Economic and Environmental Assessment for Gas Supply Chains Incorporating Shale Gas

Industrial and Engineering Chemistry Research

Supporting Information

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Content (9 pages, 3 tables and 2 figures).

This supporting information (9 pages) presents a set of tables (**Tables S1** to **S3**) and figures (**Figures S1** to **S3**) to show data for the addresses case study as well as the used nomenclature in the proposed optimization model.

Supplementary Material

S1. Case Study

This example considers the hypothetic exploitation of the shale gas located in the Northeast of Mexico, specifically in Burgos basin. In this context, there are several challenges for the exploitation of shale gas in Mexico like the lack of infrastructure and some technical aspects found only in this region such as type of geology, gas composition, depth, physical properties, etc. Once that these concerns are overcome, other challenge appears, and it is referred to generate an optimal planning strategy to satisfy the overall gas requirements through a new gas supply chain incorporating the shale gas production. In this regard, in this case study the gas demands correspond to overall gas requirements in Mexico. Thus, the implementation of the proposed methodology aims to determine the optimal supply chain for the overall gas requirements in Mexico considering the production of shale gas, conventional gas and the imported gas under the current demands. It is important to mention that most of the information required to implement the proposed methodology in this case study has been taken from PEMEX (Mexican petroleum) reports as well as other data were taken from technical reports with updated data for the Marcellus and Barnett regions,[S1,S2] which are located in United States (the largest shale gas producer). In this sense, PEMEX considers five markets to distribute the gas to all the users according to **Figure S1**, even it is shown the potential locations for two hubs (owing to that zone corresponds to Burgos basin).[S3]

Figure S1. Distribution of markets and hubs in Mexico.

As can be seen in **Figure S2**, it has been established the location for two hubs and there are considered 16 potential wells, which are grouped in four well pads. For each supply chain pathway, the environmental impact using the TRACI method was considered,[S4] having that the impact categories with the higher values were global warming, eutrophication and human health. Notice that previous investigations are focused on measuring the environmental impact by the gas production,[S5-S7] however in this paper are included the overall damage generated by all the steps in the gas network distribution by each option.

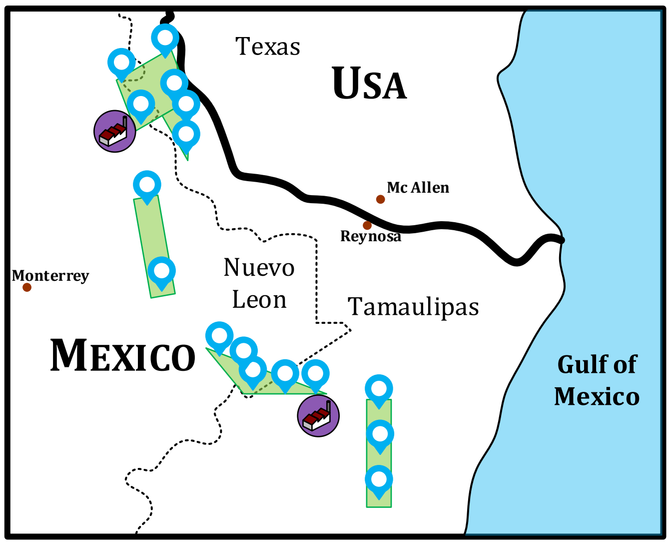

Figure S2. Location for pad wells and hubs in Burgos basin.

This example accounts for the following information:

- The gas selling prices in the markets 1-5 are 0.392217, 0.238869, 0.289, 0.277206 and 0.318492 \$MM/ MMSCF, respectively (see **Figure S1**).[S3]
- Mexico has four main conventional gas zones and the total production of each region is 792.48 MMSCFD for all the months and the unit gain (i.e., the difference among the unit selling price and the unit production cost) is 0.12 \$MM/ MMSCF.[S3]
- There are two sources to import additional gas, which correspond to gas coming from Peru and USA and the maximum availabilities in each time period are 8,076.85 MMSCFD and 104,109 MMSCFD, respectively.[S8] Also, the unit gains (difference price - cost) for the gas imported from Peru and distributed in the markets 1-5 are 1.219315×10^{-2}, 7.208529×10^{-3}, 8.838117×10^{-3}, 8.454684×10^{-3} and 9.796698×10^{-3} \$MM/ MMSCF; while unit gains for the gas imported from USA are presented in **Table S1**.

- It is considered that water and CO_2 are the fracturing fluids able to carry out the hydraulic fracturing process and their costs are 0.4 \$MM/m^3 and 0.083 \$/m^3, respectively.[S2] Notice that CO_2 represents an important option to replace the relevant amounts of water used by hydraulic fracturing process.[S9,S10]
- The fixed and variable charges for the installation of hubs are 0.066 \$MM and 2.142x10^{-5} \$MM/ MMSCF, respectively.
- The unit cost for fracturing process in well pads 1-4 are 5.76x10^{-4}, 1.92x10^{-4}, 4.8x10^{-4} and 2.88x10^{-4} \$MM/ MMSCF, respectively.[S1,S2]
- The unit transportation cost for well pads-hubs is 3.5x10^{-4} \$MM/ MMSCF km; whereas the unit transportation cost from the hubs to markets 1-5 are 37.579x10^{-4}, 75.158x10^{-4}, 75.158x10^{-4}, 112.736x10^{-4} and 112.736x10^{-4} \$MM/ MMSCF km, respectively.
- The eco-indicators for the processing in hubs are 2.9724x10^{-6}, 1.86982x10^{-8} and 1.0464x10^{-15} ton/MMSCF for global warming, eutrophication and human health, respectively.
- Besides, the overall unit eco-indicators (including extraction, transportation and processing) for global warming, eutrophication and human health with respect to the conventional gas are 3.4915337x10^{-2}, 3.85772x10^{-6} and 1.05435x10^{-12} ton/MMSCFD, respectively; whereas for imports of gas from USA are 4.7558908x10^{-2}, 2.19567x10^{-4} and 4.52367x10^{-13} ton/MMSCFD, respectively and finally for imported gas from Peru are 2.23 for global warming and 7.89x10^{-3} ton/MMSCFD for eutrophication.

Table S1. Unit gains for the gas imported from USA.

Month/Market	Unit gains for the gas imported from USA (\$MM/ MMSCF)				
	1	**2**	**3**	**4**	**5**
January	0.010549127	0.005564506	0.007194094	0.006810661	0.008152675
February	0.010869127	0.005884506	0.007514094	0.007130661	0.008472675
March	0.010869127	0.005884506	0.007514094	0.007130661	0.008472675
April	0.010719127	0.005734506	0.007364094	0.006980661	0.008322675
May	0.010689127	0.005704506	0.007334094	0.006950661	0.008292675
June	0.010289127	0.005304506	0.006934094	0.006550661	0.007892675
July	0.009949127	0.004964506	0.006594094	0.006210661	0.007552675
August	0.009829127	0.004844506	0.006474094	0.006090661	0.007432675
September	0.009689127	0.004704506	0.006334094	0.005950661	0.007292675
October	0.009589127	0.004604506	0.006234094	0.005850661	0.007192675
November	0.009999127	0.005014506	0.006644094	0.006260661	0.007602675
December	0.009239127	0.004254506	0.005884094	0.005500661	0.006842675

Moreover, **Table S2** shows the natural gas demands in each one of the five markets considered by this example and **Table S3** contains the unit environmental impacts for the working fluids and for the transportation route well pads-hubs. It should be noted that the eco-indicators related to working fluids (i.e., for the hydraulic fracturing process) represent the highest values for unit environmental impacts with respect to the rest of unit eco-indicators, which will generate an important augment in the environmental impact for the possible solutions where shale gas is required comparing with the optimal solutions where shale gas does not appear. Also notice that, for most of the cases, the eco-indicators for CO_2 are higher than water. Although, CO_2 sequestration is a potential source to obtain this fluid and considering that this process involves significant environmental benefits, the augment in eco-indicators when CO_2 is employed as fracturing fluid is generated by the compression process for CO_2 owing to the compression requirements are greater with respect to water and it is necessary to achieve higher pressures. Also, for the transportation of the fluids, the water pumping represents a lower impact with respect to CO_2 compression. Thus, the ecological footprint for compression process is capable to revert the benefits owing to CO_2 sequestration. However, this does not mean that the incorporation of CO_2 as working fluid is not relevant, in the most of the shale plays the main technical problem is related to the water availability and CO_2 offers an alternative to overcome this drawback.

Table S2. Natural gas demands in the markets.

Month/Market	Natural gas demands in the markets (MMSCFD)				
	1	**2**	**3**	**4**	**5**
January	533.41	1848.567	845.701	760.654	2173.784
February	529.922	1836.476	840.169	755.679	2159.566
March	521.934	1808.795	827.505	744.289	2127.015
April	512.502	1776.108	812.551	730.839	2088.577
May	505.641	1752.33	801.673	721.054	2060.616
June	509.036	1764.094	807.055	725.895	2074.45
July	500.769	1735.445	793.948	714.106	2040.76
August	492.158	1705.605	780.297	701.828	2005.671

September	486.396	1685.636	771.161	693.611	1982.189
October	483.25	1674.731	766.173	689.124	1969.365
November	477.395	1654.443	756.891	680.775	1945.507
December	465.738	1614.042	738.408	664.151	1898

Table S3. Unit environmental impacts in ton/MMSCFD.

Concept		Eco-indicator		
		Global Warming (ton CO_2/MMSCF)	**Eutrophication** (ton N/MMSCF)	**Human Health** (CTU cancer /MMSCF)
Pad well	**Fluid**	*For the working fluid*		
1	H_2O	600.93	0.3324	1.66119×10^{-8}
	CO_2	1201.86	0.6648	3.2238×10^{-8}
2	H_2O	200.31	0.1108	5.53729×10^{-8}
	CO_2	400.62	0.2216	1.10746×10^{-8}
3	H_2O	500.77	0.2770	1.38432×10^{-8}
	CO_2	1001.55	0.5540	2.76865×10^{-8}
4	H_2O	600.93	0.1662	8.30594×10^{-9}
	CO_2	300.46	0.3324	1.66119×10^{-8}
Pad well		*For the transportation route wells-hubs*		
1		6.92046×10^{-5}	3.195×10^{-7}	6.58255×10^{-16}
2		2.30682×10^{-5}	1.065×10^{-7}	2.19418×10^{-16}
3		5.76705×10^{-5}	2.6625×10^{-7}	5.48546×10^{-16}
4		3.46023×10^{-5}	1.5975×10^{-7}	3.29127×10^{-16}

S2. Nomenclature

Parameters

D_t	time conversion factor, d/month
$F_h^{\max-cap-hub}$	maximum capacity for the hub h, MMSCFD
$F_{i,t}^{\max-well}$	maximum capacity for the shale gas available at the well i in the time t, MMSCFD
$F_{p,t}^{\max-conv}$	maximum availability for the conventional gas at the site p in the time t, MMSCFD
$F_{e,t}^{\max-import}$	maximum availability for the importing gas in the source e in the time t, MMSCFD

$F_{j,t}^{Gas-Market}$	natural gas demands at the market j in the time t, MMSCFD
FC_{h}^{hub}	fixed charge for the hub plant in the capital cost function, \$MM
k_F	factor used to annualize the investment, y^{-1}
$M^{\mathrm{Cost}^{fluid}}$	maximum value for the working fluid cost, \$MM
$M^{EI^{fluid}}$	maximum value for the environmental impact of the working fluid, \$MM
NPV	value at present time, \$MM
$OUEI_{p,j}^{conv}$	overall unit environmental impact for the conventional gas, environmental unit/ MMSCF
$OUEI_{e,j}^{import}$	overall unit environmental impact for the imported gas, environmental unit/ MMSCF
$UC_{i,f,t}^{fuid}$	unit cost for the working fluid f, \$MM/ MMSCF
$UC_{i,t}^{fracking}$	unit cost for the fracturing in the well i, \$MM/ MMSCF
$UC_{h,t}^{process}$	unit cost for the shale gas processing at hub h, \$MM/ MMSCF
$UC_{i,h}^{trans-well-hub}$	unit transportation cost from the well i to the hub h, \$MM/ MMSCF
$UC_{h,j}^{trans-hub-market}$	unit transportation cost from the hub h to the market j, \$MM/ MMSCF
$UEI_{i,f}^{fluid}$	unit environmental impact for the working fluid, environmental unit/ MMSCF
$UEI_{h}^{process}$	unit environmental impact for the processing, environmental unit/ MMSCF
$UEI_{i,h}^{trans-well-hub}$	unit environmental impact for the transportation from wells to hubs, environmental unit/ MMSCF
$UEI_{h,j}^{trans-hub-market}$	unit environmental impact for the transportation from hubs to markets, environmental unit/ MMSCF
$UP_{h,j,t}^{gas}$	unit price for the natural gas, \$MM/ MMSCF
$UPC_{p,j,t}^{conv}$	unit difference among price and cost for conventional gas, \$MM/ MMSCF
$UPC_{e,j,t}^{import}$	unit difference among price and cost for imported gas, \$MM/ MMSCF
VC_{h}^{hub}	variable charge for the hub plant in the capital cost function, \$MM/ MMSCF

Greek Symbols

α^{hub}	exponent for the economies of scale

$\alpha_h^{proces-rawgas}$ volumetric efficiency for the processing plants

Variables

$CapCost^{hubs}$ capital cost for the hubs, \$MM

$Cost_{i,f}^{fluid-fracking}$ fracturing fluid cost, \$MM

$Cost^{fracking}$ hydraulic fracturing cost, \$MM

$Cost^{processing}$ shale gas processing cost, \$MM

$Cost^{trans-hub-market}$ total transportation cost from hubs to markets, \$MM

$Cost^{trans-well-hub}$ total transportation cost from wells to hubs, \$MM

$EI^{conv-gas}$ overall environmental impact generated by conventional gas, environmental unit

$EI_{i,f}^{fluid-fracking}$ environmental impact generated by the fracturing fluid, environmental unit

$EI^{import-gas}$ overall environmental impact generated by the imported gas, environmental unit

$EI^{processing}$ environmental impact for the shale gas processing, environmental unit

$EI^{shale-gas}$ overall environmental impact generated by the shale gas, environmental unit

$EI^{trans-well-hub}$ environmental impact for the transportation from wells to hubs, environmental unit

$EI^{trans-hub-market}$ environmental impact for the transportation from hubs to markets, environmental unit

$F_h^{cap-hub}$ capacity flowrate for hub h, MMSCFD

$F_{p,t}^{conventional}$ conventional gas production in the site p in the time t, MMSCFD

$F_{h,t}^{hub-in}$ gas flowrate entering the hub h in the time t, MMSCFD

$F_{h,t}^{hub-out}$ gas flowrate leaving the hub h in the time t, MMSCFD

$F_{e,t}^{imported}$ imported gas flowrate from the source e in the time t, MMSCFD

$F_{i,t}^{well}$ shale gas production in the well i in the time t, MMSCFD

$f_{p,j,t}^{conv-market}$ gas flowrate sent from the conventional site p to market j in the time t, MMSCFD

$f_{h,j,t}^{hub-market}$ gas flowrate sent from the hub h to the market j during the time period t, MMSCFD

$f_{e,j,t}^{import-market}$ gas flowrate sent from the importing source e to market j in the time t, MMSCFD

$f_{i,h,t}^{well-hub}$ gas flowrate sent from the well i to the hub h in the time t, MMSCFD

$Profit^{conv-gas}$ conventional gas profits, \$MM

$Profit^{import-gas}$ imported gas profits, \$MM

$Profit^{shale-gas}$ shale gas profits, \$MM

$Sales^{shale-gas}$ shale gas incomes, \$MM

TEI overall environmental impact generated by the project, environmental unit

TPP total profits, \$MM

$y_{i,f}^{fluid-fracking}$ binary variable used to select the fracturing fluid *f* in the well *i*

y_h^{hub} binary variable used to model the existence of the hub *h*

Sets

E $\{e \mid e$ is a gas importing source$\}$

F $\{f \mid f$ is a fracturing fluid$\}$

H $\{d \mid d$ is a hub/processing plant$\}$

I $\{i \mid i$ is a pad well$\}$

J $\{j \mid j$ is a market$\}$

P $\{p \mid p$ is a conventional gas production site$\}$

T $\{t \mid t$ is a time period$\}$

Subscripts and Superscripts

e gas importing source

f fracturing fluid

h hub/processing plant

i well pad

j market

p conventional gas production site

t time period

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