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Analysing Shale Gas Energy Systems using Dynamic Material Flow Analysis

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This work develops a novel dynamic material flow analysis (MFA)-based optimisation modelling framework for sustainable design of shale gas energy systems. This dynamic MFA-based framework provides high-fidelity modelling of complex material flow networks with recycling options, and it enables detailed accounting of time-dependent life cycle material flow profiles. Moreover, by incorporating a dimension of resource sustainability, the proposed modelling framework facilitates the sustainable supply chain design and operations with a more comprehensive perspective. The resulting optimisation problem is formulated as a mixed-integer linear fractional program and solved by an efficient parametric algorithm. To illustrate the applicability of the proposed modelling framework and solution algorithm, a case study of Marcellus shale gas supply chain is presented. The optimisation results help to identify clear trade-offs among economic, environmental, and resource performances in the shale gas energy system, and the MFA-based framework offers an effective way to find an optimal solution with well-balanced sustainability performance

1. Introduction

Sustainability has received increasing research attention in the design of energy systems (Gong et al., 2015). Tools and indicators are developed for assessing and benchmarking sustainability performance of different systems (Finnveden and Moberg, 2005). Among these tools, life cycle analysis (LCA) is one of the most widely applied methods to systematically quantify the environmental impacts of a product from a life cycle perspective (Guinée et al., 2011). As an analysis tool, LCA is designed to evaluate the environmental impacts based on a certain or a collection of design alternatives. However, the sustainable design generally involves a substantially large number of design alternatives (Garcia and You, 2015). Life cycle optimisation (LCO) methodology was developed, which integrates LCA with multiobjective optimisation technique into a holistic optimisation model (Yue et al., 2013). Despite the successful application of LCO in various energy systems, the framework itself has its shortcomings inherited from LCA approaches (Gao and You, 2017). Specifically, LCA might not holistically recognise resource depletion as a potential sustainability concern (Huang et al., 2012). This shortcoming of LCO can be mitigated by integrating with dynamic material flow (MFA) analysis, although there is no existing framework that integrates LCO with MFA. Therefore, it is imperative to develop an optimisation framework for energy systems design based on LCO and MFA.
As a clean transition fuel, shale gas can play an important role in the transition to a sustainable future (Middleton et al., 2017). Shale gas is an important and growing industry in the U.S. (Littlefield et al., 2017). Yet However, the design of shale gas energy systems has not yet been benefited from the rigorous MFA and LCA (Thomas, 2017). There is a growing number of publications on shale gas supply chain design focusing on various aspects of sustainability, such as water management (Gao et al., 2015), water-energy nexus (Oke et al, 2019), market uncertainty (Chebeir, 2017), estimated ultimate recovery uncertainty (Gao et al., 2017), modular manufacturing of shale gas (Gao et al., 2017), upgrading of shale gas (Yang et al., 2018), among others. However, MFA has not be considered in the existing LCO studies of shale gas supply chains (Gao et al., 2015). A resulting research challenge is integrating LCO and MFA for shale gas supply chains to support its sustainable design towards lower cost, less emissions and less water consumption.
To tackle the aforementioned research challenges, this study presents a dynamic MFA-based LCO framework in pursuit of sustainable design of shale gas energy systems. With the integration of dynamic MFA and LCA, it

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is expected to overcome their shortcomings and contribute to better sustainable designs of energy systems. Specifically, in this dynamic MFA-based LCO framework, various input, output, and recycling material/energy flows of processes are captured with precision throughout their lifetime. Meanwhile, by introducing an extra dimension of resource sustainability in addition to economic and environmental performances, the aim is to provide a better evaluation of sustainable system designs. Based on the functional unit, three fractional objective functions, corresponding to the economic, environmental, and resource sustainability performances, respectively, are defined. To illustrate the applicability of the proposed modelling framework and solution algorithm, an application to a Marcellus shale gas supply chain is presented. Through a detailed result analysis, a Pareto optimal solution balancing economic, environmental, and resource performances can be recognised, and the corresponding material flow profiles are obtained.

2. Problem statement

This work considers the sustainable design and operations of a Marcellus shale gas supply chain with the proposed dynamic MFA-based LCO framework. The life cycle system boundary is restricted to “well-to-gate” starting from the shale pad development at a wellhead to the gate of the natural gas market (Gao and You, 2015). The functional unit is defined as generating one MJ net energy from shale gas. The dynamic MFA methodology keeps track of the material flows associated with all the life cycle stages in this shale gas supply chain throughout the planning horizon. Specifically, a total of 36 key material flows are considered. To address the sustainability concern in the design and operations of shale gas supply chains, three distinct objective functions are considered in this problem. The aim is to simultaneously optimise the economic, environmental, and resource performances of this shale gas supply chain for generating one functional unit of product. Specifically, the economic performance is evaluated by the levelized cost of unit net energy output. The environmental performance is quantified with the GHG emissions (in terms of CO_2 equivalent based on 100-year time horizon). The water consumption is adopted as the resource indicator. Notably, these three objective functions are all formulated into fractional form with both numerators and denominators dependent on the design and operational decisions. Compared with their linear counterparts, the functional-unit-based fractional objectives can automatically identify the optimal amount of functional units to generate for the best sustainability performance. The net energy generation can be calculated by subtracting the energy consumption (in terms of fossil fuel, electricity, heat, etc.) throughout the shale gas supply chain from the direct energy output of produced shale gas. Therefore, this work adopts the following fractional objectives in this study:

- Minimising the levelized cost of one MJ net energy output, formulated as the total net present cost (i.e., the summation of all discounted future costs) divided by the total amount of net energy generation from shale gas;
- Minimising the GHG emissions associated with one MJ net energy output, formulated as the total life cycle GHG emissions throughout the shale gas supply chain divided by the total amount of net energy generation from shale gas;
- Minimising the water consumption associated with one MJ net energy output, formulated as the total water consumption throughout the shale gas supply chain divided by the total amount of net energy generation from shale gas.

These three objectives are optimised simultaneously considering the following design and operational decisions:

- Development of potential shale sites;
- Drilling schedule of shale wells at each shale site;
- Design of gathering pipeline networks;
- Allocation and capacity selection of processing plants;
- Shale gas production profile of each shale well;
- Water management strategy at each shale site;
- Transportation planning of water and shale gas

3. Model formulation and solution algorithm

Following the proposed MFA-based LCO framework, the resulting problem is formulated as a multiobjective MILFP problem. The general model formulation is given below.

Economic Objective: $\min \dfrac{TC}{TENG}$ (1)

Environmental Objective: $\min \dfrac{TE}{TENG}$ (2)

Resource Objectives: min $\frac{TW}{TENG}$ (3)

s.t. Mass Balance Constraints

Capacity Constraints

Logic Constraints

Economic Constraints

Environmental Constraints

Resource Constraints

Here *TC* stands for the total net present cost. *TE* is the total life cycle GHG emissions. *TW* represents the total water consumption. *TENG* indicates the total net energy generation from shale gas, which equals the direct energy output of produced shale gas minus the energy consumption throughout the shale gas supply chain. The economic, environmental, and resource objectives are all formulated in fractional form as a ratio of two linear functions, representing the functional-unit-based economic performance, environmental impact, and resource efficiency, respectively. All the constraints are linear ones with both integer and continuous variables. Therefore, the resulting problem is a multiobjective MILFP problem. Notably, large-scale MILFP problems, due to its combinatorial nature and pseudo-convexity, can be computationally intractable for general-purpose MINLP methods. To overcome this challenge, the parametric algorithm based on Newton's method is used in this study for the efficient solution of this MILFP problem (Zhong and You, 2014).

4. Application to a well-to-wire shale gas supply chain

To illustrate the applicability of the proposed dynamic MFA-based LCO framework, a case study of a "well-to-gate" shale gas supply chain based on Marcellus shale is considered (Gao and You, 2018). A total of 12 shale sites are considered, where six shale sites are existing ones with active shale wells and six shale sites are potential ones to be developed. Each shale site allows for drilling of up to five shale wells. Three potential locations are considered for the construction of midstream shale gas processing plants. A 10-year planning horizon is considered following the existing studies, which is further divided into 10 equal time periods. A 10 % discount rate is adopted for each year. The material flow profiles of 36 key materials are tracked throughout the given planning horizon. The resulting problem has 627 integer variables, 7,553 continuous variables, and 7,718 constraints. All the models and solution procedures are coded in GAMS 24.8.5. The reformulated MILP subproblems are solved using CPLEX 12.7.1.0. The optimality tolerance is set to 0.1 %. For all the Pareto-optimal solution points, the parametric algorithm converges in 3 to 5 iterations. The total computational time varies from a few CPU seconds to a few hundred seconds depending on the number of iterations.

By choosing the economic objective function as the primary objective function and transform the remaining environmental and resource objective functions into ε-constraints, an approximated 3D-Pareto optimal surface can be obtained in Figure 1 after solving a series of optimisation problems. On the Pareto optimal surface, four representative Pareto-optimal solution points are selected for further demonstration. Point A is the extreme solution with the best economic performance, namely the lowest levelized cost per unit net energy output of \$5.22/GJ. Point B is the extreme solution with the least environmental impacts, namely the lowest GHG emissions per unit net energy output of 5.70 kg CO_2-eq/GJ. Point C is the extreme solution with the best resource performance, namely the lowest water consumption per unit net energy output, which is 0.107 t/GJ. In addition to these three extreme solution points, a "good choice" solution point is selected that maintains a good balance among the three optimisation criteria. Specifically, the levelized cost of the unit net energy output of point D is 6.05 \$/GJ, 37.5 % lower than that of point B (9.68 \$/GJ) and 41.0 % lower than that of point C (10.26 \$/GJ). Meanwhile, the GHG emissions and water consumption per unit net energy output of point D are only 5.91 kg CO_2-eq/GJ and 0.110 t/GJ.

Figure 2 presents the detailed breakdowns of the economic, environmental, and resource performances regarding five key life cycle stages in the shale gas supply chain, namely water management, shale well drilling, shale gas production, shale gas processing, and transportation. The results of Pareto optimal solutions with points A to D are presented for better comparison and analysis. As can be seen, solution point A leads to the lowest levelized cost for generating unit amount of net energy, followed by point D. In terms of GHG emissions per unit net energy output, point B outperform other solution points by a small margin. Point C results in the least water consumption for unit net energy output, although all four points have similar water consumption breakdowns.

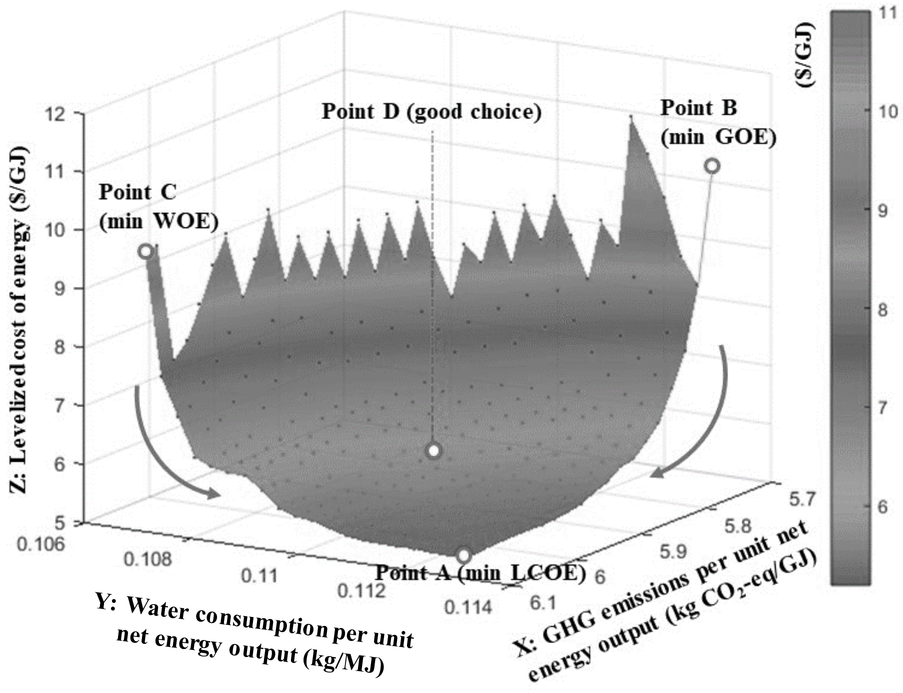

Figure 1: Pareto optimal surface for the trade-offs between economics, environmental impacts, and water use

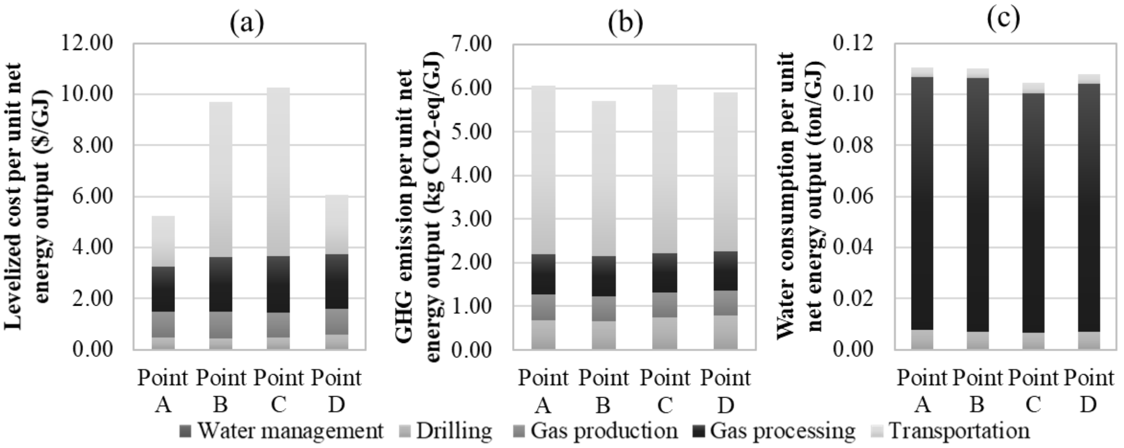

Figure 2: Breakdowns of (a) levelized cost, (b) GHG emissions, and (c) water use per unit net energy output

Next, the detailed design decisions of “good choice” solution point D is studied for more insights into the sustainable design of shale gas supply chains. A thorough MFA of point D is presented in Figure 3. The width of each flow shape is proportional to the quantity of the corresponding material flow. A total of 14 shale wells are drilled. Up to 99.7 % of the wastewater will be treated onsite with reverse osmosis technology and blended with freshwater for recycling. In the midstream, two shale gas processing plants at location 2 and location 3 are constructed. Across the shale gas supply chain, a significant amount of methane will be leaked, and both direct and indirect CO_2 emissions will be generated, resulting in the key sources of GHG emissions. This MFA identifies transportation activities as the main source of methane leakage.

Figure 4 summarises the profiles of nine key material flows, including steel, water, diesel, proppant, chemical additives, electricity, steam, TEG, and MEA, associated with Pareto optimal solution point D. As can be seen, among the nine materials, material flows of steel, diesel, proppant, and chemical additives share similar profiles, where nearly half of the total material flows occur in the first year, and a small peak is observed near year 7.

These profiles are consistent with the optimal drilling schedule of point D, indicating that these four materials flows are mainly consumed in the shale site development and well drilling phases. The other material flows, namely water, electricity, steam, TEG, and MEA, have relatively stable profiles, which match the constant shale gas output associated with point D. This observation indicates that these five materials are mainly consumed in shale gas production, processing, and transportation activities.

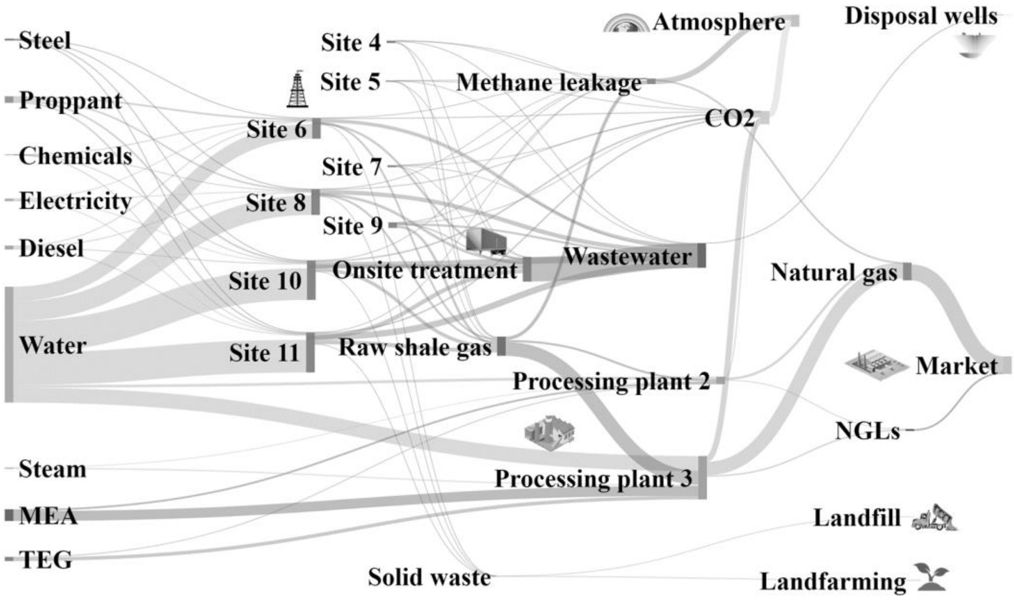

Figure 3: Material flows of Pareto optimal solution point D

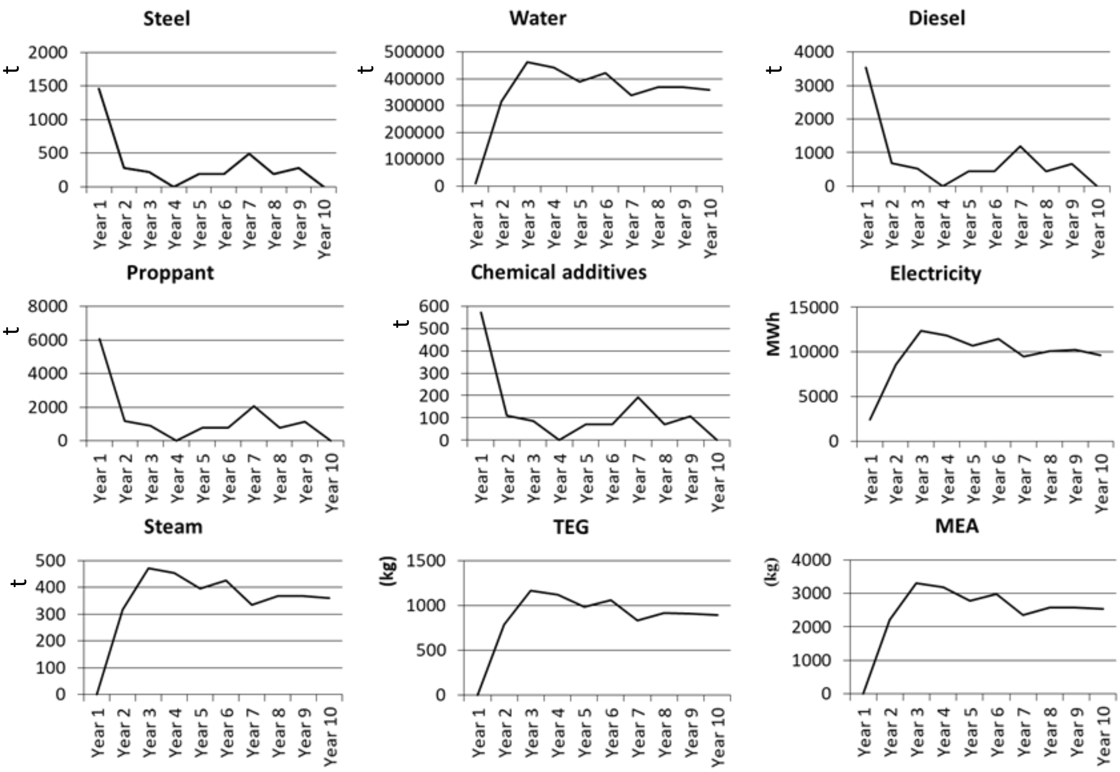

Figure 4: Key material flow profiles associated with Pareto optimal solution point D

5. Conclusions

This work developed a dynamic MFA-based framework to investigate the sustainable design of energy systems. Both the environmental impacts and resource efficiency were incorporated in a holistic optimisation model, which provides an evaluation of a system's sustainability performance. The resulting problem was formulated as a multiobjective MILFP problem that simultaneously optimised the economic, environmental, and resource performances associated with one functional unit of major product. From the optimisation results of the case study on Marcellus shale gas supply chain, there are clear trade-offs among economic, environmental, and resource performances in the shale gas energy system. The proposed MFA-based LCO framework offers an effective way to find an optimal solution with well-balanced sustainability performance.

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