Anton A. Kiss, Edwin Zondervan, Richard Lakerveld, Leyla Özkan (Eds.)
Proceedings of the 29th European Symposium on Computer Aided Process Engineering
June 16th to 19th, 2019, Eindhoven, The Netherlands.
http://dx.doi.org/10.1016/B978-0-128-18634-3.50128-4

A Framework for Multi-level Life Cycle Analysis of the Energy System

Emre Gençer,[a,*] Francis M. O'Sullivan [a]

[a]*MIT Energy Initiative, Massachusetts Institute of Technology, 77 Massachussetts Avenue, Cambridge, MA, 02139, USA*

emregencer@mit.edu

Abstract

The energy sector is undergoing a major transformation that is characterized by greater convergence of power, transportation, and industrial sectors and inter-sectoral integration. The existing techniques and tools are unable to accurately estimate the environmental impact of this paradigm shift. To develop a realistic understanding of these dynamics, we have developed a modeling framework that is designed to explore the emissions impacts of all relevant technological, operational, temporal, and geospatial characteristics of the evolving energy system. The tool is built as a MATLAB app that encapsulates MATLAB models, databases, and integrated process simulations. A modular framework constitutes the underlying analytical engine that covers all the life stages of major energy conversion pathways. The current version of the tool contains more than 900 individual pathways, which are responsible for ~80% of US greenhouse gas (GHG) emissions. Here wepresent an overview of the tool, the modeling approach and example results of case studies investigating electric power system.

Keywords: Life cycle analysis, multi-level analysis, energy systems modeling, computational tool, process simulation

1. Introduction

The global energy sector faces the grand challenge of meeting the increasing demand while profoundly reducing greenhouse gas emissions. Today's energy sector is responsible for approximately 80% of the world's total GHG emissions, and the electricity sector is the largest single emitting sector with 33% share. Industrial processes constitute 22% of emissions, while the transportation sector is responsible for 16% (Annual Energy Outlook 2018, 2018). Moving forward, the evolution of energy systems is characterized by greater convergence of power, transportation, and industrial sectors and inter-sectoral integration. Existing techniques and tools are unable to accurately estimate the environmental consequences of this paradigm shift. Understanding the implications of these dynamics requires novel tools that provide deep systems-level insights (Majumdar and Deutch, 2018). To address this pressing need, we have developed a modeling framework that is specifically designed to explore the emissions impacts of all relevant technological, operational, temporal, and geospatial characteristics of the evolving energy system.

The tool is built as a MATLAB app that encapsulates MATLAB models, databases, and integrated process simulations. A modular framework constitutes the underlying analytical engine that covers all the life stages of major energy conversion pathways. The

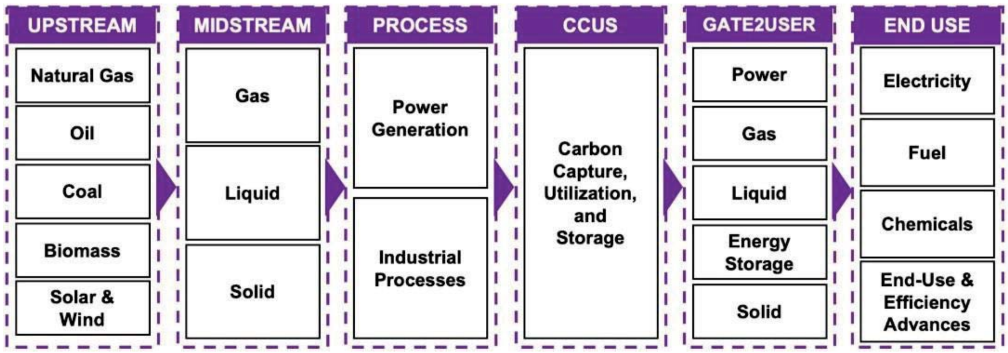


Figure 1 Summary of the contents of the tool. All major conventional and renewable energy pathways with their associated end-uses covering more than 85% of GHG emission sources in the US are represented.

first version of the tool contains more than 900 individual pathways (Figure 1), which are responsible for ~80% of US greenhouse gas (GHG) emissions. For the GHG emission hot spots, such as power plants and some chemical conversion pathways, detailed process simulation capabilities have been incorporated for in-depth analysis. In addition to performing pathway-level life cycle analysis (LCA), a central aspect of this analytical framework is the ability to assess key systems interactions and couplings. The system-level analysis is enabled by the embedded power systems and vehicle fleet models that captures market dynamics and explore dynamics of technology adoption and usage.

This paper focuses on the overview of the tool, the modeling approach as well as the results of case studies investigating electric power system. We demonstrate how the changes in the operational variability of natural-gas fired power plants impacts the system-wide emissions. Specifically, the operation of NG power plants in the evolving power system that significantly reduces plant performance and increases the emissions footprint of NG power generation. Example results of analysis of power plant dispatch profiles and detailed life cycle analysis of the US power grid using high resolution plant level simulation models and incorporation of publicly available US-wide generation and emissions data are presented (U.S. EPA, 2018a, 2018b).

2. Methodology

A crucial aspect of this analytical framework is the ability to assess key systems interactions and couplings. This allows transition options to be comprehensively assessed on the same basis. To allow performing such comprehensive analyses, we have built a flexible and modular programming architecture specifically designed to evolve as the complex energy system restructures.

The modular approach composed of four main compartments at the very high-level: User input, Control panel, Life stage modules, and Model output. To initiate the computation the necessary input parameters such as selection of complete value chain, specifications of power grid mix, geographical location, and temporal resolution should be provided by user. Control panel module constitutes the core of the tool that takes user inputs and communicates with relevant life stage modules to send and receive information as shown in Figure 2(a). The results from each life stage module are adjusted and combined in accord with the user selections given by Eq. (1). The energy consumption by fuel type is used as the basis for calculations. The efficiency of each stage is accounted for in the overall calculation denoted by ℓ. EF_i represents the emission factor from each stage given in the stage specific unit and χ is the conversion factor to adjust to the final unit. The results calculated as the sum of contribution from each stage is returned as output in desired unit and format.

$$EF = \sum_{i=1}^{6} (EF_i \times \chi_i) \prod_{j=1}^{i} \ell_j \tag{1}$$

Each life stage module consists of sub-modules. Depending on options selected, different sets of submodules are activated in parallel with the real-world operation. For example, the bituminous coal upstream operation includes all steps of extraction described by the processes involved coupled with fuels and electricity consumed. The midstream and gate2user stages are characterized by the phase of the flow. Process step is represented with high resolution to include all feedstocks and energy flows. The detailed information and data are collected from published LCA literature, reports, publicly available tools and life cyle inventory databases such as technology baselines reports (DOE NETL, 2015), GREET model (Wang, 2011), ecoinvent database.

2.1. Modeling Approach

The described programming architecture and linked modules are implemented in MATLAB. We have augmented MATLAB's capabilities by integrating with Aspen Plus process simulation software (Gençer and Agrawal, 2017a). This approach allows complementing life cycle analysis with process simulation capabilities to capture the performance and emission changes arising from technological and operational variations. It is computationally very expensive and unnecessary to simulate every process for all potential conditions. However, the developed architecture provides a platform to implement simulations of process units with high emission rates, critical for the system design, or sensitive to externalities.

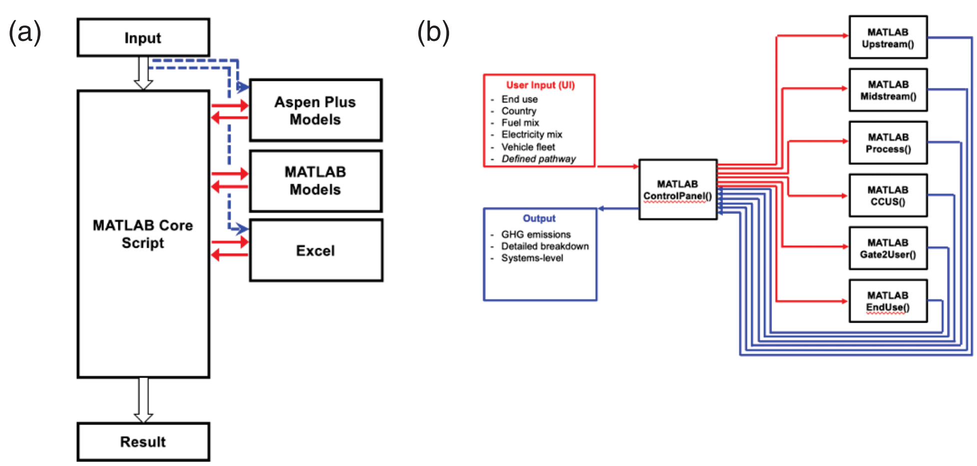


Figure 2 (a) The tool is developed in MATLAB with the added capabilities of communicating with various modeling programs such as Aspen Plus. (b) The modular structure: control panel connecting to primary life stage modules.

Figure 2(a) depicts the communication between MATLAB Core Script and auxiliary components: MATLAB Models, Aspen Plus Models, and Excel models and databases.

As needed, the tool can be equipped with more programming platforms. MATLAB is used to develop life stage modules, each one of which has its unique structure. Each module is composed of numerous custom developed MATLAB functions. Functions are designed to minimize the repetition of same scripts and framed clearly separate different tasks.

Natural gas fired power plants play a critical role in the evolving electric power system

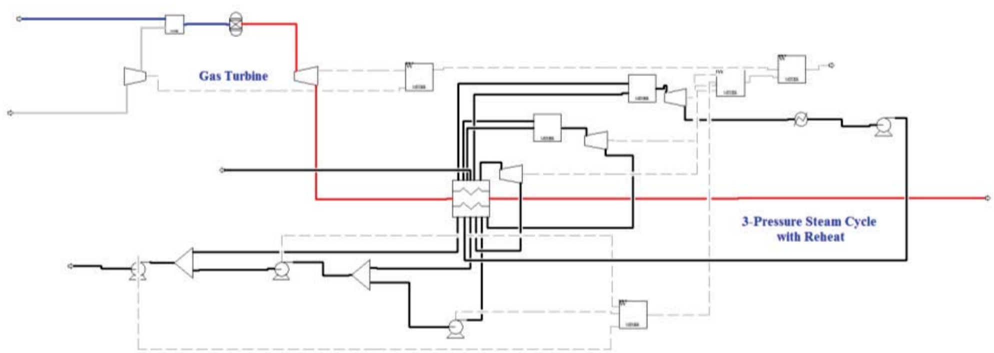


Figure 3 Process flow diagram of natural gas combined cycle unit simulated in Aspen Plus to match the performance of GE's 7FA model.

both as a lower carbon intensity alternative to coal power plants, and as balancing capacity for variable renewable energy sources. Power plant performance is sensitive to parameters such as percent loading, ambient temperature and relative humidity. To have a representative characterization of power generation units, we have developed Aspen Plus simulations for the most widely used combined cycle and gas turbine units. The performance of models is validated using the manufacturer's catalogs (Chase and Kehoe, 2013). Simulations represents steady-state operation at various conditions including percent loading (Gençer and Agrawal, 2017b).

3. System Boundaries

Pathway level analysis constitutes the backbone of the computation engine. The platform is capable of calculating all the combinations of modules, presented in Figure 1, that form a meaningful pathway. The individual pathways can be further expanded with the addition of new modules. Cradle-to-grave system boundary for every complete pathway is set and the selections are limited to allowed components. System boundary for coal-to-electricity pathway is shown

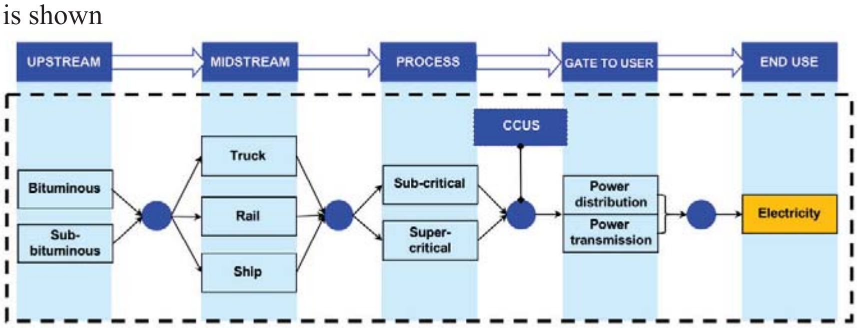
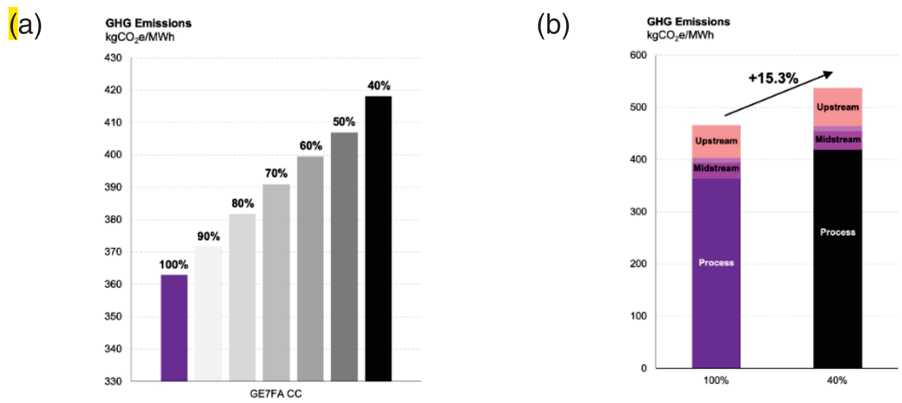


Figure 4 Coal-to-electricity pathway system boundary.



Lower plant capacity loading results in lower efficiencies and more emissions.

Figure 5 (a) GHG emissions from the flue gas of NGCC for varying loadings. (b) Cradle-to-grave life cycle emissions of shale gas-to-power pathway for 100 % and 40 % of the nameplate capacity of NGCC unit.

in Figure 4. For every life stage, there are multiple options that can be selected such as the coal type (bituminous or subbituminous), the transportation method of coal (truck, rail, or ship). Combination of these alternatives can also be specified.

3.1. Representation of Systems

Pathway-level analysis provides valuable insights however, understanding system wide emissions impact is critical. The presented modular framework is designed to perform systems-level calculations. A system is defined as a collection of individual pathways. This approach allows performing high resolution LCA based upon detailed individual pathways embedded. System can be as small as two pathways and as large as a city or a region. To determine the minimum emission option, the problem can be optimized using genetic algorithm (Gençer et al., 2015; Liu and Bakshi, 2018).

4. Results

The model can be run in pathway level or systems-level modes. The pathway level calculations are performed to estimate the life cycle GHG emissions in a given system boundary. The impact of cycling for NGCC plants is explored. Simulation results for 40 % to 100 % loading relative to nameplate capacity for a NGCC unit is shown in Figure 5(a). The emission rate increases from 362 $kgCO_2$/MWh to 419 $kgCO_2$/MWh when the power output is reduced to 40 %. The emission impact of this variation is propagated to

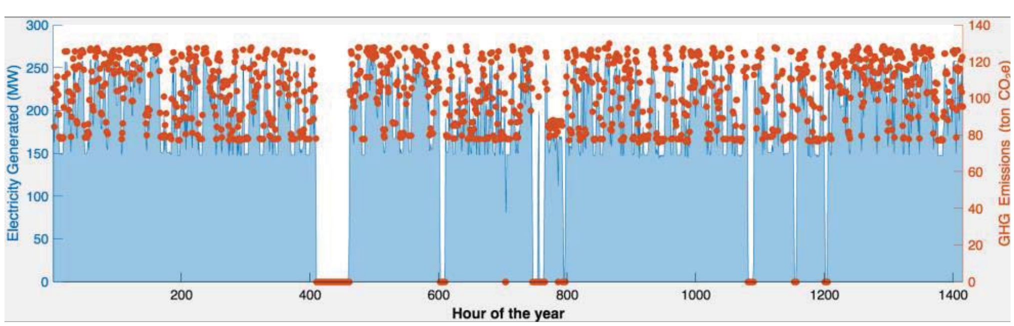


Figure 6 Hourly LCA based on observed load profile of a NGCC unit in California.

all life cycle stages of the supply chain. Cradle-to-grave life cycle analysis for the two extreme cases are performed and results are summarized in Figure 5(b). The emission intensity increases by 15.3 % relative to operation at peak efficiency. Using the embedded hourly generation profiles of thermal generation units a life cycle emissions of generators in the US has been calculated. Results for a combined cycle unit in California (Dynegy Moss Landing Power Plant Unit 1A) is shown in Figure 6, the area graph shows the hourly electricity generation and dots are the calculated full life cycle emissions in tCO_2e. For this particular unit, we observe more than 40% fluctuations in total emissions. While one reason for this change is the lower net generation, the other reason is higher emission intensity operation due to operation at off peak mode.

How different would the results be for a pathway and systems leve; analysis? What is the difference between pathway and system

5. Conclusions

The adoption of a holistic approach is increasingly important to accurately characterize the energy system. Here, we have demonstrated a novel tool to integrate the systems aspect for the conventional life cycle analysis. The underlying analytic engine constitutes of numerous individual energy pathways. The developed tool provides a consistent platform to estimate LCA of all components of the energy sector. Furthermore, the system representation is embedded into the tool for power and transportation sectors. LCA of power generation at hourly generator level resolution is estimated by integrating calculated performances from process simulations.

6. References

Annual Energy Outlook 2018. 2018.

Chase DL, Kehoe PT. GER-3574G - GE Combined-Cycle Product Line and Performance. Schenectady, NY: 2013.

DOE NETL. Cost and Performance Baseline for Fossil Energy Plants. vol. 1a. 2015.

Gençer E, Agrawal R. Strategy to synthesize integrated solar energy coproduction processes with optimal process intensification. Case study: Efficient solar thermal hydrogen production. Comput Chem Eng 2017a;105:328–47. doi:10.1016/j.compchemeng.2017.01.038.

Gençer E, Agrawal R. Synthesis of efficient solar thermal power cycles for baseload power supply. Energy Convers Manag 2017b;133:486–97. doi:10.1016/j.enconman.2016.10.068.

Gençer E, Tawarmalani M, Agrawal R. Integrated Solar Thermal Hydrogen and Power Coproduction Process for Continuous Power Supply and Production of Chemicals. vol. 37. 2015. doi:10.1016/B978-0-444-63576-1.50076-5.

Liu X, Bakshi BR. Extracting Heuristics for Designing Sustainable Built Environments by Coupling Multiobjective Evolutionary Optimization and Machine Learning. Comput Aided Chem Eng 2018;44:2539–44. doi:10.1016/B978-0-444-64241-7.50418-3.

Majumdar A, Deutch J. Research Opportunities for CO2Utilization and Negative Emissions at the Gigatonne Scale. Joule 2018;2:805–9. doi:10.1016/j.joule.2018.04.018.

U.S. EPA. Emissions & Generation Resource Integrated Database (eGRID) 2018a.

U.S. EPA. Air Markets Program Data 2018b.

Wang M. GREET Model: The Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation Model. 2011.