S19}$$

$$\sum_{p\in P} f_{t,p,k}^{cwt,in} \le F_k^{cwt,UP} \qquad \forall t \in T, k \in K \tag{S20}$$

Objective function

Different objective functions have been considered depending on the case studied. We solve a multi-objective optimization problem considering two objective functions (**Eq. (S21)** and **Eq. (S22)**). Specifically, the gross profit to be maximized includes revenue from shale gas and expenses for wellpad construction and preparation, shale gas production and water-related costs. The life cycle impact assessment minimizes environmental impacts associated with water activities.

$$\begin{aligned}
\max: GP = & \sum_{t\in T}\sum_{p\in P}\sum_{w\in RPW_p}\sum_{tt=0}^{tt\le t-1} F_{t-tt,p,w}^{gas} \cdot y_{tt+1,p,w}^{fb} \cdot \alpha_t^{gas} \\
- & \sum_{t\in T}\sum_{p\in P}[\sum_{d\in D}\alpha_d^{dis} \cdot f_{t,p,d}^{dis} \\
+ & \sum_{w\in RPW_p}(\alpha^{drill} \cdot y_{t,p,w}^{hf} + \alpha^{prod} \cdot f_{t,p,w}^{gas}) \\
+ & \sum_{f\in F}\alpha_f^{source} \cdot f_{t,p,f}^{source} \\
+ & \alpha^{fr} \cdot f_{t,p}^{imp} \\
+ & \alpha^{reuse} \cdot f_{t,p}^{imp} + \alpha^{treat} \cdot f_{t,p}^{on,in} + \alpha_p^{on} \cdot f_{t,p}^{on,in} + \beta_p^{on} \cdot y_p^{on} \\
+ & \sum_{k\in K}\alpha_k^{cwt} \cdot f_{t,p,k}^{cwt,in} \\
+ & (\sum_{f\in F} f_{t,p,f}^{source} \cdot D_{f,p}^{pad-source} + \sum_{k\in K} f_{t,k}^{cwt,in} \cdot D_{p,k}^{pad-cwt} + \sum_{pp\in P} f_{t,p,pp}^{pad,imp} \cdot D_{p,pp}^{pad-pad}) \cdot \alpha_p^{trans}] \\
+ & \alpha^{fwt} \cdot v_{fwt} + \alpha^{ft} \cdot v_{ft} + \beta^{ft}
\end{aligned} \tag{S21}$$

$$\begin{aligned}
\min: LCIA = & \sum_{t\in T}\sum_{p\in P}[\sum_{f\in F}\sigma^{source} \cdot f_{t,p,f}^{source} \\
+ & \sigma^{on} \cdot f_{t,p}^{on,in} \\
+ & \sum_{k\in K}\alpha_k^{cwt} \cdot f_{t,p,k}^{cwt,in} \\
+ & (\sum_{f\in F} f_{t,p,f}^{source} \cdot D_{f,p}^{pad-source} + \sum_{k\in K} f_{t,k}^{cwt,in} \cdot D_{p,k}^{pad-cwt} + \sum_{pp\in P} f_{t,p,pp}^{pad,imp} \cdot D_{p,pp}^{pad-pad}) \cdot \sigma^{trans}]
\end{aligned} \tag{S22}$$

Model Parameters: typical values

All data related with the case study is shown in the section (S???). However, in this section we show typical values for costs and other relevant parameter and the relevant references.

Table S.1. Cost coefficients.

Parameter	Value	Unit	Ref
Disposal cost (α_d^{dis})	90 - 120	$/m^3	[2]
Truck cost (α^{truck})	0.15	$/km/m^3	[2]
Fracturing tank cost ($\alpha^{fl}; \beta^{fl}$)	4.37; 52390	$/ m^3; $	*
Freshwater tank cost (α^{fwt})	0.59	$/ m^3	*
Pretreatment cost ($\alpha^{reuse}, \alpha^{treat}$)	0.8 - 2.0	$/m^3	[3]
Desalination cost (α_p^{ondes})	10 - 25	$/m^3	[4,5]
Demobilize, mobilize and clean out cost (β_p^{ondes})	650 - 850	$/week	*
Centralized water treatment (α_k^{cwt})	42 - 84	$/m^3	[2]
Friction reducer cost (α^{fr})	0.18 - 0.30	$/m^3	*
Freshwater withdrawal cost (α_f^{source})	1.76 - 3.50	$/m^3	[6]

* Provided by a company

Table S.2. Model parameters.

Parameter	Value	Unit	Ref
V_s^{UP}	60,000	m^3	*
$F_{t,p,w}^{well}$	2,400 - 9,300	m^3 week^{-1}	[7]
$f^{on,UP}$	4,000	m^3 week^{-1}	*
$f_k^{cwt,UP}$	16,700	m^3 week^{-1}	*
WD_w	7,500 - 37,000	m^3 week^{-1}	[7]
τ_w	1 - 5	weeks	[7]

* Provided by a shale gas company

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SHALE GAS WATER MANAGEMENT

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               LCA + Water Management Report

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BEST GLOBAL ENVIRONMENTAL ALTERNATIVE

RESULTS FOR THE CASE STUDY IN THE PAPER:

«Environmental and Economic Water Management in Shale Gas Extraction»

CONTENTS

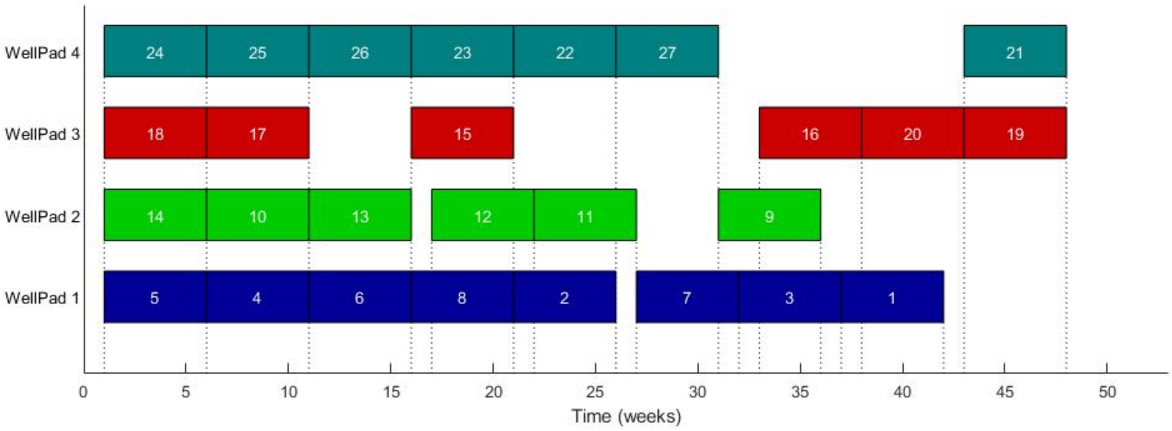
MODEL STATISTICS

```
Number of Variables                       :  11373.0
Numer of Discrete Variables               :   1165.0
Number of Equations                       :   9068.0
Number of non-zero elements               : 112950.0
Number of Iterations                      : 940439.0
CPU Generation Time (s)                   :   0.6090
CPU Solution Time (s)                     :  83.5310
Model Objective Value                     :   0.5189
```

RESULTS: SCHEDULING

The different wells must be schedule according to the following table.

```
Well 1 in wellpad 1      Starts fracking at week   37     and ends fracking at week   42
Well 2 in wellpad 1      Starts fracking at week   21     and ends fracking at week   26
Well 3 in wellpad 1      Starts fracking at week   32     and ends fracking at week   37
Well 4 in wellpad 1      Starts fracking at week    6     and ends fracking at week   11
Well 5 in wellpad 1      Starts fracking at week    1     and ends fracking at week    6
Well 6 in wellpad 1      Starts fracking at week   11     and ends fracking at week   16
Well 7 in wellpad 1      Starts fracking at week   27     and ends fracking at week   32
Well 8 in wellpad 1      Starts fracking at week   16     and ends fracking at week   21
Well 9 in wellpad 2      Starts fracking at week   31     and ends fracking at week   36
Well 10 in wellpad 2     Starts fracking at week    6     and ends fracking at week   11
Well 11 in wellpad 2     Starts fracking at week   22     and ends fracking at week   27
Well 12 in wellpad 2     Starts fracking at week   17     and ends fracking at week   22
Well 13 in wellpad 2     Starts fracking at week   11     and ends fracking at week   16
Well 14 in wellpad 2     Starts fracking at week    1     and ends fracking at week    6
Well 15 in wellpad 3     Starts fracking at week   16     and ends fracking at week   21
Well 16 in wellpad 3     Starts fracking at week   33     and ends fracking at week   38
Well 17 in wellpad 3     Starts fracking at week    6     and ends fracking at week   11
Well 18 in wellpad 3     Starts fracking at week    1     and ends fracking at week    6
Well 19 in wellpad 3     Starts fracking at week   43     and ends fracking at week   48
Well 20 in wellpad 3     Starts fracking at week   38     and ends fracking at week   43
Well 21 in wellpad 4     Starts fracking at week   43     and ends fracking at week   48
Well 22 in wellpad 4     Starts fracking at week   21     and ends fracking at week   26
Well 23 in wellpad 4     Starts fracking at week   16     and ends fracking at week   21
Well 24 in wellpad 4     Starts fracking at week    1     and ends fracking at week    6
Well 25 in wellpad 4     Starts fracking at week    6     and ends fracking at week   11
Well 26 in wellpad 4     Starts fracking at week   11     and ends fracking at week   16
Well 27 in wellpad 4     Starts fracking at week   26     and ends fracking at week   31
```

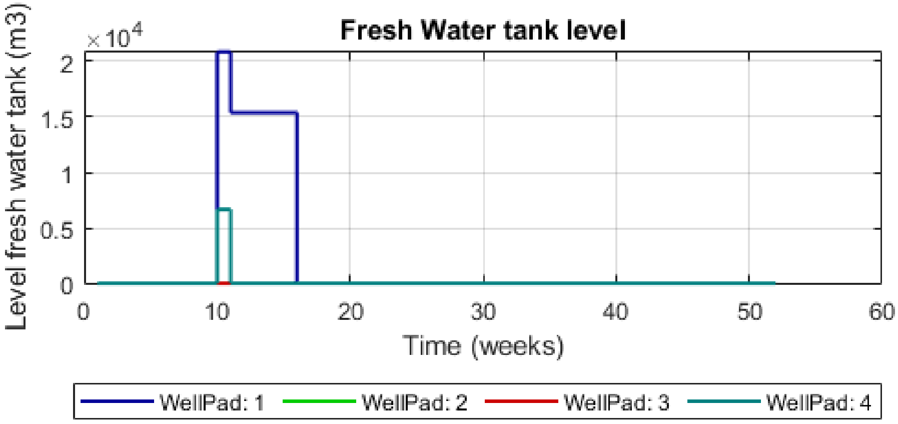


RESULTS: Storage Tanks. Volumes and Levels

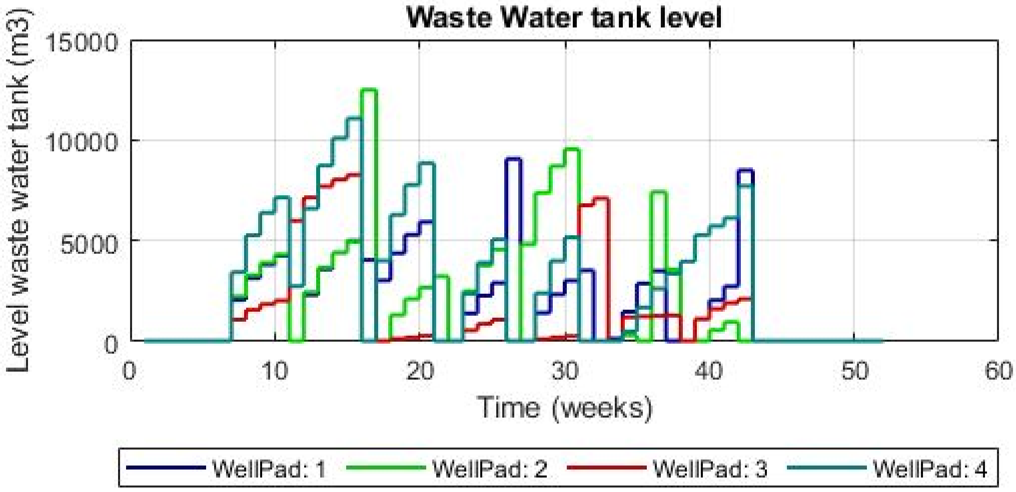
```
Volume of fresh water tanks (m3)
    Well Pad   1 :    50000.0
    Well Pad   2 :    50000.0
    Well Pad   3 :    50000.0
    Well Pad   4 :    50000.0

Volume of waste water tanks (m3)
    Well Pad   1 :    50000.0
    Well Pad   2 :    50000.0
    Well Pad   3 :    50000.0
    Well Pad   4 :    50000.0
```

FRESH Water Tank Level



WASTE Water Tank Level



RESULTS: Main Flows

```
  Total Flow from each water source to each WellPad (m3)

                  WellPad  1      WellPad  2      WellPad  3      WellPad  4      Total
Source   1 :      20847.9         0.0             0.0             6655.2         27503.0
Source   2 :      0.0             0.0             0.0             0.0             0.0
Source   3 :      24907.5         35563.9         20275.2         31464.0        12210.6
Total      :      45755.4         35563.9         20275.2         38119.2

  Total fresh water demand of each wellpad (m3)
       WellPad   1 :   126000.0
       WellPad   2 :   108000.0
       WellPad   3 :    72000.0
       WellPad   4 :   132000.0
         Total     :   438000.0

  Total flowback water in each wellpad (m3)
       WellPad   1 :    91634.5
       WellPad   2 :    78614.5
       WellPad   3 :    38240.0
       WellPad   4 :   120850.0
         Total     :   329339.1

  Total flowback recycled by each wellpad (m3)
       WellPad   1 :    80244.6
       WellPad   2 :    72436.1
       WellPad   3 :    51724.8
       WellPad   4 :    93880.8
         Total     :   298286.4

  Total flow treated on-site in each wellpad(m3)
       WellPad   1 :     4022.8
       WellPad   2 :     1185.4
       WellPad   3 :     8524.1
       WellPad   4 :     7440.2
         Total     :    21172.5

  Total flow sent to a C.W.T by each wellpad(m3)
       WellPad   1 :        0.0
       WellPad   2 :        0.0
       WellPad   3 :        0.0
       WellPad   4 :        0.0
         Total     :        0.0

  Total flow sent to disposal by each wellpad(m3)
       WellPad   1 :        0.0
       WellPad   2 :        0.0
       WellPad   3 :        0.0
       WellPad   4 :        0.0
         Total     :        0.0

  Total flow recycled between wellpads (m3)
                       WellPad  1   WellPad  2   WellPad  3   WellPad  4
       WellPad   1 :          0.0       6014.3      15117.8       4087.2
       WellPad   2 :      10032.5          0.0       5153.6       7407.1
       WellPad   3 :       2424.7       1376.7          0.0       2919.8
       WellPad   4 :       8001.2      12486.2      10322.1          0.0
```

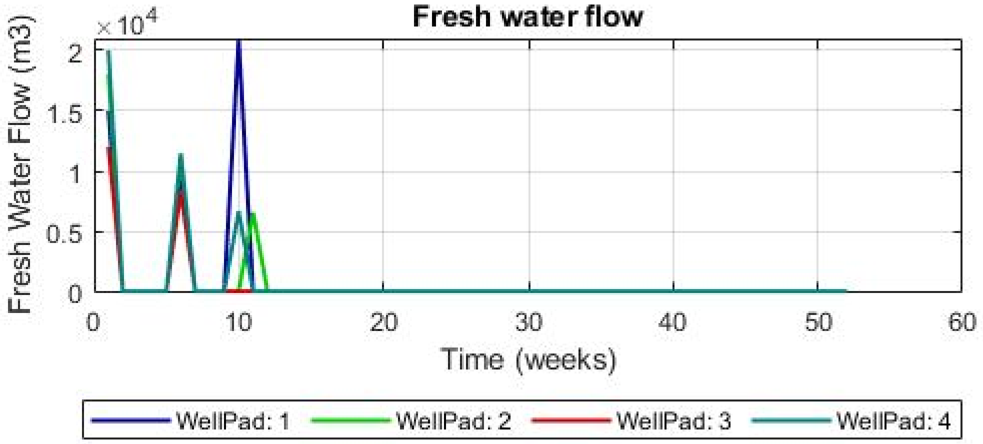
RESULTS: Global data water utilization

```
Total water demanded by WellPads (m3)  : 438000.0
Total fresh water consumption (m3)     : 139713.6
Total flowback water (m3)              : 329339.1
Total flowback water recycled (m3)     : 298286.4
Total sludge generated (m3)            :   9880.2
Total water desalinated on-site (m3)   :  21172.5
Total water desalinated off-site (m3)  :      0.0
Total water send to disposal (m3)      :      0.0

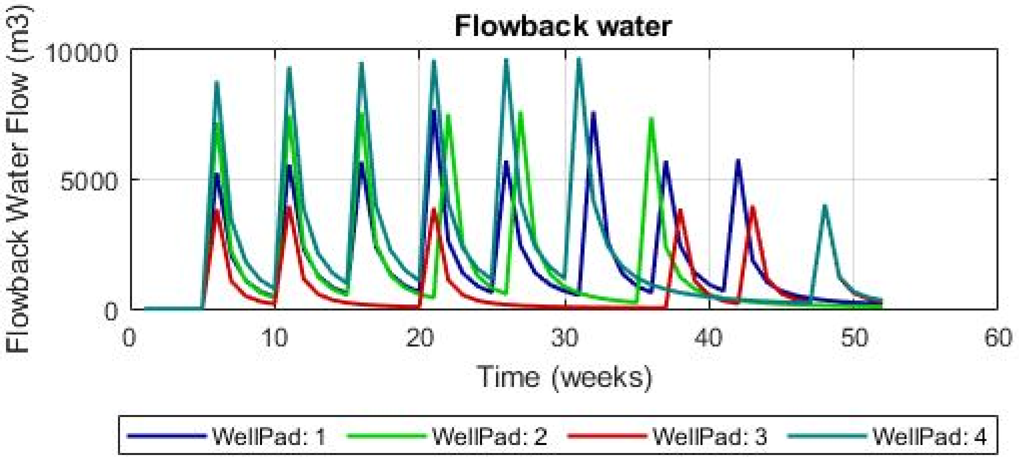
Percentage of fresh water saved (%)    :     68.1
```

RESULTS: Time dependent Water flow charts

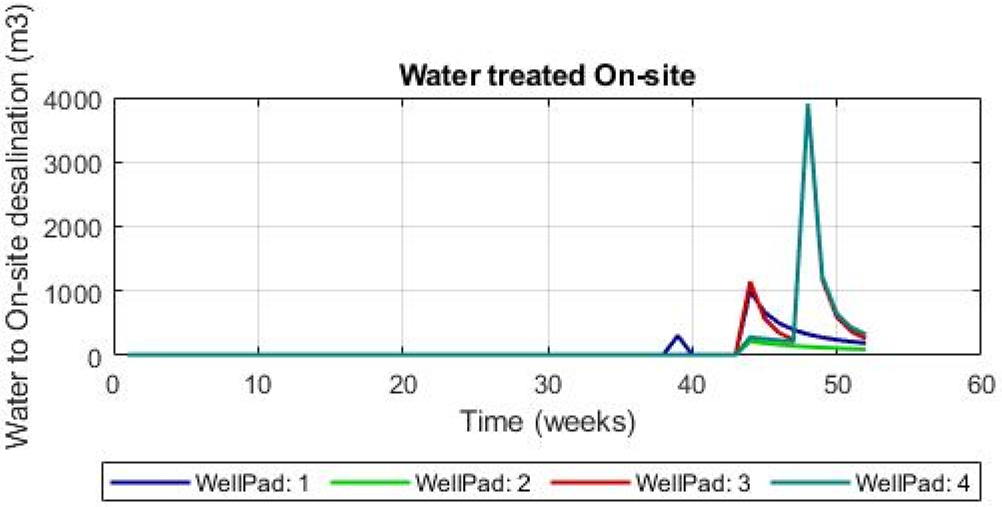
Total fresh water consumed in each wellpad



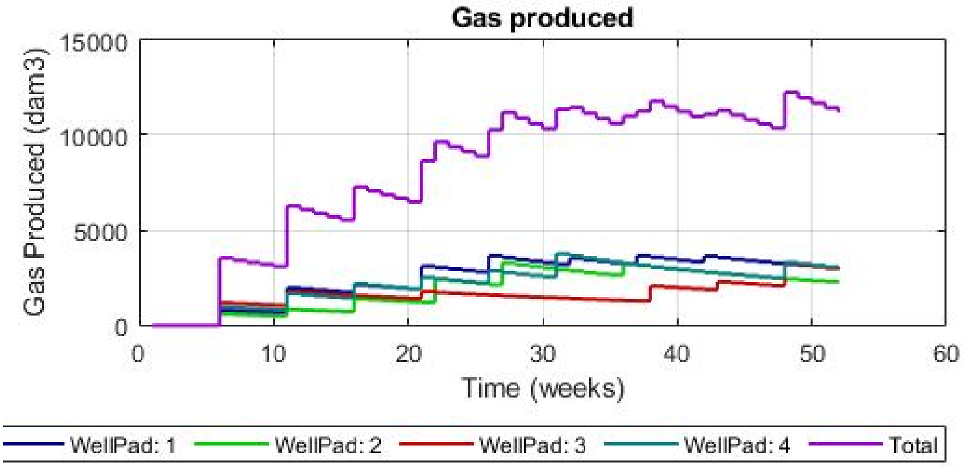
Total flowback water produced in each wellpad



Water to on-site desalination facility in each wellpad



RESULTS : Gas Production Charts



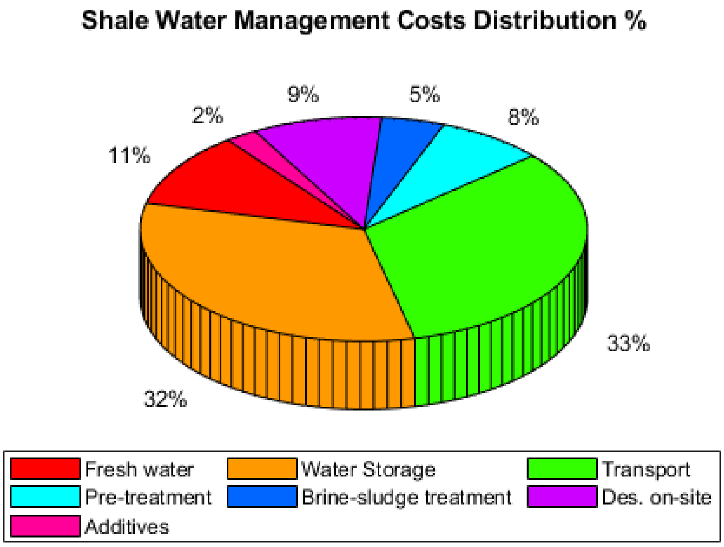
RESULTS : Cost Distribution

```
Fresh water adquisition cost(k$)       :    402.5
Water transport cost(k$)               :   1213.1
Friction reducers cost(k$)             :     86.5
Fresh water storage cost (k$)          :    118.0
Waste water Storage cost(k$)           :   1083.6
Pre-treatment cost(k$)                 :    288.3
On-site desalination cost(k$)          :    347.1
Off-site desalination cost(k$)         :      0.0
Water disposal cost(k$)                :      0.0
Brine and sludge disposal cost(k$)     :    169.4
Drilling costs(k$)                     :   7290.0
Gas production cost(k$)                :   5961.2

Total Cost (k$)                        :  16959.7

Total Gas Income (k$)                  :  59017.6
```

Water related Cost Distribution Pie Chart (drilling and gas production are not included in the chart)



RESULTS : LCA

TOTAL ENVIRONMENTAL IMPACT

```
Environmental Impact (points/dam3·gas)  :  0.51885
```

DAMAGE CATEGORIES

```
Ecosystem Quality (points/dam3·gas)     :  0.10462
Human Health (points/dam3·gas)          :  0.20497
Resources Depletion (points/dam3·gas)   :  0.20926
```

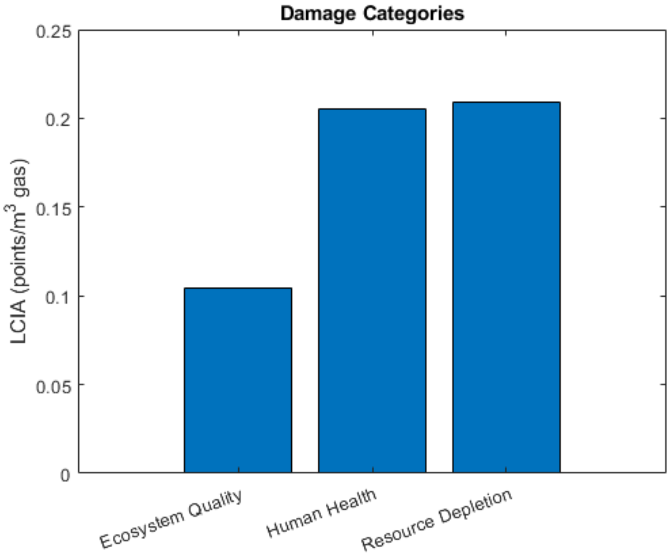
SUB-DAMAGE CATEGORIES

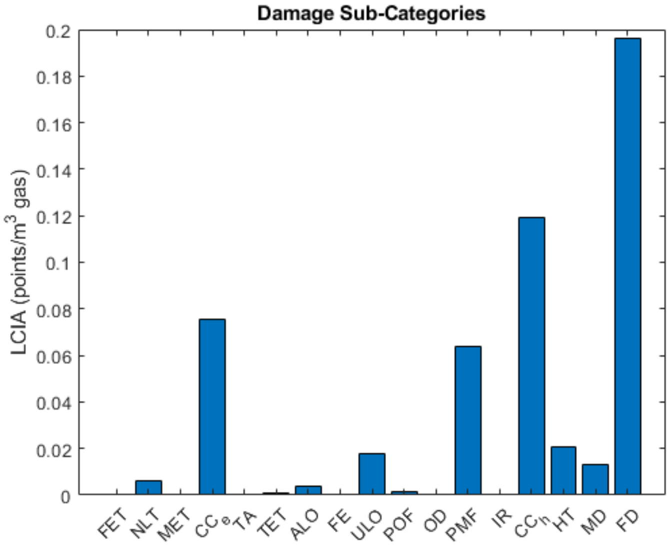
```
        Freshwater Ecotoxicity    0.00003 points/dam3·gas   ===>     0.02404  kg 1,4-DC
   Natural Land Transformation    0.00616 points/dam3·gas   ===>     0.00163  m2
            Marine Ecotoxicity    0.00001 points/dam3·gas   ===>     0.03797  kg 1,4-DC
      Climate Change, Ecosystems  0.07545 points/dam3·gas   ===>     1.66768  kg CO_2-Eq
       Terrestrial Acidification  0.00029 points/dam3·gas   ===>     0.02245  kg SO_2-Eq
         Terrestrial Ecotoxicity  0.00084 points/dam3·gas   ===>     0.00255  kg 1,4-DC
    Agricultural Land Occupation  0.00393 points/dam3·gas   ===>     0.10397  m2
       Freshwater Eutrophication  0.00005 points/dam3·gas   ===>     0.00043  kg P-Eq
           Urban Land Occupation  0.01785 points/dam3·gas   ===>     0.39002  m2

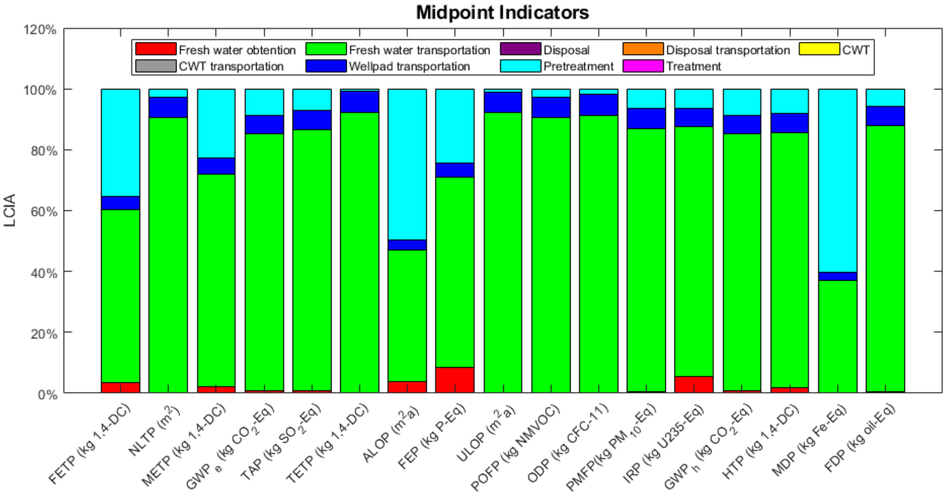
    Photochem. Oxidant Formation  0.00129 points/dam3·gas   ===>     0.03329  kg NMVOC
                 Ozone Depletion  0.00004 points/dam3·gas   ===>     0.00000  kg CFC-11
    Particulate Matter Formation  0.06368 points/dam3·gas   ===>     0.01226  kg PM_10-
Eq
             Ionising Radiation   0.00012 points/dam3·gas   ===>     0.35672  kg U235-Eq
    Climate Change, Human Health  0.11938 points/dam3·gas   ===>     2.63848  kg CO_2-Eq
                  Human Toxicity  0.02046 points/dam3·gas   ===>     1.50817  kg 1,4-DC

                  Metal Depletion  0.01295 points/dam3·gas   ===>     0.27896  kg Fe-Eq
                 Fossil Depletion  0.19632 points/dam3·gas   ===>     1.63711  kg oil-Eq
```

FIGURES LCA







Published by José A. Caballero

SHALE GAS WATER MANAGEMENT

```
================================================================
           Institute of Chemical Process Engineering

                      University of Alicante

                  LCA + Water Management Report
```

BEST ECONOMIC ALTERNATIVE

RESULTS FOR THE CASE STUDY IN THE PAPER:

«Environmental and Economic Water Management in Shale Gas Extraction»

CONTENTS

MODEL STATISTICS

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       Number of Variables                      :  11373.0
       Numer of Discrete Variables              :   1165.0
       Number of Equations                      :   9068.0
       Number of non-zero elements              : 112950.0
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       CPU Solution Time (s)                    :   3.9380
       Model Objective Value                    : 48643.1019
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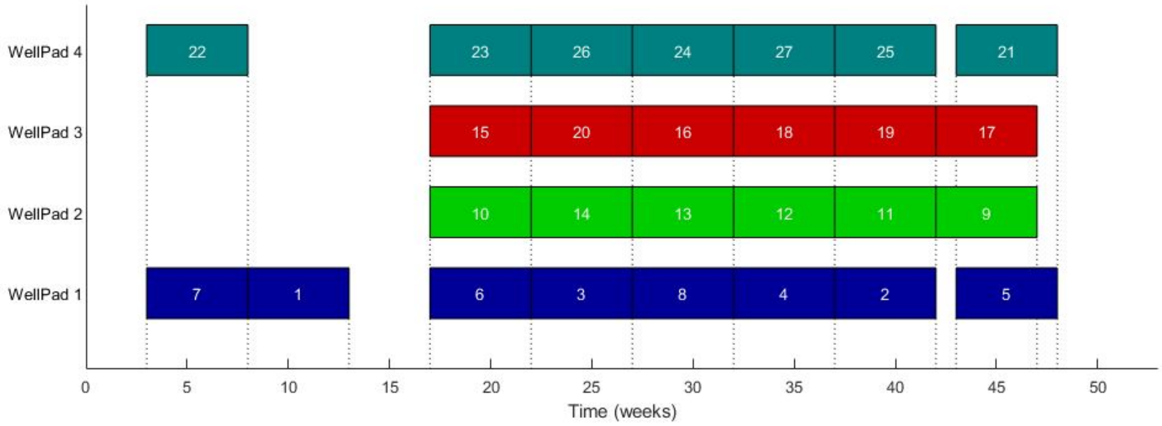
RESULTS: SCHEDULING

The different wells mus be schedule according to the following table.

```
Well 1 in wellpad 1      Starts fracking at week    8     and ends fracking at week    13
Well 2 in wellpad 1      Starts fracking at week   37     and ends fracking at week    42
Well 3 in wellpad 1      Starts fracking at week   22     and ends fracking at week    27
Well 4 in wellpad 1      Starts fracking at week   32     and ends fracking at week    37
Well 5 in wellpad 1      Starts fracking at week   43     and ends fracking at week    48
Well 6 in wellpad 1      Starts fracking at week   17     and ends fracking at week    22
Well 7 in wellpad 1      Starts fracking at week    3     and ends fracking at week     8
Well 8 in wellpad 1      Starts fracking at week   27     and ends fracking at week    32
Well 9 in wellpad 2      Starts fracking at week   42     and ends fracking at week    47
Well 10 in wellpad 2     Starts fracking at week   17     and ends fracking at week    22
Well 11 in wellpad 2     Starts fracking at week   37     and ends fracking at week    42
Well 12 in wellpad 2     Starts fracking at week   32     and ends fracking at week    37
Well 13 in wellpad 2     Starts fracking at week   27     and ends fracking at week    32
Well 14 in wellpad 2     Starts fracking at week   22     and ends fracking at week    27
Well 15 in wellpad 3     Starts fracking at week   17     and ends fracking at week    22
Well 16 in wellpad 3     Starts fracking at week   27     and ends fracking at week    32
Well 17 in wellpad 3     Starts fracking at week   42     and ends fracking at week    47
Well 18 in wellpad 3     Starts fracking at week   32     and ends fracking at week    37
Well 19 in wellpad 3     Starts fracking at week   37     and ends fracking at week    42
Well 20 in wellpad 3     Starts fracking at week   22     and ends fracking at week    27
Well 21 in wellpad 4     Starts fracking at week   43     and ends fracking at week    48
Well 22 in wellpad 4     Starts fracking at week    3     and ends fracking at week     8
Well 23 in wellpad 4     Starts fracking at week   17     and ends fracking at week    22
Well 24 in wellpad 4     Starts fracking at week   27     and ends fracking at week    32
Well 25 in wellpad 4     Starts fracking at week   37     and ends fracking at week    42
Well 26 in wellpad 4     Starts fracking at week   22     and ends fracking at week    27
Well 27 in wellpad 4     Starts fracking at week   32     and ends fracking at week    37
```

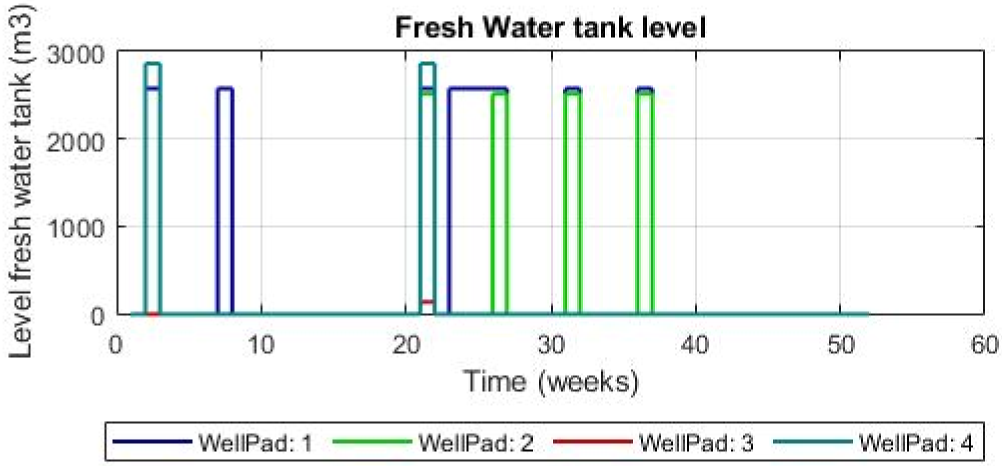


RESULTS: Storage Tanks. Volumes and Levels

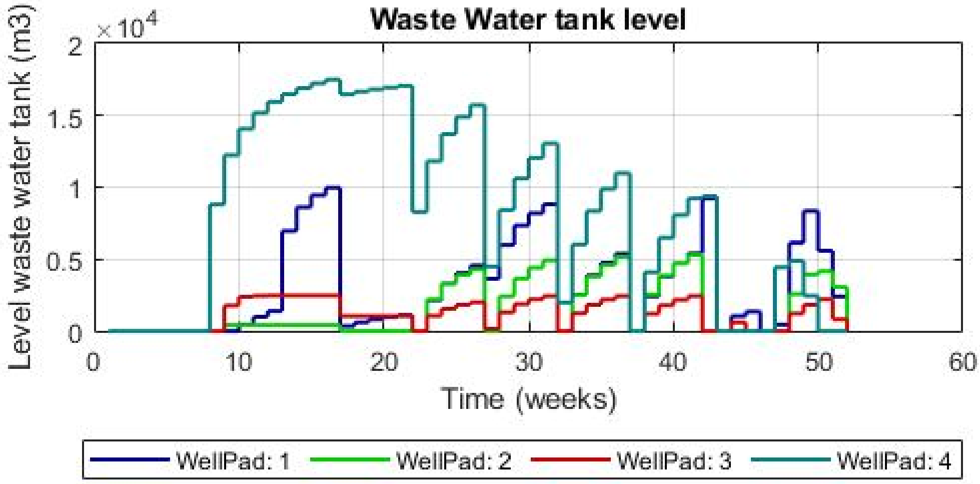
```
Volume of fresh water tanks (m3)
    Well Pad   1 :     2571.4
    Well Pad   2 :     2511.8
    Well Pad   3 :      137.1
    Well Pad   4 :     2857.1

Volume of waste water tanks (m3)
    Well Pad   1 :    10036.1
    Well Pad   2 :     5392.8
    Well Pad   3 :     2481.8
    Well Pad   4 :    17529.7
```

FRESH Water Tank Level [stairs; regular charts]



WASTE Water Tank Level



RESULTS: Main Flows

```
  Total Flow from each water source to each WellPad (m3)
              WellPad  1   WellPad  2      WellPad  3      WellPad  4           Total
Source  1 :   88714.6             0.0          1920.0             0.0         90634.6
Source  2 :       0.0             0.0             0.0             0.0             0.0
Source  3 :       0.0         46594.3             0.0         41665.0         88259.2
               Total          88714.6         46594.3          1920.0         41665.0

  Total fresh water demand of each wellpad (m3)
       WellPad   1 :   126000.0
       WellPad   2 :   108000.0
       WellPad   3 :    72000.0
       WellPad   4 :   132000.0
         Total     :   438000.0

  Total flowback water in each wellpad (m3)
       WellPad   1 :    89122.9
       WellPad   2 :    76235.8
       WellPad   3 :    38232.4
       WellPad   4 :   118500.7
         Total     :   322091.9

  Total flowback recycled by each wellpad (m3)
       WellPad   1 :    37285.4
       WellPad   2 :    61405.7
       WellPad   3 :    70080.0
       WellPad   4 :    90335.0
         Total     :   259106.2

  Total flow treated on-site in each wellpad(m3)
       WellPad   1 :    16210.8
       WellPad   2 :        0.0
       WellPad   3 :        0.0
       WellPad   4 :    37112.1
         Total     :    53322.9

  Total flow sent to a C.W.T by each wellpad(m3)
       WellPad   1 :        0.0
       WellPad   2 :        0.0
       WellPad   3 :        0.0
       WellPad   4 :        0.0
         Total     :        0.0

  Total flow sent to disposal by each wellpad(m3)
       WellPad   1 :        0.0
       WellPad   2 :        0.0
       WellPad   3 :        0.0
       WellPad   4 :        0.0
         Total     :        0.0

  Total flow recycled between wellpads (m3)
                       WellPad  1   WellPad  2   WellPad  3   WellPad  4
       WellPad   1 :          0.0        430.2      39315.5       3081.5
       WellPad   2 :       2571.8          0.0          0.0      16393.3
       WellPad   3 :       6283.3          0.0          0.0       2945.0
       WellPad   4 :          0.0       5603.9       3927.7          0.0
```

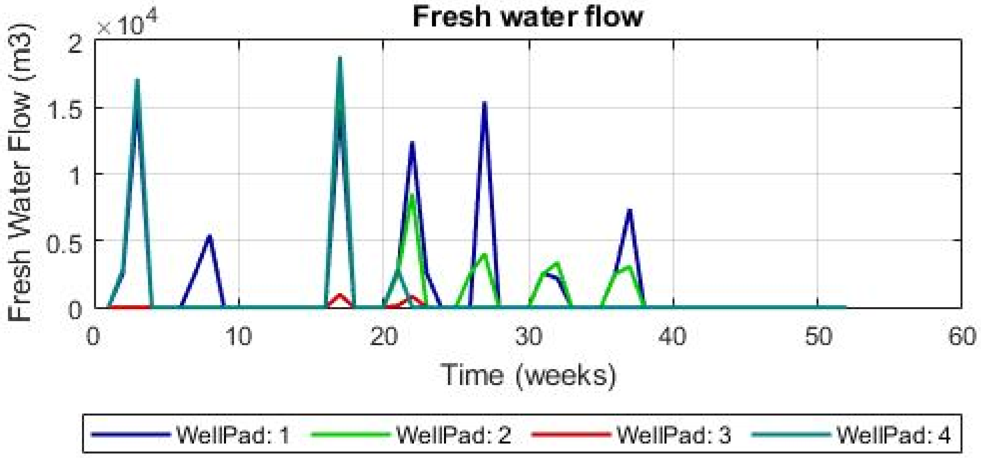
RESULTS: Global data water utilization

```
Total water demanded by WellPads (m3)  : 438000.0
Total fresh water consumption (m3)     : 178893.8
Total flowback water (m3)              : 322091.9
Total flowback water recycled (m3)     : 259106.2
Total sludge generated (m3)            :   9662.8
Total water desalinated on-site (m3)   :  53322.9
Total water desalinated off-site (m3)  :      0.0
Total water send to disposal (m3)      :      0.0

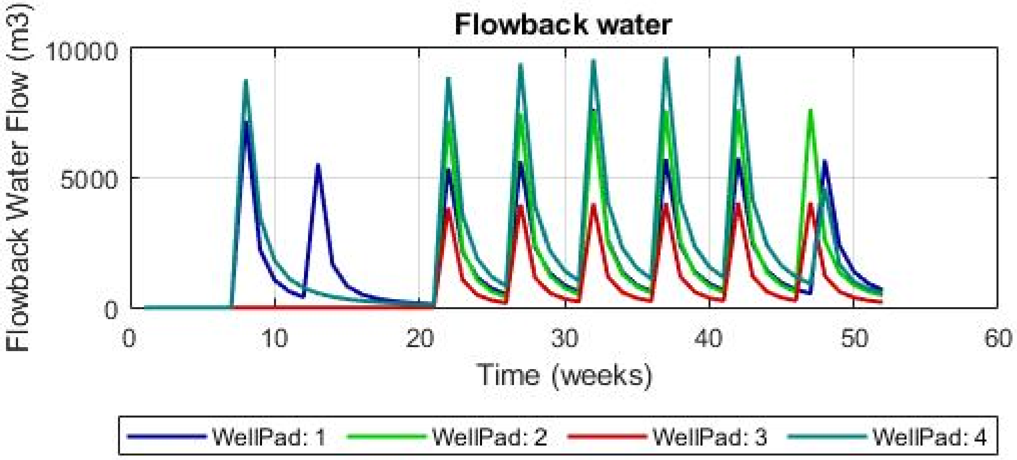
Percentage of fresh water saved (%)    :     59.2
```

RESULTS: Time dependent Water flow charts

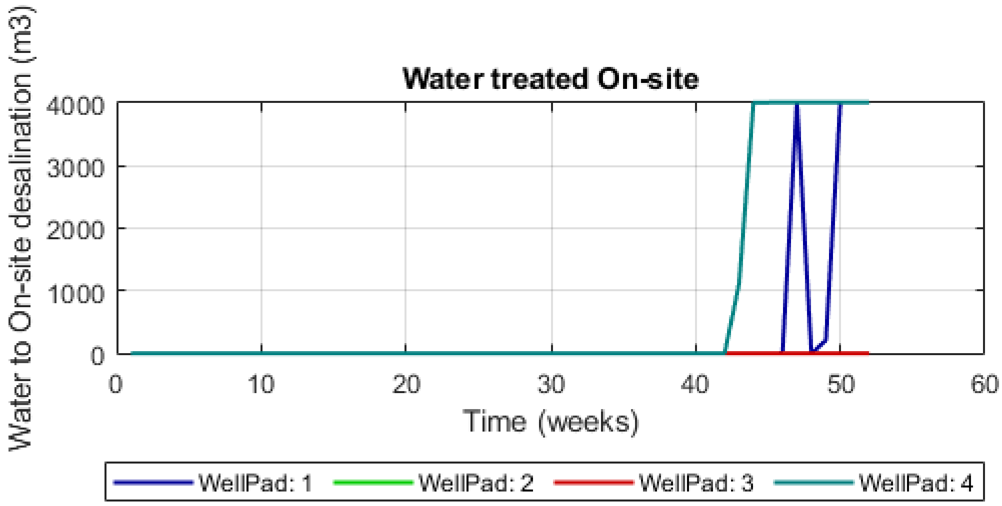
Total fresh water consumed in each wellpad



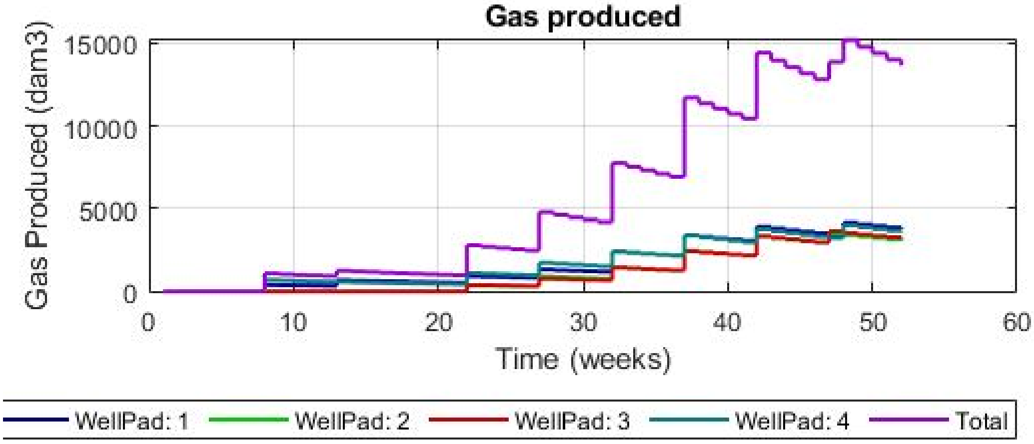
Total flowback water produced in each wellpad



Water to on-site desalination facility in each wellpad



RESULTS : Gas Production Charts



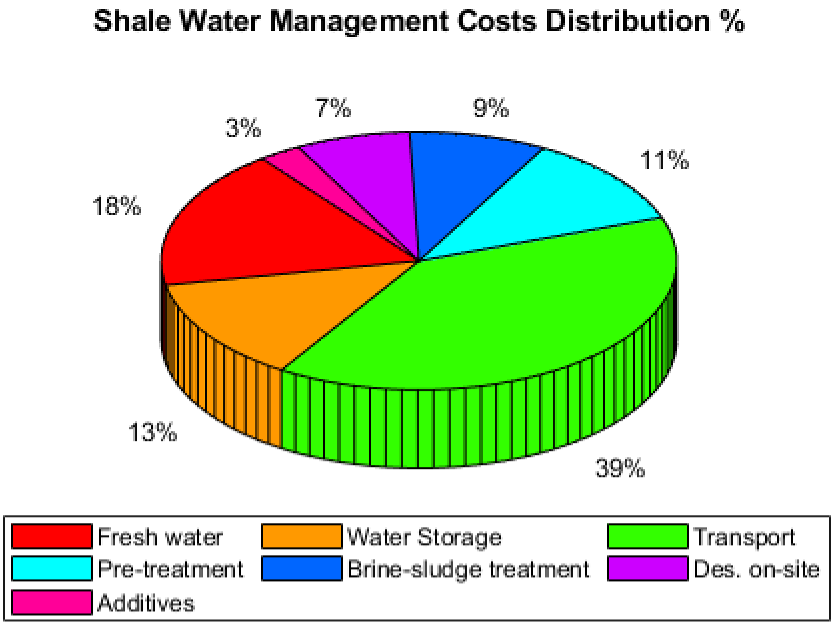
RESULTS : Cost Distribution

```
Fresh water adquisition cost(k$)       :    498.8
Water transport cost(k$)               :   1117.8
Friction reducers cost(k$)             :     75.1
Fresh water storage cost (k$)          :      4.8
Waste water Storage cost(k$)           :    364.4
Pre-treatment cost(k$)                 :    325.6
On-site desalination cost(k$)          :    203.7
Off-site desalination cost(k$)         :      0.0
Water disposal cost(k$)                :      0.0
Brine and sludge disposal cost(k$)     :    243.9
Drilling costs(k$)                     :   7290.0
Gas production cost(k$)                :   4147.9

Total Cost (k$)                        :  14272.0

Total Gas Income (k$)                  :  62915.1
```

Water related Cost Distribution Pie Chart (drilling and gas production are not included in the chart)



RESULTS : LCA

TOTAL ENVIRONMENTAL IMPACT

```
Environmental Impact (points/dam3·gas)  :  0.63906
```

DAMAGE CATEGORIES

```
Ecosystem Quality (points/dam3·gas)     :  0.12884
Human Health (points/dam3·gas)          :  0.25221
Resources Depletion (points/dam3·gas)   :  0.25802
```

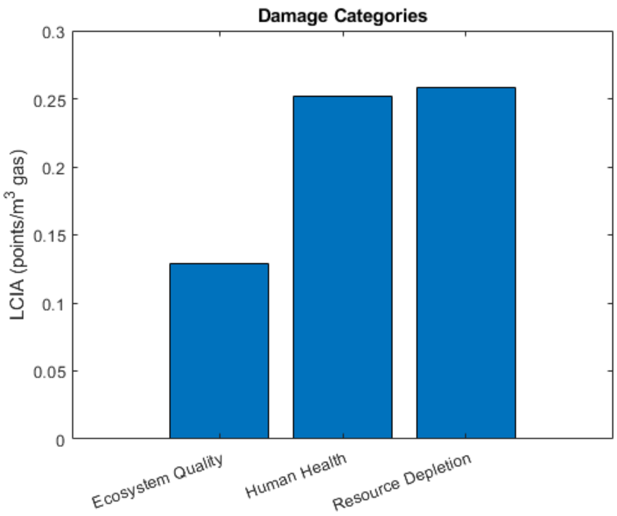
SUB-DAMAGE CATEGORIES

```
        Freshwater Ecotoxicity    0.00004 points/dam3·gas   ===>     0.03114  kg 1,4-DC
   Natural Land Transformation    0.00749 points/dam3·gas   ===>     0.00199  m2
            Marine Ecotoxicity    0.00002 points/dam3·gas   ===>     0.04805  kg 1,4-DC
    Climate Change, Ecosystems    0.09297 points/dam3·gas   ===>     2.05471  kg CO_2-Eq
     Terrestrial Acidification    0.00035 points/dam3·gas   ===>     0.02757  kg SO_2-Eq
       Terrestrial Ecotoxicity    0.00102 points/dam3·gas   ===>     0.00309  kg 1,4-DC
  Agricultural Land Occupation    0.00522 points/dam3·gas   ===>     0.13825  m2
     Freshwater Eutrophication    0.00006 points/dam3·gas   ===>     0.00055  kg P-Eq
         Urban Land Occupation    0.02167 points/dam3·gas   ===>     0.47347  m2

  Photochem. Oxidant Formation    0.00160 points/dam3·gas   ===>     0.04054  kg NMVOC
               Ozone Depletion    0.00005 points/dam3·gas   ===>     0.00000  kg CFC-11
  Particulate Matter Formation    0.07813 points/dam3·gas   ===>     0.01505  kg PM_10-
Eq
            Ionising Radiation    0.00014 points/dam3·gas   ===>     0.43868  kg U235-Eq
  Climate Change, Human Health    0.14708 points/dam3·gas   ===>     3.25081  kg CO_2-Eq
                Human Toxicity    0.02520 points/dam3·gas   ===>     1.85754  kg 1,4-DC

               Metal Depletion    0.01748 points/dam3·gas   ===>     0.37656  kg Fe-Eq
              Fossil Depletion    0.24054 points/dam3·gas   ===>     2.00593  kg oil-Eq
```

FIGURES LCA


Damage Categories
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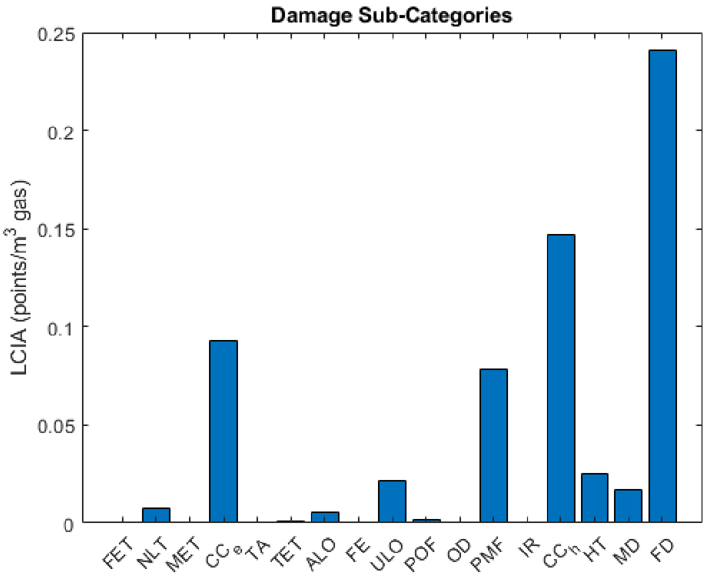
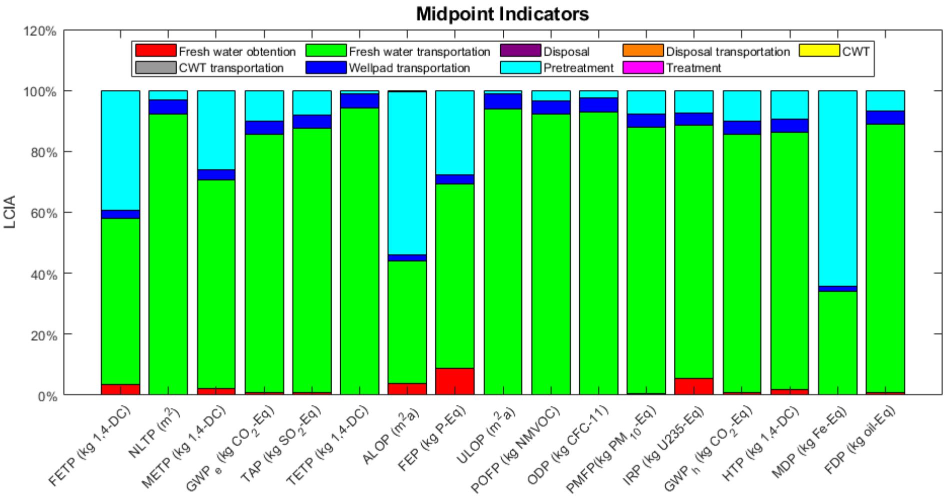
0.25
0.2
0.15
0.1
0.05
0
Ecosystem Quality
Human Health
Resource Depletion


Damage Sub-Categories
LCIA (points/m^3 gas)
0.25
0.2
0.15
0.1
0.05
0
FET
NLT
MET
CC$_e$
TA
TET
ALO
FE
ULO
POF
OD
PMF
IR
CC$_h$
HT
MD
FD


Midpoint Indicators
Fresh water obtention
Fresh water transportation
Disposal
Disposal transportation
CWT
CWT transportation
Wellpad transportation
Pretreatment
Treatment
LCIA
120%
100%
80%
60%
40%
20%
0%
FETP (kg 1,4-DC)
NLTP (m^2)
METP (kg 1,4-DC)
GWP$_e$ (kg CO$_2$-Eq)
TAP (kg SO$_2$-Eq)
TETP (kg 1,4-DC)
ALOP (m^{2}a)
FEP (kg P-Eq)
ULOP (m^{2}a)
POFP (kg NMVOC)
ODP (kg CFC-11)
PMFP(kg PM$_{10}$-Eq)
IRP (kg U235-Eq)
GWP$_h$ (kg CO$_2$-Eq)
HTP (kg 1,4-DC)
MDP (kg Fe-Eq)
FDP (kg oil-Eq)

SHALE GAS WATER MANAGEMENT

```
===============================================================
         Institute of Chemical Process Engineering

                  University of Alicante

               LCA + Water Management Report

==================================================================
```

MINIMUM FRESH WATER CONSUMPTION ALTERNATIVE

RESULTS FOR THE CASE STUDY IN THE PAPER:

«Environmental and Economic Water Management in Shale Gas Extraction»

CONTENTS

MODEL STATISTICS

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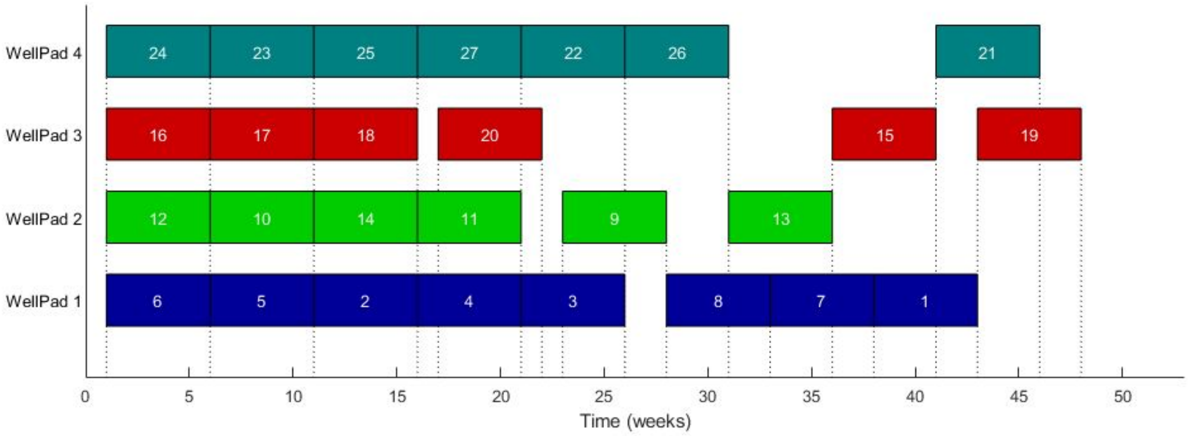
Number of Variables                     :  11373.0
Numer of Discrete Variables             :   1165.0
Number of Equations                     :   9068.0
Number of non-zero elements             : 112950.0
Number of Iterations                    : 991149.0
CPU Generation Time (s)                 :   0.5940
CPU Solution Time (s)                   : 122.5790
Model Objective Value                   : 138897.1536
```

RESULTS: SCHEDULING

The different wells must be schedule according to the following table.

```
Well 1 in wellpad 1      Starts fracking at week   38     and ends fracking at week   43
Well 2 in wellpad 1      Starts fracking at week   11     and ends fracking at week   16
Well 3 in wellpad 1      Starts fracking at week   21     and ends fracking at week   26
Well 4 in wellpad 1      Starts fracking at week   16     and ends fracking at week   21
Well 5 in wellpad 1      Starts fracking at week    6     and ends fracking at week   11
Well 6 in wellpad 1      Starts fracking at week    1     and ends fracking at week    6
Well 7 in wellpad 1      Starts fracking at week   33     and ends fracking at week   38
Well 8 in wellpad 1      Starts fracking at week   28     and ends fracking at week   33
Well 9 in wellpad 2      Starts fracking at week   23     and ends fracking at week   28
Well 10 in wellpad 2     Starts fracking at week    6     and ends fracking at week   11
Well 11 in wellpad 2     Starts fracking at week   16     and ends fracking at week   21
Well 12 in wellpad 2     Starts fracking at week    1     and ends fracking at week    6
Well 13 in wellpad 2     Starts fracking at week   31     and ends fracking at week   36
Well 14 in wellpad 2     Starts fracking at week   11     and ends fracking at week   16
Well 15 in wellpad 3     Starts fracking at week   36     and ends fracking at week   41
Well 16 in wellpad 3     Starts fracking at week    1     and ends fracking at week    6
Well 17 in wellpad 3     Starts fracking at week    6     and ends fracking at week   11
Well 18 in wellpad 3     Starts fracking at week   11     and ends fracking at week   16
Well 19 in wellpad 3     Starts fracking at week   43     and ends fracking at week   48
Well 20 in wellpad 3     Starts fracking at week   17     and ends fracking at week   22
Well 21 in wellpad 4     Starts fracking at week   41     and ends fracking at week   46
Well 22 in wellpad 4     Starts fracking at week   21     and ends fracking at week   26
Well 23 in wellpad 4     Starts fracking at week    6     and ends fracking at week   11
Well 24 in wellpad 4     Starts fracking at week    1     and ends fracking at week    6
Well 25 in wellpad 4     Starts fracking at week   11     and ends fracking at week   16
Well 26 in wellpad 4     Starts fracking at week   26     and ends fracking at week   31
Well 27 in wellpad 4     Starts fracking at week   16     and ends fracking at week   21
```

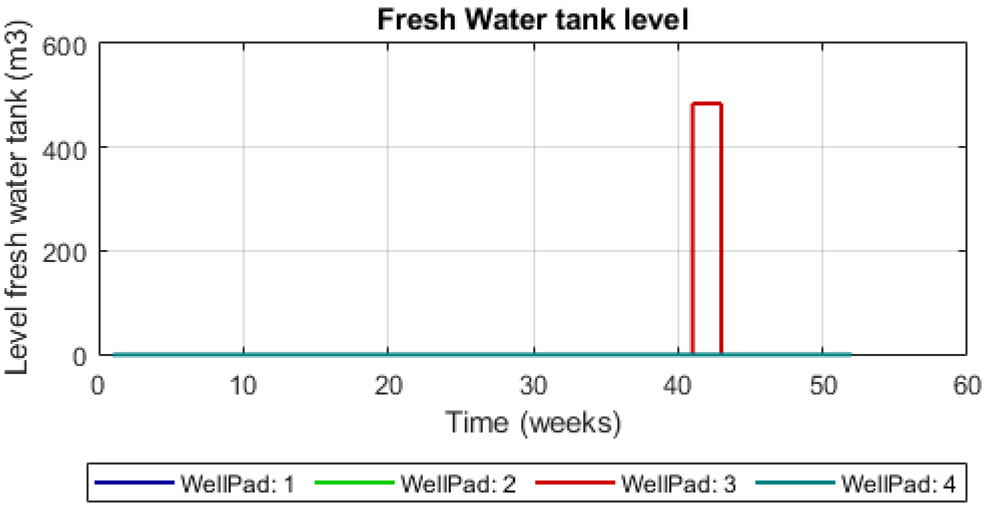


RESULTS: Storage Tanks. Volumes and Levels

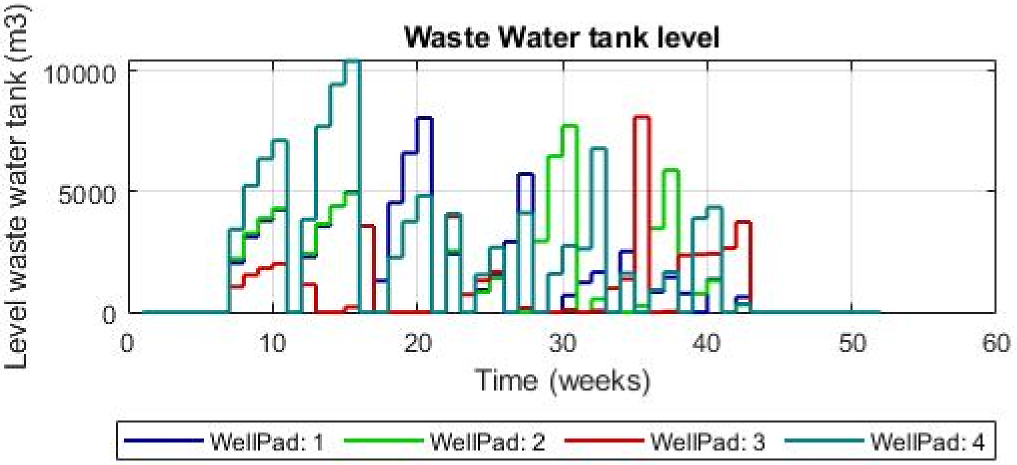
```
Volume of fresh water tanks (m3)
    Well Pad   1 :    50000.0
    Well Pad   2 :    50000.0
    Well Pad   3 :    50000.0
    Well Pad   4 :    50000.0

Volume of waste water tanks (m3)
    Well Pad   1 :    50000.0
    Well Pad   2 :    50000.0
    Well Pad   3 :    50000.0
    Well Pad   4 :    50000.0
```

FRESH Water Tank Level



WASTE Water Tank Level



RESULTS: Main Flows

```
  Total Flow from each water source to each WellPad (m3)
              WellPad 1      WellPad 2        WellPad 3       WellPad 4           Total
Source 1 :          0.0             0.0           483.0             0.0           483.0
Source 2 :          0.0             0.0             0.0             0.0             0.0
Source 3 :      24907.5         39559.4         31930.0         42017.2        138414.1
Total           24907.5         39559.4         32413.0         42017.2

  Total fresh water demand of each wellpad (m3)
       WellPad   1 :   126000.0
       WellPad   2 :   108000.0
       WellPad   3 :    72000.0
       WellPad   4 :   132000.0
         Total     :   438000.0

  Total flowback water in each wellpad (m3)
       WellPad   1 :    91596.1
       WellPad   2 :    78609.0
       WellPad   3 :    38483.7
       WellPad   4 :   121070.7
         Total     :   329759.5

  Total flowback recycled by each wellpad (m3)
       WellPad   1 :   101092.5
       WellPad   2 :    68440.6
       WellPad   3 :    39587.0
       WellPad   4 :    89982.8
         Total     :   299102.9

  Total flow treated on-site in each wellpad(m3)
       WellPad   1 :     5184.4
       WellPad   2 :     1196.6
       WellPad   3 :     6728.6
       WellPad   4 :     7654.3
         Total     :    20763.8

  Total flow sent to a C.W.T by each wellpad(m3)
       WellPad   1 :        0.0
       WellPad   2 :        0.0
       WellPad   3 :        0.0
       WellPad   4 :        0.0
         Total     :        0.0

  Total flow sent to disposal by each wellpad(m3)
       WellPad   1 :        0.0
       WellPad   2 :        0.0
       WellPad   3 :        0.0
       WellPad   4 :        0.0
         Total     :        0.0

  Total flow recycled between wellpads (m3)
                       WellPad  1   WellPad  2   WellPad  3   WellPad  4
       WellPad   1 :          0.0       4790.5      11290.4      10081.5
       WellPad   2 :      17129.2          0.0      11789.7      10417.0
       WellPad   3 :      12132.2       4711.8          0.0       7635.4
       WellPad   4 :      14868.6      23015.4      10663.7          0.0
```

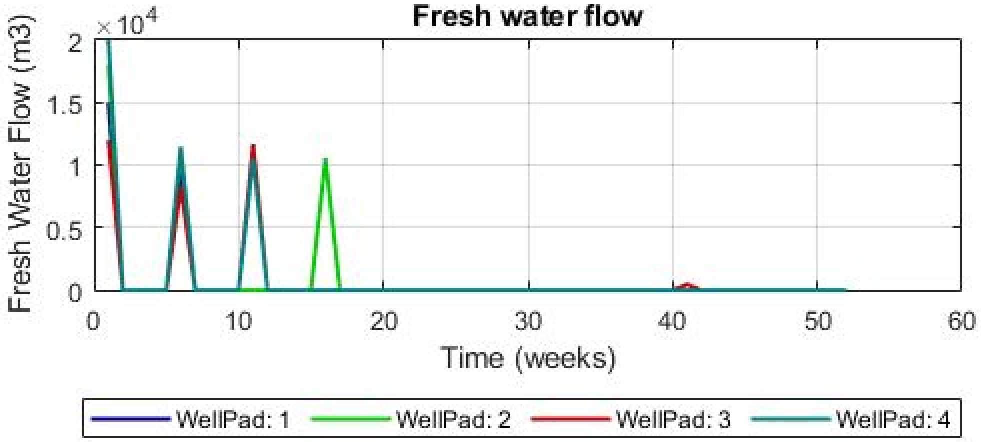
RESULTS: Global data water utilization

```
Total water demanded by WellPads (m3)  : 438000.0
Total fresh water consumption (m3)     : 138897.1
Total flowback water (m3)              : 329759.5
Total flowback water recycled (m3)     : 299102.9
Total sludge generated (m3)            :   9892.8
Total water desalinated on-site (m3)   :  20763.8
Total water desalinated off-site (m3)  :      0.0
Total water send to disposal (m3)      :      0.0

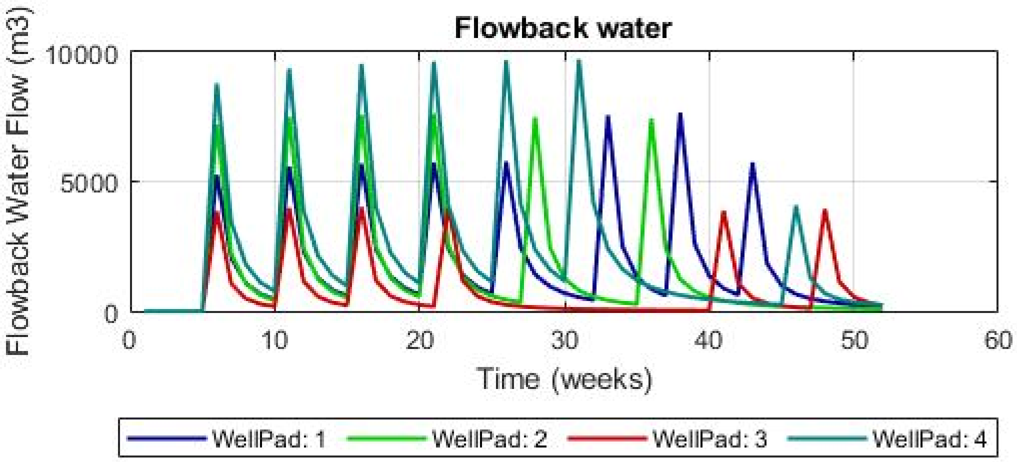
Percentage of fresh water saved (%)    :     68.3
```

RESULTS: Time dependent Water flow charts

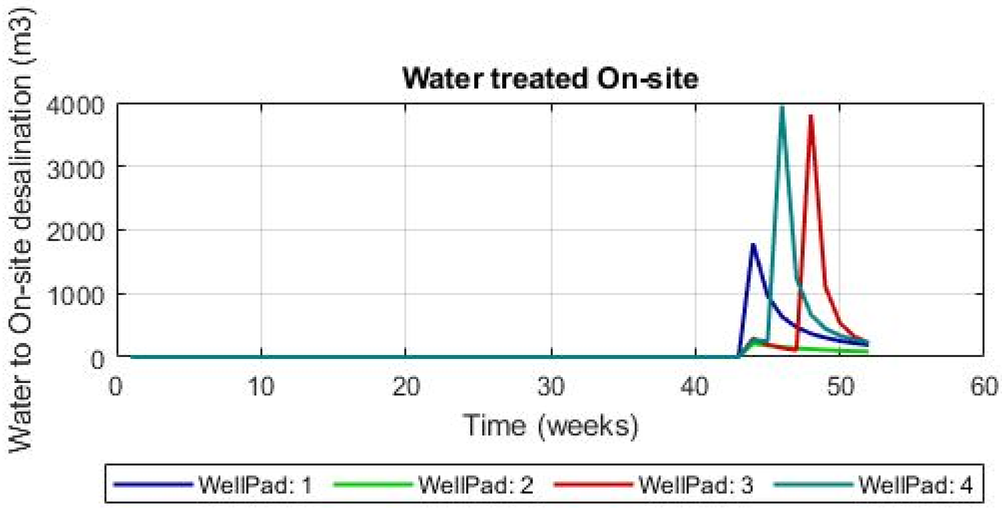
Total fresh water consumed in each wellpad



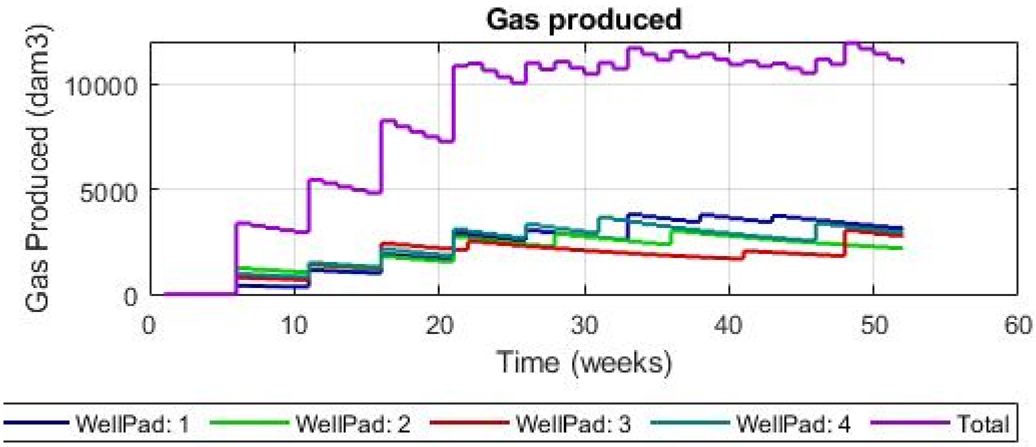
Total flowback water produced in each wellpad



Water to on-site desalination facility in each wellpad



RESULTS : Gas Production Charts



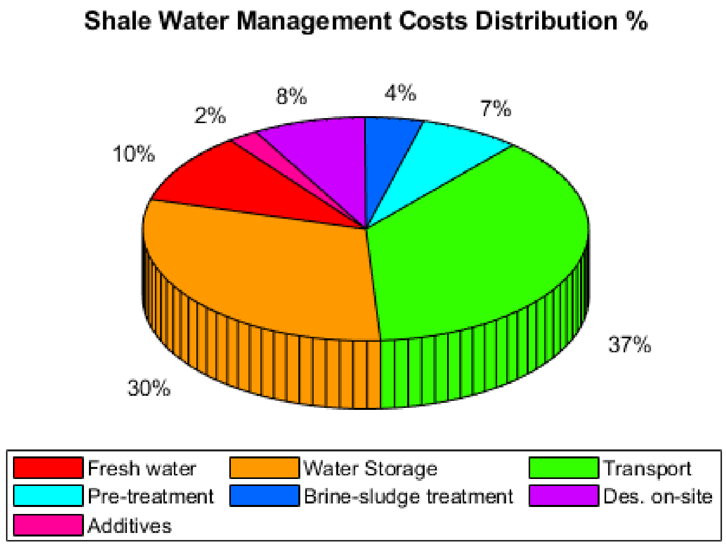
RESULTS : Cost Distribution

```
Fresh water adquisition cost(k$)       :    408.2
Water transport cost(k$)               :   1483.8
Friction reducers cost(k$)             :     86.7
Fresh water storage cost (k$)          :    118.0
Waste water Storage cost(k$)           :   1083.6
Pre-treatment cost(k$)                 :    288.1
On-site desalination cost(k$)          :    323.0
Off-site desalination cost(k$)         :      0.0
Water disposal cost(k$)                :      0.0
Brine and sludge disposal cost(k$)     :    168.5
Drilling costs(k$)                     :   7290.0
Gas production cost(k$)                :   6050.9

Total Cost (k$)                        :  17300.9

Total Gas Income (k$)                  :  58593.7
```

Water related Cost Distribution Pie Chart (drilling and gas production are not included in the chart)



RESULTS : LCA

TOTAL ENVIRONMENTAL IMPACT

```
Environmental Impact (points/dam3·gas)  :  0.54656
```

DAMAGE CATEGORIES

```
Ecosystem Quality (points/dam3·gas)     :  0.11022
Human Health (points/dam3·gas)          :  0.21597
Resources Depletion (points/dam3·gas)   :  0.22037
```

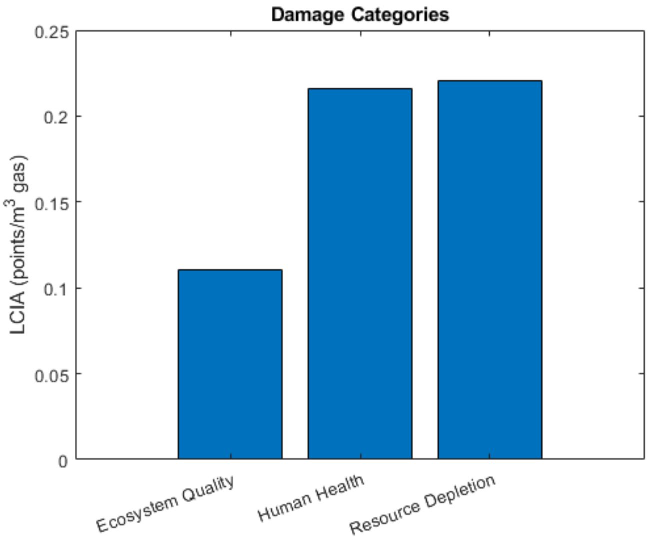
SUB-DAMAGE CATEGORIES

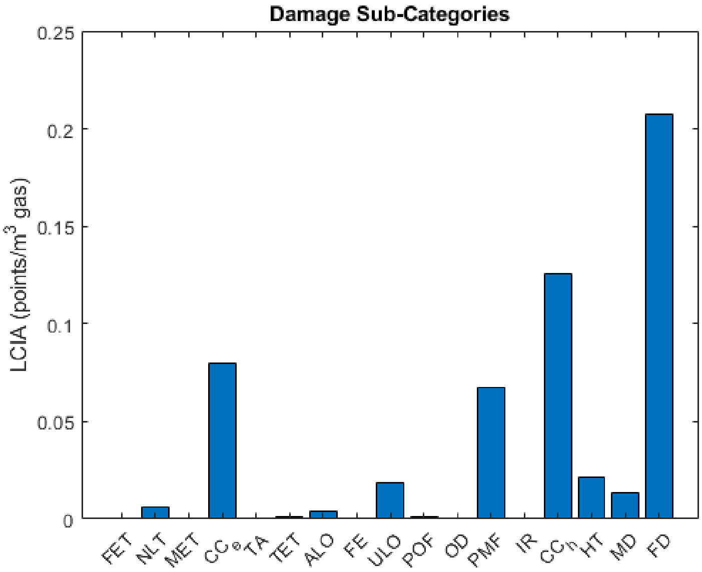
```
        Freshwater Ecotoxicity    0.00003 points/dam3·gas   ===>     0.02487  kg 1,4-DC
   Natural Land Transformation    0.00652 points/dam3·gas   ===>     0.00173  m2
            Marine Ecotoxicity    0.00001 points/dam3·gas   ===>     0.03962  kg 1,4-DC
    Climate Change, Ecosystems    0.07947 points/dam3·gas   ===>     1.75645  kg CO_2-Eq
     Terrestrial Acidification    0.00030 points/dam3·gas   ===>     0.02367  kg SO_2-Eq
       Terrestrial Ecotoxicity    0.00089 points/dam3·gas   ===>     0.00270  kg 1,4-DC
  Agricultural Land Occupation    0.00404 points/dam3·gas   ===>     0.10654  m2
     Freshwater Eutrophication    0.00005 points/dam3·gas   ===>     0.00044  kg P-Eq
         Urban Land Occupation    0.01890 points/dam3·gas   ===>     0.41288  m2

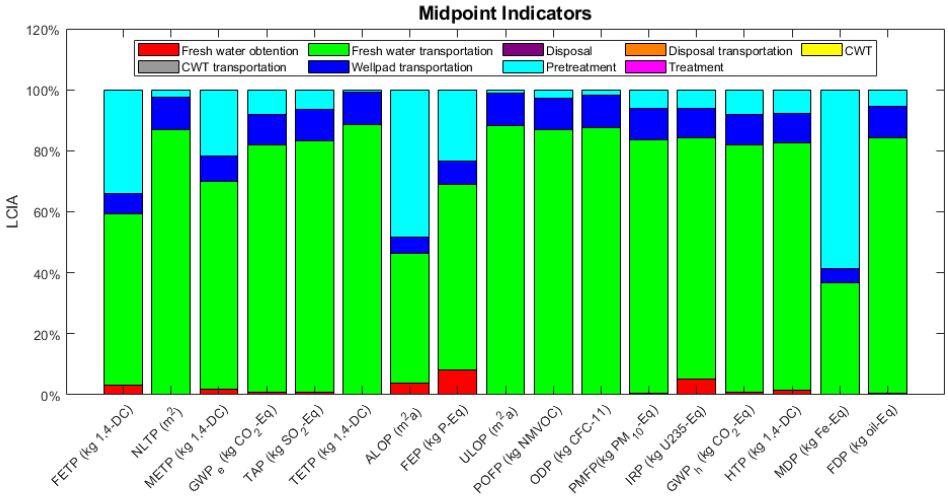
  Photochem. Oxidant Formation    0.00136 points/dam3·gas   ===>     0.03520  kg NMVOC
               Ozone Depletion    0.00004 points/dam3·gas   ===>     0.00000  kg CFC-11
  Particulate Matter Formation    0.06716 points/dam3·gas   ===>     0.01293  kg PM_10-
Eq
            Ionising Radiation    0.00012 points/dam3·gas   ===>     0.37521  kg U235-Eq
  Climate Change, Human Health    0.12573 points/dam3·gas   ===>     2.77893  kg CO_2-Eq
                Human Toxicity    0.02155 points/dam3·gas   ===>     1.58815  kg 1,4-DC

               Metal Depletion    0.01321 points/dam3·gas   ===>     0.28467  kg Fe-Eq
              Fossil Depletion    0.20716 points/dam3·gas   ===>     1.72753  kg oil-Eq
```

FIGURES LCA







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