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Handling Uncertain Feedstock Compositions in Shale Gas Processing System Designs with Simulation-based Robust Equipment Capacities

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The international gas market has been revolutionized by the advent of shale gas. As the shale gas production rate from a shale well declines over time, the mixture composition of raw shale gas gathered from multiple shale wells can be uncertain. This paper addresses the robust design and synthesis of shale gas processing and natural gas liquids (NGLs) recovery processes under uncertain feedstock compositions. The process feedstock comes from 8 shale wells with different raw shale gas compositions and the processed pipeline gas is to satisfy the fuel demand of a real world power plant. We employ monoethanolamine absorption, triethylene glycol absorption, and turboexpander-based NGLs recovery in the process designs to remove acid gases, water, and NGLs, respectively. Based on detailed process simulation and techno-economic analysis for each raw shale gas composition, we develop a robust process design with the minimum total direct cost of each operation unit needed to satisfy the pipeline gas demand. The robust process design can handle feedstock from the 8 shale wells with varying production flowrates. We perform a life cycle analysis for the robust design according to the Eco-indicator 99 methodology. The unit annualized cost is $1.8/GJ. Raw shale gas production and cooling utility generation are the major contributors to the environmental impacts of shale gas processing and NGLs recovery.

1. Introduction

Unconventional natural gas from shale, i.e. shale gas, is regarded as a game changer in the global energy industry (Kerr, 2010). Since horizontal drilling and hydraulic fracturing were successfully applied in shale gas production (Gao et al., 2015a), shale gas has reached its golden age and the total shale gas production in the US is predicted to increase by 40 % by 2040 (Gao et al., 2015b). As a result, an increasing number of midstream facilities and transportation pipelines need to be designed and deployed (Gao et al., 2017). Shale gas processing plants remove valuable natural gas liquids (NGLs) and undesired components from raw shale gas to meet product specifications in downstream distribution networks (He and You, 2014). The rapid expansion of the shale gas industry will lead to the design and development of many new shale gas processing plants for various functions (Gao et al., 2015b). There is great economic potential and practical need to address the optimal design and synthesis of shale gas processing processes (Gong et al., 2015).
There are a few process designs for shale gas processing and NGLs recovery (He et al., 2015). However, existing process designs assume fixed feedstock compositions, which cannot be guaranteed in real world operations (Luyben, 2013). Shale gas from various shale wells shows different compositions and processing needs (Bullin and Krouskop, 2009). As a shale gas processing plant is designed to process raw shale gas gathered from multiple shale wells, the feedstock composition fluctuates with the changes in raw shale gas production rates (He et al., 2016). If a processing plant is designed to process raw shale gas with fixed compositions, a large amount of off-spec gas will be produced when the amounts of undesired components surpass their processing capacities (Getu et al., 2013). In order to maintain stable supply of qualified gas products, uncertain feedstock compositions must be considered and addressed at the design stage, just like other uncertain sources in shale gas energy systems (Gao et al., 2015c).
In this work, we develop a robust design of shale gas processing and NGLs recovery processes under uncertain feedstock compositions. We investigate the shale gas demand of a real world power plant and design a shale gas processing and NGLs recovery process for 8 raw shale gas sources. The process consists of three sections:

acid gas removal (AGR), dehydration, and NGLs recovery. We perform detailed process simulation and techno-economic analysis for the 8 raw shale gas compositions. A robust process design is proposed based on the capacities and total direct costs (TDC) of operation units in the 8 individual process designs. The robust design generates qualified pipeline products as long as the feedstock comes from the considered 8 raw shale gas sources. To identify the hotspots of environmental impacts for the robust design, we further conduct a life cycle analysis according to the Eco-indicator 99 methodology.

2. Uncertainty in feedstock compositions

The shale gas processing facility in this work is designed to meet a practical need: the processed pipeline gas will be purchased and consumed by a 1,150 MW natural gas power plant located in Texas, US. An energy conversion efficiency of 51.5 % is considered in the natural gas power plant. In order to satisfy the power generation demand, a pipeline gas with 2,233 MW is required as the fuel of the power plant. 8 raw shale gas streams (Table 1) are gathered from different shale wells in the gulf coast region and serve as the feedstock of shale gas processing. There are 9 major components in raw shale gas: CH_4, C_2H_6, C_3H_8, C_4H_{10}, C5+ (represents the hydrocarbon molecules with more than 4 carbon atoms), CO_2, H_2S, N_2, and H_2O. As shown in Eq.(1), the concentration of a component i in the feed c_i^{feed} is determined by the concentration $c_{i,j}$ of component i in stream j and the flowrate v_j of stream j. It is shown that the production rate of a shale well gradually declines over time (Gao et al., 2015d). In addition, more wells can be completed in the similar area to increase the production rate. As a result, the stream flowrate v_j rarely remains a fixed value in practice and a fluctuation in stream flowrates can cause significant changes in the feed composition. In this work, we focus on the change in stream flowrates and assume the composition of each stream is relatively stable. As a result, a feed composition is a convex combination of the 8 compositions with varying weights and the 8 compositions are extreme conditions among all possible feed compositions. A robust design of shale gas processing can handle all the combinations while satisfying the downstream demand. The robust design in this work is based on the designs of the 8 compositions.

$$c_i^{feed} = \sum_j c_{i,j} v_j \Big/ \sum_j v_j , \quad \forall i \tag{1}$$

Table 1: Shale gas compositions (Pring, 2012)

Raw shale gas streams		1	2	3	4	5	6	7	8
Composition (mole %)	CH_4	94.64	95.62	95.75	94.81	79.90	78.48	72.62	81.05
	C_2H_6	0.05	0.08	0.08	0.16	11.61	12.68	14.47	11.10
	C_3H_8	0.00	0.00	0.00	0.00	3.98	4.44	6.37	3.91
	C_4H_{10}	0.00	0.00	0.00	0.00	2.12	2.11	3.42	1.75
	C5+	0.00	0.00	0.00	0.00	1.22	1.02	1.59	0.94
	CO_2	4.93	3.92	3.78	4.46	0.73	0.86	1.11	0.79
	H_2S	0.23	0.23	0.23	0.23	0.23	0.23	0.23	0.23
	N_2	0.03	0.04	0.04	0.22	0.09	0.06	0.07	0.11
	H_2O	0.12	0.12	0.12	0.12	0.12	0.12	0.12	0.12

3. Process description

The goal of a shale gas processing plant is to remove undesired constituents and separate valuable NGLs so that the resulting gas product meets the specifications for transmission and downstream utilization (Speight, 2013). There are three sections in the process design for the 8 raw shale gas feedstocks, namely, AGR, dehydration, and NGLs recovery. As shown in Figure 1, the AGR process is based on MEA absorption given that MEA has a high solution capacity for H_2S and CO_2 in contrast with other amine absorbents. The shale gas feed is first sent into the bottom of an absorber and the acid gases are absorbed by a lean amine solution introduced from the top of the absorber. The treated gas, or sweet shale gas, leaves the top of the tower and is sent to the next section. The rich amine solution is then fed to a stripper column, and the liquid product from the bottom of the stripper becomes the lean amine stream after it is cooled and pressurized. The gas product containing primarily H_2S and CO_2 is sent to the sulfur recovery process. The high CO_2/H_2S ratios will cause a low sulfur recovery if the gas is sent to a Clause process directly. Instead we employ an acid gas enrichment process to concentrate H_2S before it can be handled by a Clause process.

The sweet shale gas stream from the AGR section is water-saturated. However, both operating the cryogenic units in the NGLs recovery section and transporting gas product in pipelines require a low concentration of water. In Figure 2, we consider a TEG absorption process to remove the extra water because of TEG's high absorption efficiency, less energy-intensive regeneration, nontoxicity, and no interaction with the hydrocarbons. The sweet shale gas from the last section is fed to a phase separator to remove any free liquid, and then contacts with a lean TEG stream countercurrently. Most dry shale gas is introduced to the NGLs recovery section, while a small portion of the dry shale gas is used as the stripping gas in a two-stage stripper column system. The rich TEG stream is depressurized and flashed to remove most hydrocarbons, and the remaining solution becomes the lean TEG solution after going through the stripper columns.

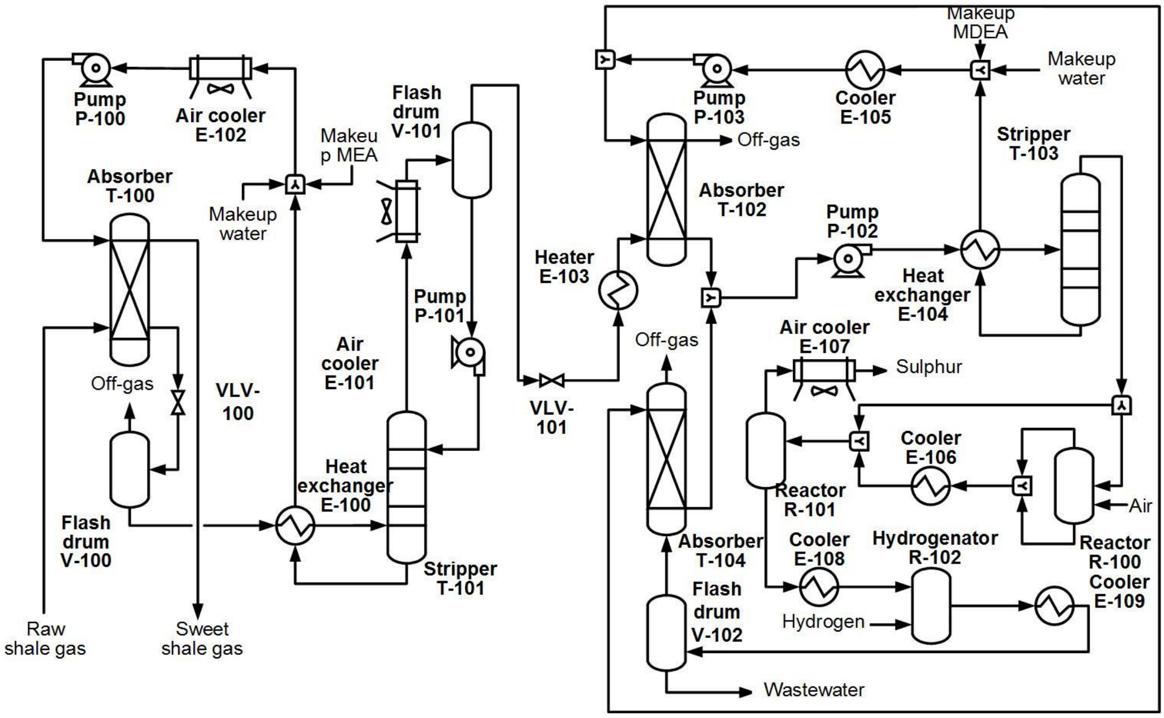


Figure 1: Process flowsheet of acid gas removal process

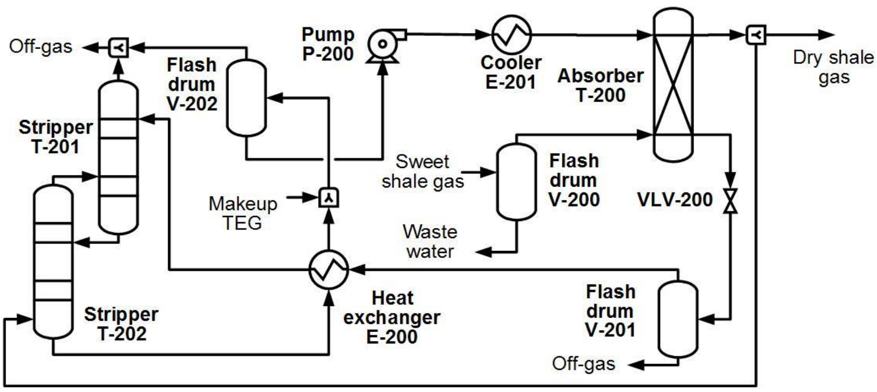


Figure 2: Process flowsheet of dehydration process

Sequentially, the dry shale gas is fed to a NGLs recovery process in order to separate valuable NGLs. The dry gas is pre-cooled in a cold box. The liquid product is injected into the demethanizer, while the vapour product is split into two streams. One stream is further cooled by a heat exchanger, a cooler, and a Joule-Tomson valve. A flash drum immediately separates the gas product, while the liquid product is fed to the first stage of the demethanizer. The other stream is introduced into a turbo-expander, which generates electricity and drives a compressor. It is later fed to the middle of the demethanizer. For transportation purpose, pipeline gas should be pressurized to 60 bar, which is much higher than the pressure of the purified gas from the cold box. As a result, a three-stage compression system pressurizes the gas before it is injected into the distribution system. The liquid product from the bottom of the demethanizer it is injected into the NGLs distribution system after pressurized by a pump. If the dry shale gas from the last section does not contain much NGLs, the NGLs recovery units will be bypassed and the product will be directly pressurized by the compressor system.

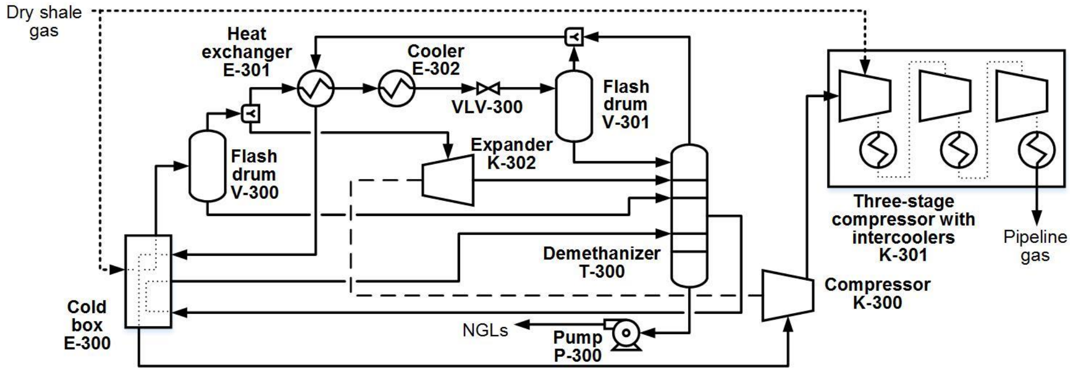


Figure 3: Process flowsheet of NGLs recovery process

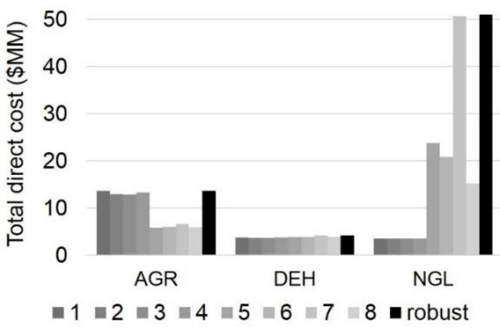
4. Results and discussion

We perform detailed ASPEN HYSYS simulation for 8 scenarios, corresponding to 8 raw shale gas compositions in Table 1. The mass and energy balance results are shown in Table 2. As mentioned in the previous section, the processed pipeline gas is to meet the fuel demand of a natural gas power plant. Therefore, the higher heating values of all pipeline gas must be at least 2,233 MW. As most NGLs are separated from the pipeline gas product, the more NGLs are contained in the feedstock, the more raw shale gas will be sent to the plant and processed. Raw shale gas feeds 1–4 have relatively high methane concentrations. As a result, the corresponding feed flowrates are lower. Additionally, the acid gas concentrations in these feedstocks are higher, resulting in higher energy consumption in the AGR section. In contrast, raw shale gas feeds 5–8 show much higher NGLs concentrations, so higher feed flowrates are required to satisfy the pipeline gas demand.

Table 2: Mass and energy balance results for 8 shale gas compositions

Scenario	1	2	3	4	5	6	7	8
Raw shale gas, m^3/s	62.7	62.1	62.0	62.5	72.8	73.9	79.2	71.8
Solvent, 10^{-3} kg/s	1.3	1.3	1.3	1.3	3.8	4.2	5.4	3.8
Hydrogen, 10^{-4} kg/s	6.7	6.7	6.7	6.7	7.8	8.1	8.3	7.8
Process water, kg/s	0.2	0.2	0.3	0.2	0.1	0.1	0.2	0.1
Electricity, MW	3.7	3.6	3.6	3.7	8.1	8.1	8.2	8.1
Heating, MW	89.6	85.6	85.2	88.0	23.3	24.9	26.8	23.3
Cooling, MW	39.7	38.9	38.8	39.4	33.3	33.0	36.2	32.2
Pipeline gas, MW	2,233.0	2,233.0	2,233.0	2,233.0	2,233.0	2,233.0	2,233.0	2,233.0
NGLs, MW	0	0	0	0	1,099.0	1,052.4	1,499.1	893.0
Sulfur, kg/s	0.2	0.2	0.2	0.2	0.2	0.2	0.3	0.2

Based on the mass and energy balance results, we employ ASPEN economic analyser to evaluate TDC of each operation unit in all scenarios. The TDCs are then categorized into three groups, corresponding to the three process sections. The TDCs for all 8 scenarios are shown in figure 4. It can be seen that process designs with raw shale gas feeds 1–4 demonstrate higher TDCs of the AGR section and lower TDCs in the NGLs recovery section. In fact, the corresponding dry gas from the dehydration section already satisfies the pipeline gas specification in the first four scenarios. Therefore, only the three-stage compressor system is utilized in the NGLs recovery section. In contrast, the TDCs of the NGLs recovery section for the process designs with raw shale gas feeds 5–8 are much higher. This is due to the fact that more raw shale gas in such scenarios must be processed to satisfy the pipeline gas demand, and the extra NGLs adds to the equipment capacity. The TDCs of the dehydration section do not demonstrate significant differences among the 8 scenarios. This is because the sweet gas are water-saturate no matter what raw shale gas feedstock compositions are considered. As a result, the total amount of water to be removed is largely dependent on the total flowrate of the sweet gas to be processed. As shown in Table 2, raw shale gas feeds 5–8 have higher flowrate and they contain less acid gas to be removed in the first section. Therefore, the dehydration burdens, or the TDCs, for these scenarios are slightly heavier.



Gas	Design 1	2	3	4	5	6	7	8	Rob.
1	✓	×	×	×	×	×	×	×	✓
2	✓	✓	×	✓	×	×	×	×	✓
3	✓	✓	✓	✓	×	×	×	×	✓
4	✓	×	×	✓	×	×	×	×	✓
5	×	×	×	×	✓	×	✓	×	✓
6	×	×	×	×	✓	✓	✓	×	✓
7	×	×	×	×	×	×	✓	×	✓
8	×	×	×	×	✓	✓	✓	✓	✓

Figure 4: Total direct cost distribution and product qualities of different designs with respect to various gas compositions. Check and cross represent qualified and unqualified product for pipeline gas specifications

We propose a robust design of shale gas processing and NGLs recovery based on the TDCs in Figure 4. A robust design employs equipment units with the largest capacity among all the scenarios. Given that a larger capacity corresponds to a larger TDC, we compare the TDC of each equipment unit and calculate the maximum TDC among all scenarios. The robust TDCs are $ 13.6 MM, $ 4.2 MM, and $ 51.0 MM for the three respective sections. It is noted that the robust TDCs are slightly larger than those of the largest TDCs among different scenarios because the largest TDCs of several units can come from a design with a smaller TDC of the section. As shown in Figure 4, the robust process design is able to handle all raw shale gas compositions, while the other deterministic design can handle no more than half of the compositions.

Table 3: Economic evaluation results

Scenario	1	2	3	4	5	6	7	8	Robust
Total direct cost, $MM	20.9	20.2	20.1	20.6	33.5	30.8	61.5	25.0	68.8
Indirect expense, $MM	6.7	6.5	6.4	6.6	10.7	9.9	19.7	8.0	22.0
Total plant capital cost, $MM	27.6	26.6	26.5	27.3	44.2	40.6	81.2	33.0	90.9
Annual operating cost, $MM	8.2	7.8	7.8	8.0	9.3	9.4	10.1	9.3	10.1
Raw material cost, $MM	109.8	109.8	109.8	109.8	164.1	167.6	192.1	158.9	192.1
Total annualized cost, $MM	118.8	118.4	118.4	118.6	174.6	178.1	204.4	169.1	204.7
Unit annualized cost, $/GJ	1.8	1.8	1.8	1.8	1.8	1.8	1.8	1.8	1.8

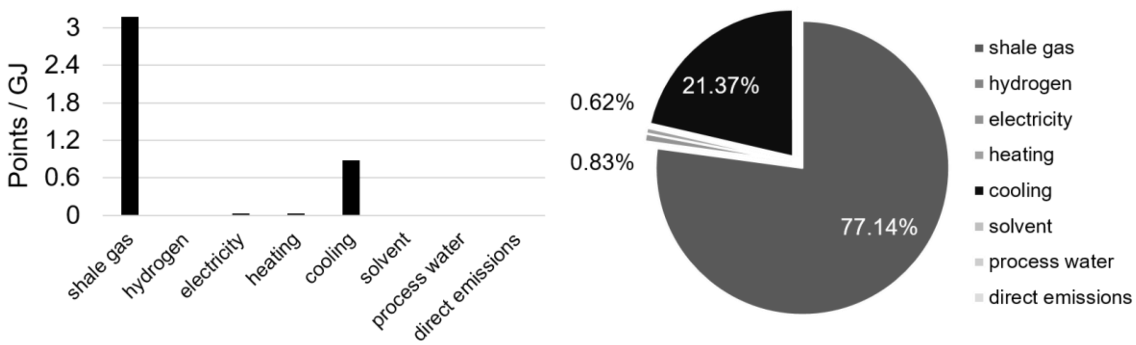


Figure 5: Eco-indicator 99 distribution of the robust process design

We perform an economic evaluation for all scenarios and the robust design as shown in Table 3. The indirect expenses are calculated as 32 % of the corresponding TDCs. The annual operating cost accounts for electricity, heating, cooling, solvent, and water consumption. In addition, the raw material cost accounts for the raw shale gas and hydrogen purchase expenses. The total annualized cost (TAC) sums up the annualized total plant capital cost, annual operating cost, and the raw material cost. The unit annualized cost is evaluated as the ratio of the TAC divided by the total annual energy input of the raw shale gas feed. The indirect expense and total plant capital cost of the robust design are calculated based on its TDC. Moreover, the annual operating cost and raw material cost of the robust process design are evaluated as the worst case among the 8 scenarios. It can be seen that even though the TAC of the robust design is more than 70 % of those of the scenarios 1–4, the unit annualized costs of all scenarios are nearly identical. The processing costs are 0.1 to 0.2 $/GJ.

We perform a cradle-to-gate life cycle analysis to evaluate the endpoint environmental impacts of the robust design according to the Eco-indicator 99 methodology. The functional unit is to process 1 GJ of the raw shale gas. The system boundary accounts for CO_2 and SO_2 direct emissions from the processing plant, and the indirect emissions associated with feedstock and utility production. Indirect emissions associated with feedstock transportation are ignored. It can be seen from Figure 5 that raw shale gas production contributes to 77.1 % the entire environmental impact. The second largest share comes from cooling utility generation.

5. Conclusions

We develop a robust design of shale gas processing and NGLs recovery processes that can remove acid gas, water, and NGLs from raw shale gas feedstocks. We perform detailed process simulation and techno-economic analysis for 8 raw shale gas compositions. The robust process design consists of the largest operation units in the 8 individual process designs and is capable of generating qualified pipeline products as long as the feedstock comes from the 8 raw shale gas sources. To identify the hotspots of environmental impacts for the robust design, we further conduct a life cycle analysis according to the Eco-indicator 99 methodology. The robust design has a unit annualized cost of 1.8 $/GJ. The largest contributors to the environmental impacts are raw shale gas production and cooling utility generation.

References

Bullin K.A., Krouskop P.E., 2009. Compositional Variety Complicates Processing Plans for US Shale Gas. Oil & Gas Journal, 107, 50-55.

Gao J., You F., 2015a. Optimal Design and Operations of Supply Chain Networks for Water Management in Shale Gas Production: MILFP Model and Algorithms for the Water-Energy Nexus. AIChE Journal, 61, 1184-1208.

Gao J., You F., 2015b. Deciphering and handling uncertainty in shale gas supply chain design and optimization: Novel modeling framework and computationally efficient solution algorithm. AIChE Journal, 61, 3739-3755.

Gao J., You F., 2015c. Shale Gas Supply Chain Design and Operations towards Better Economic and Life Cycle Environmental Performance: MINLP Model and Global Optimization Algorithm. ACS Sustainable Chemistry & Engineering, 3, 1282-1291.

Gao J., You F., 2017a. Game Theory Approach to Optimal Design of Shale Gas Supply Chains with Consideration of Economics and Life Cycle Greenhouse Gas Emissions. AIChE Journal, DOI: 10.1002/aic.15605

Gao J., You F., 2017b. Design and Optimization of Shale Gas Energy Systems: Overview, Research Challenges, and Future Directions. Computers & Chemical Engineering, DOI: 10.1016/j.compchemeng.2017.01.032

Getu M., Mahadzir S., Long N.V.D., Lee M., 2013. Techno-economic analysis of potential natural gas liquid (NGL) recovery processes under variations of feed compositions. Chemical Engineering Research & Design, 91, 1272-1283.

Gong J., You F., 2015. Sustainable Design and Synthesis of Energy Systems. Current Opinion in Chemical Engineering, 10, 77-86.

He C., You F., 2014. Shale Gas Processing Integrated with Ethylene Production: Novel Process Designs, Exergy Analysis, and Techno-Economic Analysis. Industrial & Engineering Chemistry Research, 53, 11442-11459.

He C., You F., 2015. Toward more cost-effective and greener chemicals production from shale gas by integrating with bioethanol dehydration: Novel process design and simulation-based optimization. AIChE Journal, 61, 1209-1232.

He C., You F., 2016. Deciphering the true life cycle environmental impacts and costs of the mega-scale shale gas-to-olefins projects in the United States. Energy & Environmental Science, 9, 820-840.

Kerr R. A., 2010. Natural Gas From Shale Bursts Onto the Scene. Science, 328, 1624-1626.

Luyben W.L., 2013. Effect of Natural Gas Composition on the Design of Natural Gas Liquid Demethanizers. Industrial & Engineering Chemistry Research, 52, 6513-6516.

Palma V., Ricca A., Martino M., Meloni E., 2016, Innovative Catalytic Systems for Methane Steam Reforming Intensification. Chemical Engineering Transactions, 52, 301-306.

Pring M., 2012. Condensate Tank Oil and Gas Activities. Austin, TX, USA: Eastern Research Group, Inc.

Speight, J.G., 2013. Chapter 4 - Shale Gas Properties and Processing. In: SPEIGHT, J. G. (ed.) Shale Gas Production Processes, Gulf Professional Publishing, Boston, USA.