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Sustainable Design and Operations of Shale Gas Supply Chains Using Integrated Hybrid Life Cycle Optimization Models

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In this paper, we address the sustainable design and operations of shale gas supply chains by proposing an integrated hybrid life cycle optimization (LCO) modelling framework. Unlike the traditional process-based LCO that suffers system truncation, the integrated hybrid LCO supplements the truncated system with a comprehensive economic input-output system. Meanwhile, the integrated hybrid LCO retains the precision in modelling major unit processes within the well-to-wire system boundary compared with the economic input-output-based LCO models. With the help of the integrated hybrid LCO framework, we can automatically identify the optimal sustainable alternatives in the design and operations of shale gas supply chains. To demonstrate the applicability, we present a case study of a well-to-wire shale gas supply chain located in the UK. According to the optimization results, the lowest levelized cost of electricity generated from shale gas is £51.8 /MWh, and the optimal life cycle GHG emissions are 473.5 kg CO_2-eq/MWh.

1. Introduction

In recent decade, the combined application of horizontal drilling and hydraulic fracturing has led to a shale revolution. According to the most recent report by the U.S. Energy Information Administration (EIA), there are 35,782 Trillion cubic feet (Tcf) risked shale gas in-place for 41 countries, of which 7,299 Tcf shale gas is considered technically recoverable (EIA, 2018). Meanwhile, 16.76 trillion cubic feet of dry natural gas was produced from shale resources in the U.S., comprising about 60 % of the total U.S. dry natural gas production (EIA, 2018). Motivated by this, numerous mathematical programming models are proposed for the optimal design and planning of shale gas energy systems (Asala et al., 2017). Accompanying the rapid expansion of shale gas industry, there are increasing concerns on the environmental impacts associated with shale gas extractions (Weber and Clavin, 2012). Life cycle assessment (LCA) is a systematic way to investigate the environmental impacts of shale gas (Fernandez et al., 2017). Based on the LCA approach, a series of life cycle optimization (LCO) models are proposed, which enables automatic identification of the optimal design and operational alternatives in shale gas supply chains (Gao and You, 2015). However, all the existing shale gas LCO models in the literature rely on the process-based LCO framework (Gong et al., 2015). Although process-based LCA provides more accurate and detailed process information, it underestimates the true environmental impacts due to system truncation. An alternative is the economic input-output (EIO)-based LCA, which utilizes national EIO data coupled with sectoral environmental impact factors to evaluate the environmental impacts of a product system. Nevertheless, by aggregating industries and commodities, the process-scale details are missing in the EIO-based LCA (Gao and You, 2017). Thus, it is necessary to propose new LCO frameworks to overcome the drawbacks of tradition LCO models, and thus achieve more sustainable decisions in the design and operations of shale gas supply chains.

To address this research challenge, an integrated hybrid LCA method is presented in this paper. The integrated hybrid LCO framework is established by combining the strengths of both process-based LCA and EIO-based LCA (Yue et al., 2016). The process details associated with major processes within the system boundary are guaranteed by explicit process analysis, and the truncated system is supplemented by the EIO systems. Additionally, upstream and downstream cutoff matrices are introduced to explicitly capture the interactions

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between the process systems and the macroeconomic systems. In this study, the life cycle greenhouse gas (GHG) emissions are chosen as the environmental impact indicator (Yang and You, 2017). This integrated hybrid LCO framework enables automatic identification of the optimal design and operational alternatives in a "well-to-wire" shale gas supply chain. The resulting LCO problem is formulated as a mixed-integer nonlinear programming (MINLP) problem that is computationally intractable for general-purpose global optimizers. Thus, a tailored global optimization algorithm integrating the parametric algorithm and a branch-and-refine algorithm is applied for efficient solution of the MINLP problem. A case study on shale gas supply chain design in UK is presented to illustrate the applicability of the proposed hybrid LCO model and global optimization algorithm.

2. Problem statement

In this study, the integrated hybrid LCO framework is adopted (Peters and Hertwich, 2006). The mathematical formulation for calculating the environmental impacts using the integrated hybrid LCO is given as follows (Suh and Huppes, 2005).

$$\text{Total environmental impact} = \begin{bmatrix} E_p & E_{io} \end{bmatrix} \begin{bmatrix} A_p & -C_d \\ -C_u & I - A_{io} \end{bmatrix}^{-1} \begin{bmatrix} y \\ 0 \end{bmatrix} \tag{1}$$

where A_p is the process matrix that represents the exchanges of goods among processes within the process system boundary. A_{io} is the direct requirements matrix describing the interdependencies among industrial sectors within the EIO systems. C_u and C_d are the upstream cutoff matrix and downstream cutoff matrix, respectively. E_p and E_{io} are the environmental extension vectors corresponding to the process systems and the EIO systems, respectively. $\begin{bmatrix} y & 0 \end{bmatrix}^T$ is the functional unit column indicating the amount of final product that is produced per functional unit. With this integrated hybrid LCO methodology, the comprehensive life cycle environmental impacts of shale gas associated with both the foreground process systems and the background EIO systems can be quantified. For the process systems, a "well-to-wire" system boundary is considered. The life cycle stages considered in the process systems include shale pad construction, shale well drilling, hydraulic fracturing and completion, water acquisition, wastewater treatment, shale gas production, processing, transportation, and end use of shale gas for electricity generation at CCGT power plants. Consistent with the "well-to-wire" process system boundary, a functional unit of generating one Megawatt-hour (MWh) electricity from shale gas is adopted.

A planning horizon consisting of a set of time periods is given, so the resulting hybrid LCO problem is a multi-period optimization problem. There are a set of shale sites. Some of them already exist with drilled shale wells, and the remaining shale sites are potential ones to be developed. At each shale site, the maximum number of wells that can be drilled is known. In addition, the production profile, estimated ultimate recovery, and shale gas composition of each shale well are given. Both drilling and hydraulic fracturing activities require freshwater supply and generate wastewater simultaneously. Thus, it is necessary to make corresponding decisions regarding water management. Two wastewater treatment options are considered, including centralized wastewater treatment (CWT) facilities and onsite wastewater treatment units. For the latter, three typical wastewater treatment technologies are considered, namely multi-stage flash (MSF), multi-effect distillation (MED), and reverse osmosis (RO). The technological information regarding each water treatment option, such as the treatment capacities, energy efficiency, and recovery factors, is given. Raw shale gas can be produced at shale sites once the corresponding shale wells are completed. The raw shale gas is first sent to processing plants, where impurities, such as water, acid gas, and nitrogen are removed, and the pipeline-quality natural gas and heavier hydrocarbons (He and You, 2014), known as natural gas liquids (NGLs), are separated (Gong and You, 2018). The transportation of raw shale gas from shale sites to processing plants requires the construction of gathering pipelines. There are a set of pipeline specs with given capital costs and capacities to select from. The processing plants include existing ones with fixed processing capacities and potential ones to be designed and constructed. After the processing plants, natural gas is sent to a set of CCGT power plants for electricity generation. The distribution of natural gas from processing plants to power plants also requires the readiness of transmission pipelines. The transportation distance between each pair of locations is given. For the power plants, the electricity demand in each time period and the electricity generation efficiency are given.

To simultaneously optimize the economic and environmental performances associated with production of one functional unit, the following fractional objectives are considered:

- Minimizing the levelized cost of electricity (LCOE) generated from shale gas.
- Minimizing the total life cycle GHG emissions per MWh of electricity generation.

These economic and environmental objectives are optimized considering the following decisions:

- Development planning of shale sites;

- Drilling schedule, production profile, and water management strategies at each shale site;
- Locations and capacities of shale gas processing plants;
- Installation and spec selection of transportation pipelines, as well as planning of corresponding transportation activities;
- Electricity generation profiles at CCGT power plants.

3. Model formulation and solution algorithm

A multi-objective, multi-period MINLP model is developed to address the sustainable design and operations of shale gas supply chains.

$$\text{Economic Objective: } \min\ LCOE = \frac{TC^{cap} + \sum_{t\in T} \frac{TC^{oper}}{\left(1+dr\right)^{t}}}{TGE} \tag{2}$$

$$\text{Environmental Objectives: } \min\ UE = \frac{TE^{pro} + TE^{IO}}{TGE} \tag{3}$$

s.t. Economic Constraints
Environmental Constraints
Mass Balance Constraints
Capacity Constraints
Bounding Constraints
Logic Constraints

As stated in the problem statement section, *LCOE* indicates the levelized cost of electricity, which is formulated as the summation of total capital cost (TC^{cap}) and the total discounted value of operating cost (TC^{oper}) divided by the total electricity generation (*TGE*). *UE* denotes the life cycle GHG emissions associated with one MWh of electricity generation, formulated as the summation of process emissions (TE^{pro}) and IO emissions (TE^{IO}) divided by the total electricity generation. These objectives are optimized subject to the following constraints:

- Economic constraints calculating the capital and operating costs associated with all the design and operational decisions across the shale gas supply chain.
- Environmental constraints calculating the GHG emissions resulting from both the process systems and the EIO systems following the integrated hybrid LCA approach.
- Mass balance constraints describing the detailed input-output mass balance relationships among shale sites, processing plants, and CCGT power plants throughout the shale gas supply chain.
- Capacity constraints describing the capacity restrictions of different unit processes, including water management options, gas processing, transportation, and demand of electricity generation at power plants.
- Composition constraints describing the reuse specification of onsite treatment technologies.
- Bounding constraints linking the supply chain design decisions with corresponding operational decisions, including those associated with processing plants and transportation pipelines.
- Logic constraints describing the logic relationships among strategic decisions, including those regarding well drilling, wastewater treatment, construction of processing plant, and pipeline instalment.

Both the economic and environmental objective functions are formulated as fractional terms to reflect the functional-unit-based life cycle performances. There are nonlinear terms introduced in the economic objective function to calculate the capital cost of processing plants. Thus, the resulting problem is a nonconvex MINLP problem. Due to the combinatorial nature and pseudo-convexity of fractional objectives as well as separable concave terms for capital cost estimation, mixed-integer nonlinear fractional programming problems have been known as computationally challenging problems for general-purpose MINLP solvers. Therefore, a tailored global optimization algorithm is applied that integrates the parametric algorithm with a branch-and-refine algorithm to tackle this computational challenge (You and Grossmann, 2011).

4. Application to a shale gas supply chain

A case study of a “well-to-wire” shale gas supply chain in the UK is presented to illustrate the proposed integrated hybrid LCO model. In this study, the data are obtained from the most recent LCA study for UK shale gas, as well as the Ecoinvent database v3.3 (Ecoinvent database v3.3, 2017) to construct the process-based LCI (Stamford and Azapagic, 2014). A total of 40 basic processes are considered in the process systems. For the EIO systems, A two-region IO model as reported in the literature is adopted (Wiedmann et al., 2011). The

100-year global warming potential (GWP) factors reported in the fifth assessment report by IPCC is applied to convert these GHG emissions to carbon dioxide equivalents. In this shale gas supply chain, there were seven existing shale sites with active shale wells, and eight potential shale sites to be developed. Each shale site allowed multiple shale wells to be drilled. A total of four processing plants were considered, among which two processing plants already existed with given capacities, and two processing plants were potential ones to be designed. The pipeline-quality sales gas obtained at processing plants was distributed to six CCGT power plants for electricity generation. A 10-year planning horizon and 40 time periods with equal time intervals were considered. The resulting MINLP problem has 414 integer variables, 11,797 continuous variables, and 15,370 constraints. All the models and solution procedures are coded in GAMS 24.7.3 on a PC with an Intel® Core™ i7-6700 CPU and 32GB RAM, running the Windows 10 Enterprise, 64-bit operating system. Furthermore, the MILP subproblems are solved using CPLEX 12.7.0.

By solving the resulting MINLP problem, a Pareto-optimal curve consisting of 10 Pareto-optimal solutions is presented in Figure 1. The *x*-axis represents the life cycle GHG emissions for generating one MWh of electricity from shale gas. The *y*-axis represents the LCOE across the shale gas supply chain. Two extreme Pareto-optimal solutions are selected, namely point A with the lowest life cycle GHG emissions and point B with the lowest LCOE, for further investigation and comparison. Additionally, the cost breakdowns as well as GHG emission breakdowns for the two extreme Pareto-optimal solutions are provided by pie charts and donut charts, respectively. The sizes of these charts are proportional to the absolute values of GHG emissions and total cost.

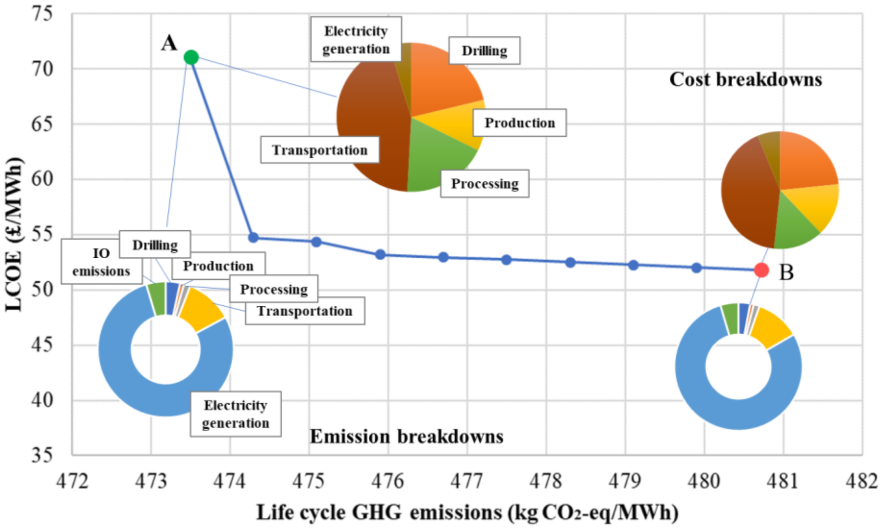

Figure 1: Pareto-optimal curve illustrating the trade-offs between LCOE and life cycle GHG emissions

Pareto-optimal solution point A has the lowest life cycle GHG emissions of 473.5 kg CO_2-eq/MWh and the highest LCOE of £71.1/MWh. By contrast, point B has lowest LCOE of £51.8/MWh, but the corresponding life cycle GHG emissions are 480.7 kg CO_2-eq/MWh. The upstream activities across the shale gas supply chain, including shale well drilling, gas production, processing, and transportation activities contribute the most to the total cost. However, downstream electricity generation plays a dominant role in terms of life cycle GHG emissions. Apart from electricity generation, upstream activities, including well drilling and gas transportation, as well as the EIO systems, also contribute significant amounts of GHG emissions.

To further investigate the key impact factors associated with the life cycle GHG emissions, the following GHG emission breakdowns based on the 40 basic processes of the process system are presented in Figure 2. Fugitive emissions of CO_2 and CH_4 are identified as the major impact factors, which in total contribute about 93 % of the total process GHG emissions. Other processes, including electricity generation, tap water production, and gas transportation, also contribute a significant amount of GHG emissions throughout the process systems.

Figure 3 summarizes and presents the optimal drilling schedules of solution point A (minimizing the life cycle GHG emissions) and point B (minimizing the LCOE). More shale wells are drilled in the optimal solution of point A than that of point B. Specifically, a total of 105 shale wells are drilled in the optimal solution of point A, and 82 shale wells are drilled in the optimal solution of point B. Here the development of shale site 15 in the optimal solution of point A is highlighted. With these extra wells at shale site 15 drilled, the corresponding shale gas production of point A is expected to be larger than that of point B.

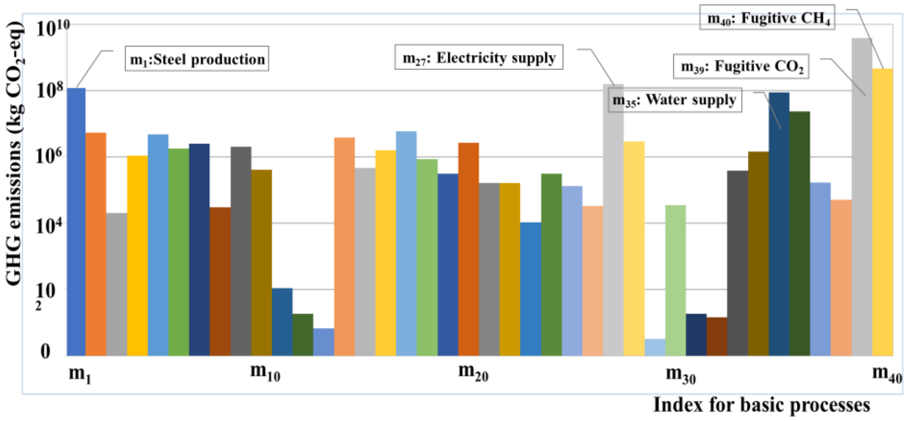

Figure 2: Life cycle GHG emission breakdowns based on the 40 basic processes (indexed by m) of the process systems

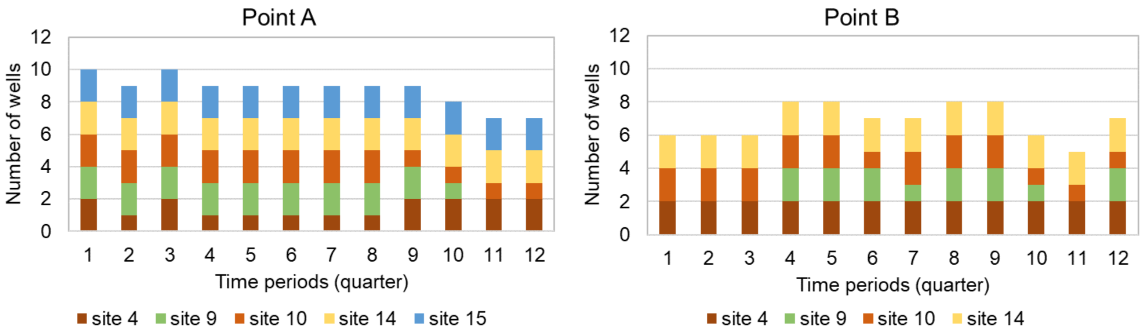

Figure 3: Optimal drilling schedules of solution points A and B

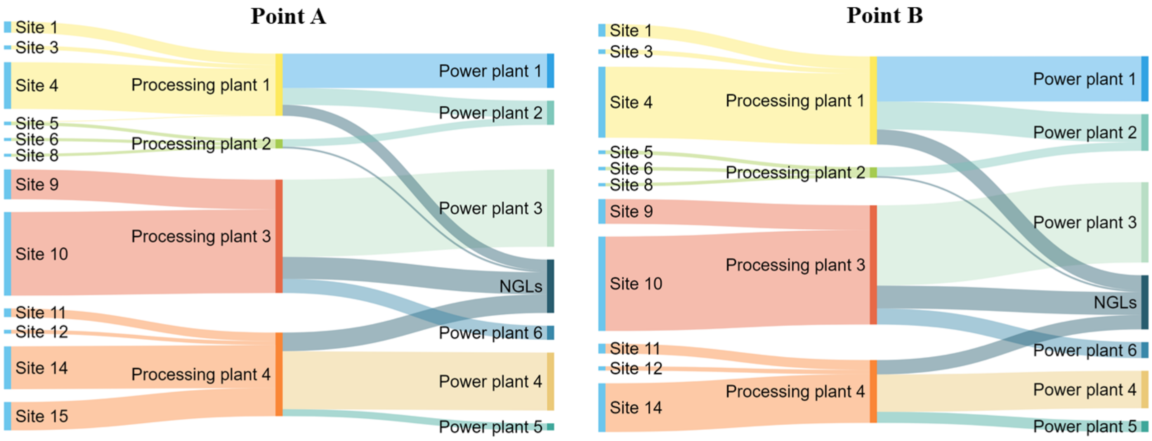

Figure 4: Summary of shale gas supply chain design and flow information

The optimal shale gas supply chain designs with corresponding mass flows are summarized in Figure 4, which is given in the form of a Sankey diagram. Although the structures of both shale gas supply chains in points A and B are similar, the overall shale gas production at each shale site, the capacities of processing plants, and the distribution planning of sales gas are different in these two solution points. Specifically, shale site 15 is developed in point A, which further leads to a larger shale gas production near processing plant 4. Thus, the working capacity of shale gas processing plant 4 is 3.50 billion standard cubic feet per year in point A, greater than the 3.18 Bscf per year processing capacity in point B. Similarly, the capacity of processing plant 3 in point A is 6.27 Bscf per year, greater than the 6.05 Bscf per year of processing plant 3 in point B. The sales gas from processing plant 1 is mainly consumed by power plants 1 and 2. All the sales gas from processing plant 2 is sent to power plants.

5. Conclusions

In this study, an integrated hybrid LCO model is developed to automatically identify the optimal design and operational alternatives in a “well-to-wire” shale gas supply chain considering both economic and environmental criteria. In contrast to the traditional process-based LCA approach, this integrated hybrid LCA approach provided a way to estimate the total environmental impacts resulted from both the process systems and the EIO systems. Based on the optimization results of a UK case study, it is concluded that environmental impacts induced by the EIO systems could constitute a significant part of the overall life cycle environmental impacts of shale gas, especially with pessimistic LCI estimations or certain environmental categories.

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