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Integrating Time-Varying Environmental Indicators into an Energy Systems Modeling and Optimization Framework for Enhanced Sustainability

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ABSTRACT

Data-driven decision-making is crucial in the transition to a low-carbon economy, especially as global industries strive to meet stringent sustainability goals. Traditional life cycle assessments often rely on static emission factors, overlooking the dynamic nature of the energy grid. As renewable energy penetration increases, grid carbon intensity fluctuates significantly across time and regions, due to the inherent intermittency of renewable sources like wind and solar. This variability introduces discrepancies in emission estimations if time-averaged factors are applied, leading to sub-optimal process operations and unintended environmental consequences. To this end, we present a real-time emission-aware optimization framework, which is implemented through a mixed-integer linear programming formulation that can determine optimal design configurations and operation schedules while simultaneously mitigating emissions by utilizing electricity price forecasts, time-varying emission factors, sporadic weather data, and supply and demand variability. The optimization model integrates life cycle assessment criteria to evaluate various environmental inputs, categorized into direct on-site emissions (Scope 1), indirect emissions from energy use (Scope 2), and upstream, downstream, and construction-related emissions associated with the process system (Scope 3). The framework, demonstrated through a detailed hydrogen production case study, showcases the effect of time-varying emissions by generating a set of optimal solutions that balance the trade-offs between environmentally sustainable and economical operational strategies.

Keywords: Real-time carbon accounting, Life cycle assessment, Time-varying indicators, Sustainability, Optimization

INTRODUCTION

Climate change remains a critical challenge in the 21st century, necessitating comprehensive strategies to mitigate greenhouse gas (GHG) emissions across various sectors. In this context, life cycle assessment (LCA) has emerged as a pivotal tool for evaluating the environmental impacts of products and processes. Central to LCA is the accurate quantification of emissions, which has traditionally relied on static average emission factors (AEFs) [1]. However, growing concerns about the temporal and spatial variability of emissions have highlighted the need for more dynamic approaches, such as the use of marginal emission factors (MEFs) [2]. Marginal emission factors quantify the incremental change in emissions resulting from a unit change in electricity demand or supply. Unlike AEFs, which represent the average emissions over a fixed period, MEFs account for real-time grid conditions and the specific generation mix at a given moment. This distinction is especially critical in regions with a high

share of renewable energy sources, where the marginal electricity emission factor often differs from the average emission factor calculated of the given fuel mix [3]. Consequently, MEFs provide a more accurate representation than AEFs, particularly in grids with diverse renewable sources such as wind and solar, which exhibit high intermittency. The dynamic nature of MEFs provides a more accurate representation of the environmental impact of electricity use, especially in the context of flexible and time-dependent systems like hydrogen production, electric vehicle charging, and energy storage [4]. Adopting MEFs enables policymakers and industry stakeholders to design interventions that align with low-carbon electricity availability, thereby enhancing the efficacy of decarbonization efforts. For instance, scheduling energy-intensive processes during periods of low marginal emissions can significantly reduce overall GHG impacts. Furthermore, MEFs facilitate a better understanding of the interplay between electricity demand patterns and grid emissions, offering valuable insights for optimizing energy transitions [5].

This paper explores the significance and effects of using MEFs instead of static emission factors in an energy systems modeling and optimization framework. By advocating for the adoption of MEFs, this study aims to contribute to a more nuanced and impactful approach to emission accounting, thereby advancing global efforts toward sustainable development.

SYSTEM UNDER INVESTIGATION

Goal, Scope, and Boundary System

The objective of this case study is to meet a daily hydrogen demand of 240,000 kg by integrating various hydrogen production technologies. The primary focus is on minimizing costs and emissions, with particular attention to the impact of employing marginal emission factors rather than static emission factors. To highlight the influence of emissions on hydrogen production, the Houston area in Texas has been selected as a representative location for potential hydrogen infrastructure development [6]. A superstructure, illustrated in Figure 3, has been developed to incorporate both conventional steam methane reforming (SMR) and proton exchange membrane (PEM) processes for hydrogen production. The system considers three energy sources: the electrical grid and two renewable power purchase agreements (PPAs), specifically solar and wind energy. The electrical grid comprises multiple energy generation sources, including nuclear, hydropower, solar, wind, natural gas, and coal/lignite, each characterized by distinct global warming potentials. Table 1 presents the global warming potentials, expressed in kg CO_2-eq/MWh, which are used to calculate the time-varying emission factors of the electrical grid. Figure 1 illustrates the hourly dynamic behavior of the Electric Reliability Council of Texas (ERCOT), highlighting the contributions of various energy sources to meet hourly energy demand. It is important to note that the energy mix is determined in advance through fuel mix forecasting, as performed by ERCOT. This forecasting relies on predictive models that estimate electricity demand and the availability of renewable energy sources, such as wind and solar, based on weather patterns and historical data. Figure 2 demonstrates the significant variation in emission factors resulting from fluctuations in the contributions of these energy sources. The calculated marginal emission factor of the ERCOT grid ranges from 276.06 to 403.75 kg CO_2-eq./MWh, with an average value of 353.80 kg CO_2-eq./MWh. This average aligns closely with the emission factor reported by the Environmental Protection Agency (EPA), which is 351.31 kg CO_2-eq./MWh [7].

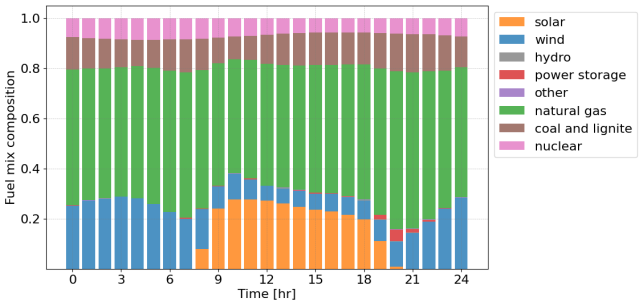

Figure 1. Time-varying energy mix of the ERCOT grid.

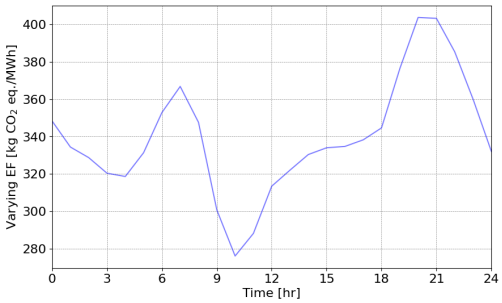

Figure 2. Time-varying emission factor of the grid on an hourly resolution.

Table 1: Various energy sources generating power within the ERCOT grid – *adapted from Ecoinvent V3.10.*

Energy Source	GWP 100 [kg CO_2 eq./MWh]
Coal and lignite	960.00
Natural gas	407.00
Nuclear	50.00
Wind	≈0.00
Solar	≈0.00
Hydropower	≈0.00

Data Sourcing and Assumptions

Operational data for the SMR, and CCS, were

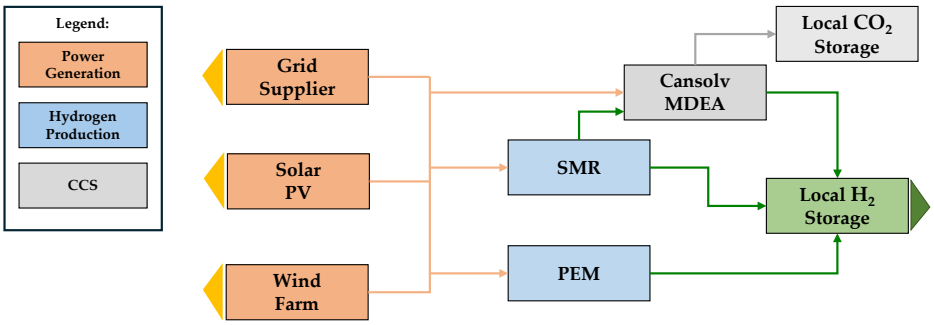

Figure 3: Proposed superstructure integrating two renewable energy sources—wind and solar—alongside a grid supplier, a conventional steam methane reformer, and a proton exchange membrane hydrogen production unit. The system operates within a life cycle boundary framework that accounts for both scope 1 and scope 2 emissions.

sourced from the National Energy Technology Laboratory (NETL) and Zang et al., both of which comprehensively discuss the operational aspects of hydrogen production processes [8,9]. Data for the PEM process were obtained from the National Renewable Energy Laboratory's (NREL) report on proton exchange membrane water electrolyzers and Gerloff N. [10,11]. Emission factors for all resources utilized in this study were extracted from Ecoinvent version 3.10, while characterization factors for converting emissions into carbon dioxide equivalent values were derived from the Sixth Assessment Report of the Intergovernmental Panel on Climate Change (IPCC) [12,13]. Lastly, Figure 4 presents the hourly electricity pricing data sourced from ERCOT, along with the capacity factors reflecting solar and wind variability in Texas. These data are integrated into the model to formulate a linear programming problem, enabling the development of economical and environmentally optimized production schedules. The implementation was conducted on a Windows 11 system equipped with a 13th Gen Intel(R) Core(TM) i7-13700 processor and 32 GB of DDR5 RAM, while using Gurobi to solve the optimization problem.

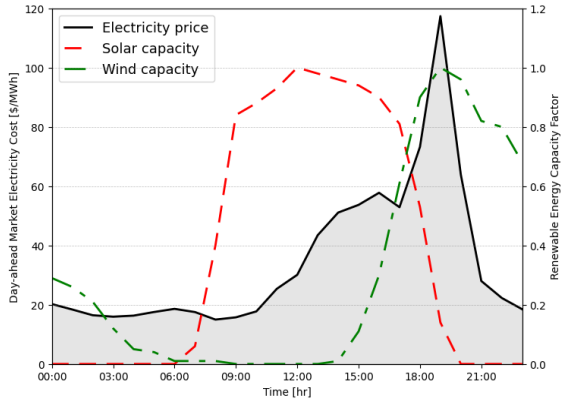

Figure 4. Varying day-ahead market electricity prices and renewable energy availability

Methodology

The proposed framework is designed to be applicable and adaptable over different research sectors, extending beyond the specific case study of hydrogen production. The framework's foundation lies in a resource-process approach, which categorizes system components into resource inputs, conversion processes, and associated outputs [14]. This modular and systematic structure allows the framework to accommodate a wide range of process systems, provided they adhere to this fundamental programming structure.

By decoupling the methodological design from the specifics of any one application, the framework achieves a level of generality suitable for addressing diverse optimization problems in various sectors. Examples include chemical manufacturing, energy systems, and other industrial processes that involve resource transformation and utilization. This adaptability ensures the framework's relevance in solving problems related to cost minimization, and emissions reduction. The generalizable nature of the framework not only enhances its utility for interdisciplinary applications, but also ensures its scalability for future advancements in sustainable process system scheduling and design.

Time-varying Emission Factor Formulation

To fully encapsulate the time-varying aspect of electrical grid power generation, Eq. 1 is utilized to quantify the varying emission factor. The total energy generation, E_t, must be known at each time step, which is multiplied by the contribution percentage, $Co_{r,t}$, of each energy producing source, which is then multiplied with their corresponding global warming potential, $GWP_{r,t}$.

$$EF_t = E_t \times \sum_{r \in R} Co_{r,t} . GWP_{r,t} \quad \forall\, t \in T \tag{1}$$

Scope-wise Emission Approach

Within this quantification framework, Eq. 2 captures emissions associated with both resource consumption and discharge. The total resource emissions, em_r, are

calculated as the sum of emissions from resource consumption and discharge at time, $t \in T_{sch}$. Specifically, the emissions from total resource consumption, $c_{r,t}$, are determined by multiplying the consumed quantity by the corresponding emission factor, $EF_{r,t}$, for the resource, r. Similarly, the emissions from resource discharge, $s_{r,t}$, are calculated by multiplying the discharged quantity by its associated emission factor. This formulation ensures a comprehensive accounting of resource-related emissions within the system's lifecycle.

$$em^r = \sum_{t \in T^{sch}} \sum_{r \in R} (EF_{r,t} \cdot c_{r,t} + EF_{r,t} \cdot s_{r,t}) \quad (2)$$

Secondly, on-site emissions, referred to as process emissions, are quantified using Eq. 2. These emissions are determined by the production quantity and the emission factors associated with the resources utilized during the production phase. Specifically, the process emissions at a given location are calculated by summing the emission contributions of each resource used. This is achieved by multiplying the emission factor, $EF_{r,t}$, of a resource by the conversion factor, $\eta_{p,r,t}$, which represents the efficiency of process, $p \in P$, in converting the resource into the desired product. The result is then multiplied by the total production quantity, $p_{p,t}$, of the process at the location of interest. This formulation ensures an accurate representation of emissions directly attributable to production activities at specific locations.

$$em^p = \sum_{t \in T^{sch}} \sum_{r \in R} EF_{r,t} \times \sum_{p \in P} \eta_{p,r,t} \cdot p_{p,r,t} \quad (3)$$

RESULTS & DISCUSSION

The Cost Minimization Scenario

When optimizing for cost, the use of time-varying emission factors is found to have no impact on the production schedule as seen in Figure 5. Regardless of the chosen emission quantification approach, the cost-minimized optimal configuration consistently involves using SMR without CCS. This is due to the total emissions generated are not weighted in the optimization process when prioritizing profitability. However, while the production schedules remain identical, the quantification of total emissions differs between the two approaches. Using the time-varying emission factor approach results in total emissions of 2,861 metric tons (MT) of CO_2-eq., whereas the constant emission factor approach yields 2,864 MT of CO_2-eq.

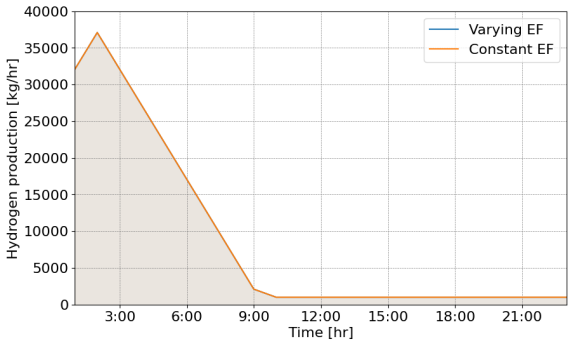

Figure 5. Hydrogen production profile using time-varying and constant emission factors while minimizing the cost objective.

This represents a difference of up to 3,000 kg CO_2-eq. within a 24-hour period. These findings highlight the influence of a dynamically changing energy mix, demonstrating that specific times of the day may be more favorable for increasing production rates due to lower emission factors. Figure 6 demonstrates that, despite the objective function being focused on cost minimization, the renewable PPAs for solar and wind energy, with fixed rates of $52.69/MWh and $60.11/MWh respectively, are more cost-effective during specific periods of the day. As a result, these renewable energy sources are prioritized over the more volatile grid electricity prices during those times.

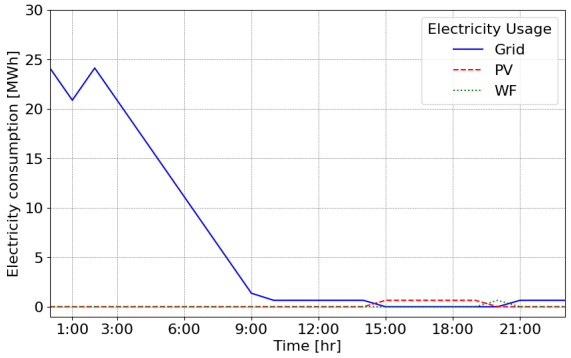

Figure 6. Energy consumption from different sources required to produce hydrogen in the cost minimization scenario.

Emission Minimization Scenario

When the objective function is adjusted to prioritize minimizing total emissions, Figure 7 illustrates a shift in the optimal production schedule when utilizing time-varying emission factors. An important observation is that SMR coupled with CCS is the preferred technology configuration when minimizing emissions. In contrast, PEM is not utilized, as its high energy demand would significantly increase grid power consumption, ultimately leading to higher overall emissions. The Maximum production in Figure 7 is concentrated in the earlier hours of the day,

specifically between 9:00 AM and 12:00 PM, coinciding with the period when the grid's emission factor is at its lowest. During this timeframe, the emission factor ranges from 270 to 300 kg CO_2-eq./MWh consumed, highlighting the environmental benefits of strategically aligning production with periods of lower grid emissions.

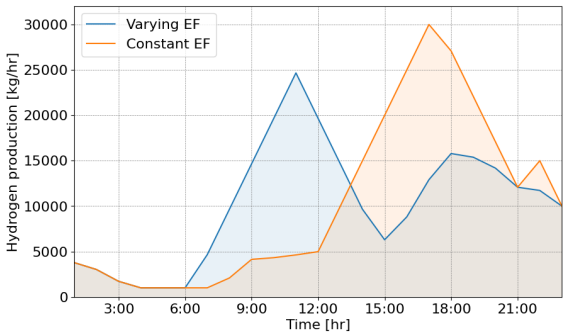

Figure 7. The difference in hydrogen production profiles when minimizing the total emission objective.

Table 2 reveals a significant difference in total emissions between the two carbon accounting approaches, with a disparity of 8,365 kg CO_2-eq. Additionally, while the change in the levelized cost of hydrogen (LCOH) is minimal, its impact becomes more pronounced when scaled to meet the daily hydrogen demand. Specifically, this minor deviation translates to a $4,800 difference in daily hydrogen value, which would accumulate to an annual difference of $1,752,000.

Table 2: Difference in LCOH and total emissions occurring when time-varying emission factors are utilized.

Scenario	LCOH [kg/H_2]	Total Emission [kg CO_2 eq.]
Time-varying EF	3.85	728,722
Average EF	3.87	737,087

A comparison of the energy consumption patterns in Figures 8 and 9 reveals that both approaches fully utilize the available solar and wind energy resources. However, the use of the grid supplier distinctly highlights the impact of varying emission factors on the timing and quantity of energy consumption required to meet the daily hydrogen production demand. In Figure 9, grid energy consumption is significantly constrained by the time-varying emission factor. In contrast, under the average emission factor scenario, there are no restrictions on when grid power can be consumed. As a result, the model is only constrained by the ramping and production limitations of the technology utilized. This demonstrates how the dynamic nature of grid emissions influences energy allocation strategies.

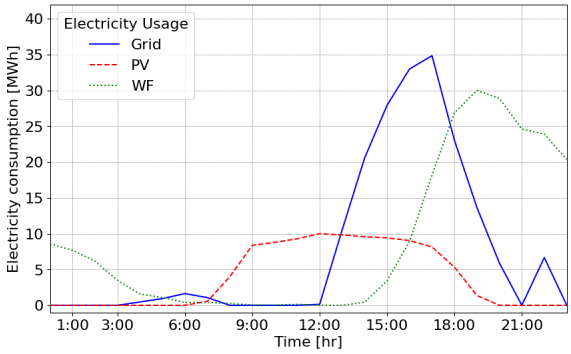

Figure 8. The energy consumption of different sources while utilizing an averaged emission factor approach.

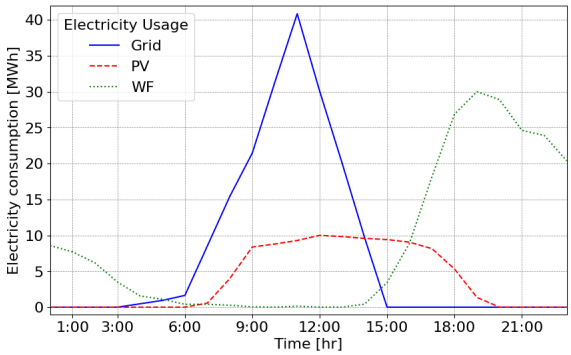

Figure 9. The energy consumption of different sources while utilizing a time-varying emission factor approach.

CONCLUSION & ONGOING WORK

Time-varying environmental indicators provide deeper insights into emission accounting by addressing the uncertainty of major contributors such as grid suppliers. However, this concept can be further expanded to not only cover dynamic energy production, but also create varying emission factors for any resource that is dependent on being produced by using electricity from grid suppliers. Cooperative decision-making between energy suppliers and plant management is also essential to enhance precise and accurate real-time carbon accounting and emission factor calculation. A key area of the ongoing work is to introduce social quantification metrics into the optimization framework to evaluate broader societal impacts and have a triple-bottom-line optimization approach. Furthermore, efforts are put into investigating the temporal dynamics of greenhouse gas residence times and their influence on global warming potential over various time horizons, which could lead to having time-varying global warming potentials that can be used to calculate dynamically changing emissions present in the atmosphere. These efforts aim to refine the framework and facilitate the transition toward a more sustainable and emission-conscious hydrogen production sector.

DIGITAL SUPPLEMENTARY MATERIAL

The supplementary materials for this study are accessible at Marcopdsousa-TAMUparametric. The data file *"RT 20 August 2024"* includes raw data for Day-Ahead Market (DAM) and natural gas prices, as well as maximum electricity production factors for solar and wind power in the Houston area, which is retrieved from ERCOT. The repository contains the optimization models used in this study. The *"Constant_EF"* model optimizes hydrogen production using the average emission factor approach, as defined by the Environmental Protection Agency (EPA). The *"Time_varying_EF"* model incorporates the calculated time-varying emission factors into the optimization framework. These resources are provided to enhance reproducibility and collaboration on the subject. For further inquiries or assistance, please contact *Marcopdsousa@tamu.edu*.

ACKNOWLEDGEMENTS

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