A NOVEL FORECASTING FRAMEWORK FOR ENERGY AND A SYSTEMS ENGINEERING METHODOLOGY TOWARDS CIRCULAR ECONOMY

A Dissertation

by

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ABSTRACT

The rising energy demands and the burgeoning population combined with concerns about the risks of climate change mandate a cost-conscious transition towards low-carbon or carbon-neutral energy, that will not limit the economic growth. Such transition introduces major challenges, and thus requires holistic strategies and systematic approaches during its execution. In this work, process and energy systems engineering thinking along with mathematical optimization and machine learning are utilized to address some of the outstanding issues related to the energy transition and the circular economy (CE) implementation.

First, a novel forecasting framework to calculate the average as well as the market (spot) price of energy in the United States is presented. The complex energy landscape is thoroughly analyzed to accurately determine the two key factors of this framework: the total demand of the energy products directed to the end-use sectors, and the corresponding price of each product in the form of either a monthly or a spot price. Spot prices are available to date, while data for the demand and the monthly price of energy products lag several months. This issue is overcome with the introduction of state-of-the-art forecasting methodologies that allow accurate forecasting for the demand and the prices of the energy products up to 48 and 12 months respectively. The forecasting capabilities of the framework are rigorously tested over a long period of 184 months, while its effectiveness is demonstrated by addressing four policy questions of significant public interest.

Then, a literature review listing Process Systems Engineering approaches that have been developed and can be used to facilitate the transition towards CE has been conducted. Thereafter, a novel CE system engineering framework for the modeling and optimization of food supply chains is introduced, demonstrating efficient ways for the re-utilization of products and materials along with the extensive usage of renewable energy sources. Due to the conflicting objectives involved, a multi-objective optimization strategy for trade-off analysis capturing different demand scenarios and uncertainty factors is also presented. Finally, a micro-level CE assessment framework with sector-specific indicators as well as overall and category-based metrics is proposed, allowing the robust and holistic assessment of multi-scale, multi-faceted, and interconnected CE supply chains.

DEDICATION

To my wife, Ismini, for her endless support and constant encouragement

To my parents, Evangelia and George, for instilling in me the love of learning

To my aunt, Georgia, for teaching me to strive for excellence

To my mother-in-law, Fotini, for her generosity, kindness and selflessness

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NOMENCLATURE

$	United States Dollar (USD)
CE	Circular Economy
EPIC	Energy Price Index
ESPIC	Energy Spot Price Index
REPIC	Residential Energy Price Index
CEPIC	Commercial Energy Price Index
INEPIC	Industrial Energy Price Index
TEPIC	Transportation Energy Price Index
CPI	Consumer Price Index
GHG	Greenhouse Gas
IEA	International Energy Agency
BTU	British Thermal Unit
MMBtu	Million British Thermal Units
EIA	U.S Energy Information Administration
NAICS	North American Industry Classification System
CHP	Combined Heat and Power
OPEC	Organization of the Petroleum Exporting Countries
OECD	Organization for Economic Co-operation and Development
PSE	Process Systems Engineering
HGL	Hydrocarbon Gas Liquid
NG	Natural Gas
RBOB	Reformulated Gasoline Blendstock for Oxygenate Blending

WTI	West Texas Intermediate
ETF	Exchange-Traded Fund
REC	Renewable Energy Certificate
RTN	Resource Task Network
IMF	International Monetary Fund
ETS	Emissions Trading System
LCA	Life Cycle Assessment
RPS	Renewable Portfolio Standards
NREL	National Renewable Energy Laboratory
PI	Process Intensification
RAPID	Rapid Advancement in Process Intensification Deployment
SDGs	Sustainable Development Goals
FSC	Food Supply Chains
CEO	Coffee Energy Output
CCC	Coffee Cherries Consumption
CWC	Coffee Water Consumption
CWG	Coffee Waste Generation
CEM	Coffee CO_2 Emissions
RMSE	Root Mean Squared Error
sMAPE	symmetric Mean Absolute Percentage Error
MAE	Mean Absolute Error
STL	Seasonal and Trend decomposition using Loess
ARIMA	Auto Regressive Integrated Moving Average
AIC	Akaike Information Criterion
AICc	Corrected Akaike Information Criterion

NN	Neural Network
MLP	Multi-Layer Perceptron Neural Network
ELM	Extreme Learning Machine Neural Network
RNN	Recurrent Neural Network
CNN	Convolutional Neural Network
DNN	Deep Neural Network
LSTM	Long Short-Term Memory Neural Network
MICRON	MIcro CirculaR ecOnomy iNdex
MILP	Mixed Integer Linear Programming
MINLP	Mixed Integer Non linear Programming

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1. INTRODUCTION

1.1 The Energy Challenge

According to United Nations estimates, the current world population of 7.7 billion is projected to reach 9.7 billion in 2050, and peak at nearly 11 billion in 2100 [22]. As population grows and people seek to improve their quality of life, it is expected that by 2070 the world will be using at least 50% more energy than it does today [23]. Nevertheless, 770 million people did not have access to electricity in 2019 [24], while another billion was struggling with unreliable supplies of electricity [25]. In the meantime, GHG emissions have risen at a rate of 1.5% per year in the last decade, with the total GHG emissions reaching a record high of 55.3 $GtCO_2e$ in 2018, from which 37.5 $GtCO_2e$ per year comes from fossil CO_2 emissions related to energy and industrial use. Without a sign of GHG emissions peaking in the next few years, United Nations projects that by 2030 the emissions would need to be 25% and 55% lower than those in 2018 so as to put the world on the least-cost pathway for limiting global warming to below 2°C and 1.5°C respectively [26]. But the challenge is not just to mitigate climate change, but to do this while providing more reliable and accessible energy supplies. Therefore, a broad transformation of global energy is required towards achieving energy access, climate goals and air quality [25].

1.2 The Concept Circular Economy

Rising populations place huge stresses on natural resources. Extraction and depletion of raw materials and waste created throughout the supply chain of products have enormous environmental and socioeconomic impacts. One way to reduce these impacts is through the move towards the Circular Economy (CE) [27]. CE aims to solve resource, waste, and emission challenges confronting society by creating a production - to - consumption total supply chain that is restorative, regenerative, and environmentally benign [28]. Research challenges are highlighted and Process Systems Engineering (PSE) research opportunities are identified so as to assist in the understanding, analysis and optimization of CE supply chains. As such, a systems engineering framework for the optimization of food supply chains under CE considerations is presented. Moreover, a quantitative, holistic and robust CE assessment framework at the micro level of the economy is developed in an effort to accurately measure the various aspects of CE and identify potential areas of improvement towards the transition to a CE economic model.

1.3 What is the Price of Energy?

It is evident that energy affects every single individual and entity in the world. Moving towards a broad transformation of global energy, it is crucial to precisely quantify the "price of energy", and study how it evolves through time, through major political and social events, and through changes in energy and monetary policies. To this respect, the different types and sources of energy need to be identified along with their corresponding economic, pricing, supply and demand attributes. This task is complex and challenging.

Different types and sources of energy are used and produced in today's world. Primary energy sources include fossil fuels (i.e. petroleum, natural gas and coal), nuclear energy, and renewables, while electricity is considered as a secondary energy source since it is generated from primary energy sources. In addition, the energy sources are measured in different physical units. For example: liquid fuels are measured in barrels or gallons, natural gas in cubic feet, coal in short tons, and electricity in kilowatts and kilowatthours. Thus, one standard physical unit is required, and in this context BTU will be used since it is commonly used for comparing different types of energy to each other in the United States.

Similarly, the different types and sources of energy along with the various energy feedstocks and products are governed by their unique pricing, demand and supply mechanisms. For example, the main method for pricing crude oil in international trade is the market-related pricing system, the adoption of which by many oil exporters in 1986-1988 opened a new chapter in the history of oil price formation. It represented a shift from a system where the prices were administered by the large multinational oil companies in the 1950s and 1960s and then by OPEC between 1973-1988, to a system in which prices are set by "markets" [29]. Moreover, EIA considers seven key factors that could influence oil markets. These factors include the supply in the OPEC and non-OPEC countries, the demand in the OECD and non-OECD countries, the OECD inventories, the spot prices of oil and its products and various financial markets indicators [30].

But even though oil and natural gas are substitutes in many processes, they do not follow the same pricing system. Although, the oil indexation became the leading pricing mechanism for natural gas in the 20th and early 21st century in Europe, in recent years, gas-to-gas competition seems to have become the dominant price mechanism [31]. Also, the crude oil price has a small impact on the natural gas price, while the coal price has no effect [32]. Unlike oil, the price of natural gas is governed mainly by supply and demand, weather conditions, availability and prices of other fuels, and the level of economic growth [33].

These two indicative examples reveal the complexities and unique features of the energy landscape which cause the nonexistence of a "unified" price of energy.

1.4 Literature Review

To address the above-mentioned challenges, a detailed analysis of the fundamentals of the energy landscape is needed. The US energy landscape is a complex and extensive network of energy feedstocks and products across multiple sectors. This complexity is due to the fact that the various energy feedstocks can be utilized in many different ways. More specifically, they can be directed straight to the end-use sectors, or converted and refined to be directed to the end-use sectors and/or to the intermediate energy consuming sector, or directed straight to the intermediate energy consuming sector.

The requirement for energy as an input to provide products and/or services is defined as energy *demand* [34]. Since some of the energy feedstocks can be directed to the end-use sectors, the term *products* in this context refers to the components sent to the end-use sectors, including the primary energy sources e.g. natural gas, coal etc. The components that are directed to the end-use sectors should be delineated, ensuring that all energy demand is accounted for while avoiding any double counting of any energy demand. It is of utmost importance to maintain a holistic and concrete approach in defining and counting the various energy products so as to be precise and consistent throughout this context. This is essential, since the total demand of the energy products directed to the end-use sectors along with their respective prices constitute the cornerstone of the developed forecasting framework.

To this respect, extensive literature review has been conducted ensuring familiarity and comprehension of such a complex energy landscape, and presented in Chapters 2, 3 and 4. This includes research in the development of process superstructures [35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55], energy supply chain analyses [56, 57, 58, 59], and strategic planning frameworks [60, 61, 62, 63, 64, 65, 66, 67, 68, 69] that utilize single and hybrid energy feedstocks (biomass, coal, natural gas, municipal solid waste) to produce liquid fuels and chemicals, as well as reviews in the current state of energy technologies [70, 71, 72, 73, 74, 75, 76].

Furthermore, the role of PSE in the transition towards CE has also been studied. In particular, a literature review that lists the PSE approaches that have been developed and can be used in this direction is presented in Chapter 5. The literature gaps have been identified and areas with great potential that shall be explored are suggested. In Chapter 6, the literature of food supply chains and the necessary steps towards CE food supply chains are reviewed, while an extensive literature review for the identification and assessment of the alternative pathways for the waste and by-products valorization across the supply chain of coffee is demonstrated. Finally, the lack of effective CE metrics and assessment indicators at the micro level along with the key challenges causing this research gap are summarized and highlighted in Chapter 7.

1.5 The US Energy Landscape

The US Energy Information Administration (EIA) defines the energy consuming end-use sectors as the residential, commercial, industrial and transportation sectors of the economy because they purchase or produce energy for their own consumption and not for resale. The electric power sector is defined as an intermediate energy – consuming sector which provides electricity to the four major energy sectors i.e. residential, commercial, industrial and transportation [34, 77]. The definitions of each of the four end-use sectors and the electric power intermediate energy - consuming sector are provided verbatim by EIA [34, 77] as follows:

- **Residential Sector:** An energy – consuming sector that consists of living quarters for private households. Common uses of energy associated with this sector include space heating, water heating, air conditioning, lighting, refrigeration, cooking, and running a variety of other appliances. The residential sector excludes institutional living quarters.

- **Commercial Sector:** An energy – consuming sector that consists of service-providing facilities and equipment of businesses; Federal, State, and local governments; and other private and public organizations, such as religious, social, or fraternal groups. The commercial sector includes institutional living quarters. It also includes sewage treatment facilities. Common uses of energy associated with this sector include space heating, water heating, air conditioning, lighting, refrigeration, cooking, and running a wide variety of other equipment. *Note:* This sector includes generators that produce electricity and/or useful thermal output primarily to support the activities of the above-mentioned commercial establishments.

- **Industrial Sector:** An energy – consuming sector that consists of all facilities and equipment used for producing, processing, or assembling goods. The industrial sector encompasses the following types of activity manufacturing (NAICS*codes 31-33); agriculture, forestry, fishing and hunting (NAICS code 11); mining, including oil and gas extraction (NAICS code 21); and construction (NAICS code 23). Overall energy use in this sector is largely for process heat and cooling and powering machinery, with lesser amounts used for facility heating, air conditioning, and lighting. Fossil fuels are also used as raw material inputs to manufactured products. *Note:* This sector includes generators that produce electricity and/or useful thermal output primarily to support the above mentioned industrial activities.

- **Transportation Sector:** An energy – consuming sector that consists of all vehicles whose primary purpose is transporting people and/or goods from one physical location to another. Included are automobiles; trucks; buses; motorcycles; trains, subways, and other rail ve-

*The North American Industry Classification System (NAICS) is the standard used by Federal statistical agencies in classifying business establishments for the purpose of collecting, analyzing, and publishing statistical data related to the US business economy (https://www.census.gov/eos/www/naics/)

hicles; aircraft; and ships, barges, and other waterborne vehicles. Vehicles whose primary purpose is not transportation (e.g., construction cranes and bulldozers, farming vehicles, and warehouse tractors and forklifts) are classified in the sector of their primary use.

- **Electric power sector:** An energy – consuming sector that consists of electricity only and combined heat and power (CHP) plants whose primary business is to sell electricity, or electricity and heat, to the public – i.e., North American Industry Classification System 22 plants.

The Figures 1.1 to 1.5 illustrate the landscape for each energy feedstock. Please note that the gray arrows are not taken into account so as to avoid double counting (indirect use).

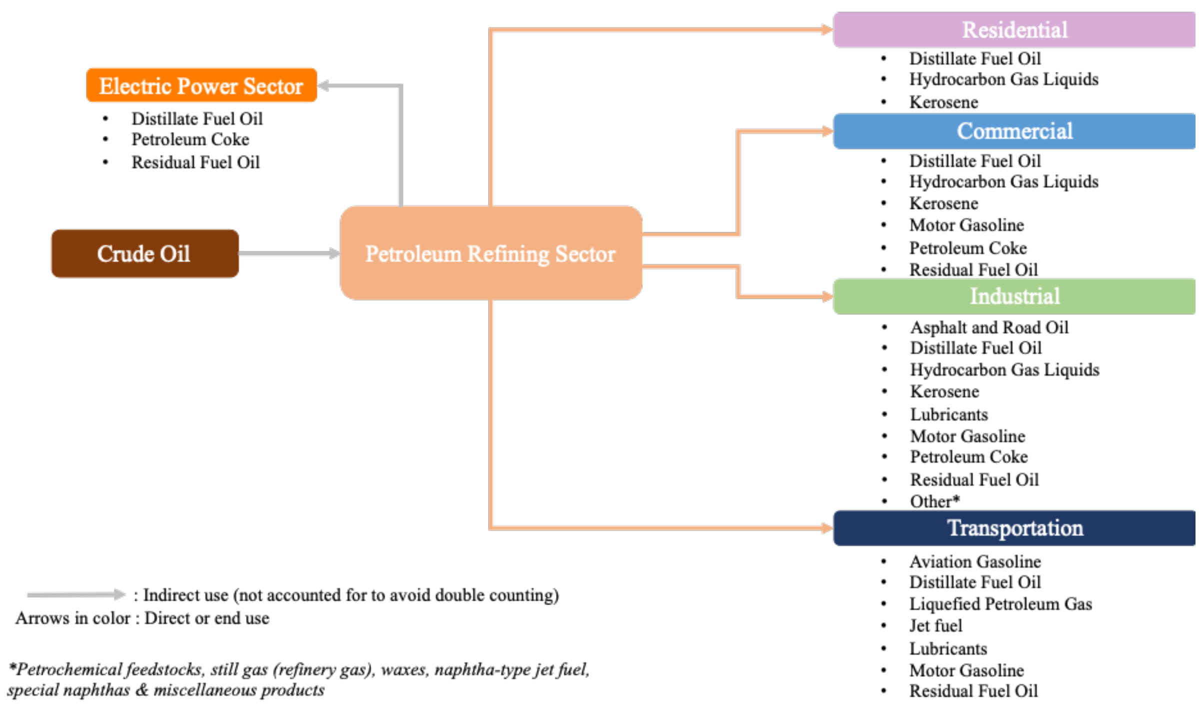

Figure 1.1: Landscape of Crude Oil in the United States

Figure 1.6 illustrates in detail the complete US energy landscape for the different energy feedstocks [78]. Each energy feedstock (source) has a unique color for easy visualization of the dif-

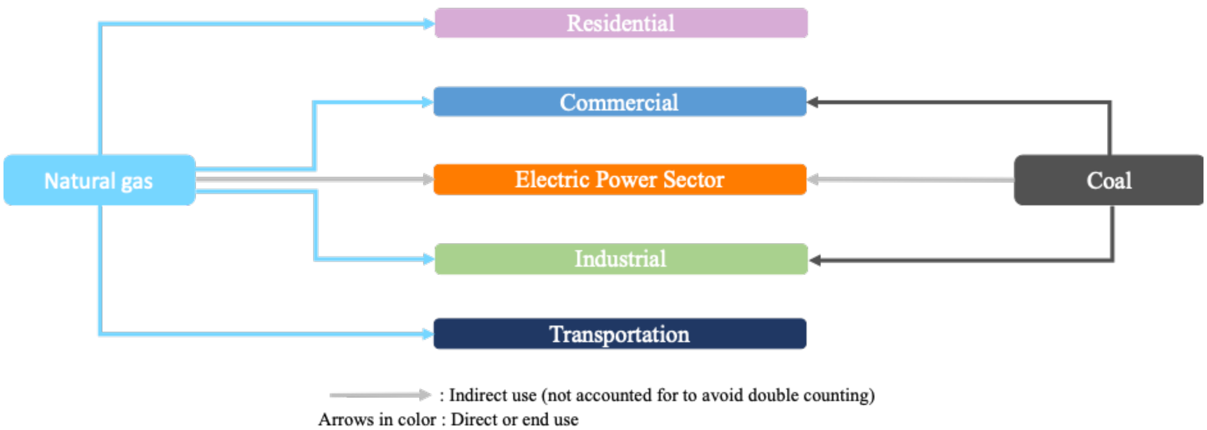

Figure 1.2: Landscape of Natural Gas and Coal in the United States

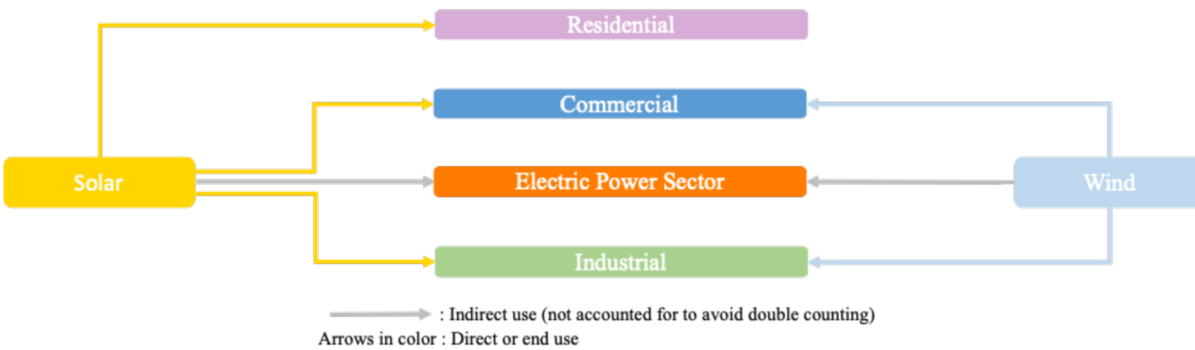

Figure 1.3: Landscape of Solar and Wind in the United States

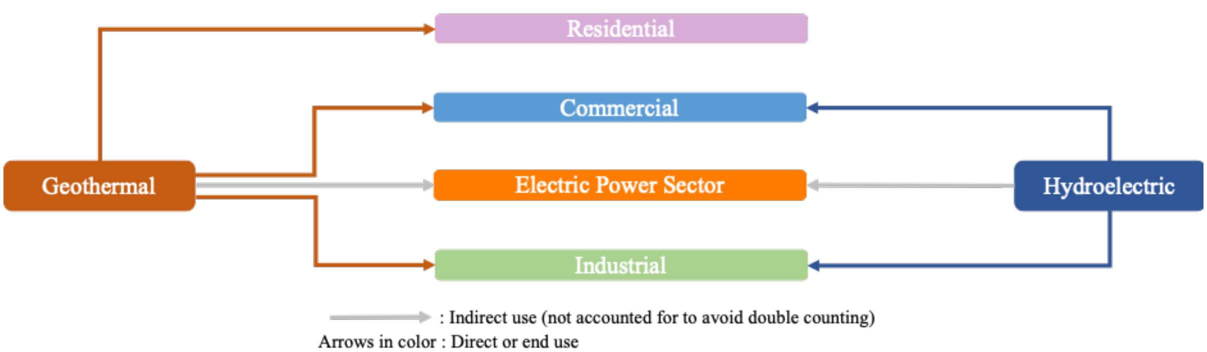

Figure 1.4: Landscape of Geothermal and Hydroelectric in the United States

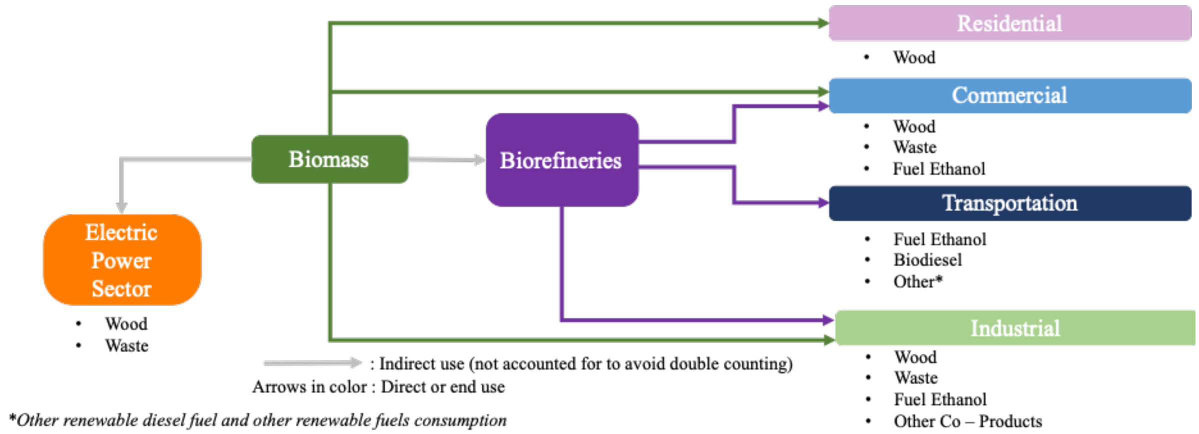

Figure 1.5: Landscape of Biomass in the United States

ferent pathways. Arrows connect energy feedstocks with the sectors that are consumed in. A gray arrow represents indirect use of an energy feedstock in an intermediate energy sector. A colored arrow (other than gray) represents direct use and matches with the color of its corresponding energy feedstock. It is also directed to the end-use sector that this energy feedstock is consumed in.

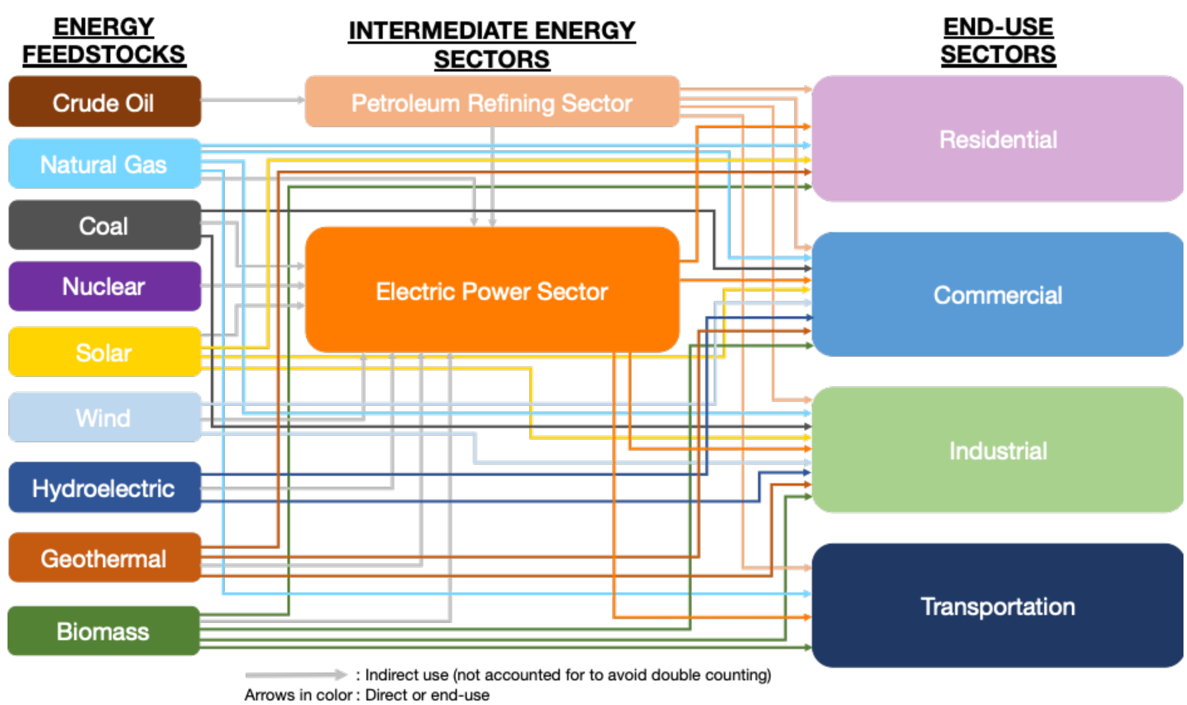

Figure 1.6: US Energy Consumption by Source and End-Use Sector

As mentioned above, to avoid double counting, the feedstocks directed into the electric power sector are not directly taken into account, because electricity is sold from the electric power sector as a product to the four end-use sectors. Therefore, the arrows going into the electric power sector are not counted, whereas the arrows leaving the electric power sector are counted.

1.6 Dissertation Objectives

This dissertation aims to address some of the outstanding questions regarding the energy transition and circular economy implementation. In particular, the main focus areas here are twofold. First, the study and analysis of the entire energy landscape that enhances our understanding with regards to the supply-demand and pricing mechanisms across all energy feedstocks and products. This will ultimately enable the design and implementation of effective energy policies for mitigating climate change and empowering the energy transition. Second, the development of analytical, systems engineering methodologies for the modeling and optimization of food supply chains under CE principles, which will be supported by CE indicators and metrics to holistically assess the alternative pathways towards circularity.

With regards to the first objective, a novel, quantitative framework that defines and quantifies a unified price of energy is introduced. Energy Price Index - EPIC, which is determined by both the demand and the prices of the energy products, represents the average monthly price of energy to the end-use consumers in \$/MMBtu. Having to deal with a lag of several months on data availability, a novel forecasting framework is developed to estimate the current as well as future values of EPIC using state-of-the-art optimization, statistical and machine learning methods. This framework allows accurate forecasts for the demand and the prices of the energy products up to 48 and 12 months respectively. For accomplishing the first objective, potential applications of this framework in the areas of policy, economics, finance and engineering are presented, revealing the effectiveness of EPIC as a tool to evaluate, design and optimize different policy questions. Seeking also to express the daily price of energy, the Energy Spot Price Index - ESPIC, is introduced. The ESPIC quantifies the daily average market price of energy in \$/MMBtu, and is also determined by the demand and the spot prices of the energy products. Due to its inherent attributes, ESPIC has also enormous potential applications as a financial instrument for investors who seek to get exposure to the entire energy market.

The second objective requires the development of novel methodologies for the implementation of the convergence from a linear to a CE food supply chain as well as for the holistic evaluation of this transition. As a first step, the objectives and goals of CE along with the challenges towards this transition are presented. Since a holistic approach is required for this transition, PSE approaches that can be readily used along with research gaps to facilitate this transition are identified. As a second step, a novel CE system engineering framework and decision-making tool for the modeling and optimization of food supply chains is introduced. The framework works as follows: First, the alternative pathways for the production of the desired product and the valorization of wastes and by-products are identified. Then, a Resource-Task-Network representation that captures all these pathways is utilized, based on which a mixed-integer linear programming (MILP) model is developed. This approach allows the holistic modeling and optimization of the entire food supply chain, taking into account any of its special characteristics, potential constraints as well as different objectives. Considering that typically CE introduces multiple, often conflicting objectives, a multi-objective optimization strategy for trade-off analysis is deployed. A representative case study for the supply chain of coffee is discussed, illustrating the steps and the applicability of the framework. Single and multi-objective optimization formulations under five different coffee-product demand scenarios are also discussed.

Additionally, and since the transition towards environmental, economic and social advancements requires analytical tools for quantitative evaluation of the alternative pathways, an analytical decision-making tool for evaluating and comparing the circularity of different companies or scenarios at micro level is introduced. The tool provides i) a set of indicators and metrics with sector-specific dimensions, ii) quantitative, holistic and robust CE overall and category-based metrics, iii) media for data visualization and analysis of CE indicators, and iv) an analytical tool to assess multi-national businesses and the multi-scale, multi-faceted and interconnected CE supply chains. Using a GRI-based, quantitative tool that takes into account all goals of CE holistically, companies are able to track their transition towards CE, conduct temporal analysis, and compare and benchmark their performance against their peers and industry's standards. The applicability and the capabilities of the developed CE assessment framework is demonstrated through case studies in the Energy & Utilities, Manufacturing and Automotive sectors where category-based and overall circularity indices are calculated over a period up to 10 years.

2. A NOVEL FORECASTING FRAMEWORK: THE ENERGY PRICE INDEX * † ‡

2.1 Background & Motivation

Energy markets are sensitive and volatile to technological breakthroughs and innovations, changes in monetary and fiscal policies, major global events and consumer trend changes [79, 80, 81]. Various governmental agencies, political and commercial organizations, think tanks as well as researchers and academics worldwide, consider various energy policies and their effects when dealing with the increasing concerns in energy independence, energy scarcity, energy sustainability, and pollution caused by the utilization of energy [82, 83, 84, 85, 86, 87]. Furthermore, with strategic political and commercial decisions and policies being assessed in economic terms, it is of utmost importance to accurately determine the price of energy so as to evaluate their effectiveness. Undoubtedly, energy affects every person and entity. Therefore, it is essential to accurately quantify "the price of energy" and grasp how it is affected by major breakthroughs, political events, as well as energy and monetary policies.

2.2 Introduction

Given the absence of such a pre-existing tool, a novel forecasting framework, the Energy Price Index (EPIC) is introduced, which can be used as a benchmark to calculate the average price of energy to the end-use consumers in the United States - US. The complex energy landscape of the US has been carefully analyzed in Section 1.5 to determine the products that are directed to the

*Reprinted from "A hybrid forecasting framework with statistical and machine learning methods for the energy sector" by S.G. Baratsas, R.C. Allen, E.N. Pistikopoulos, Computers & Chemical Engineering, 2021, with permission from Elsevier and Copyright Clearance Center. A summary of the work is given in this chapter with additional details provided in Appendix E.

†Reprinted from "A framework to predict the price of energy for the end-users with applications to monetary and energy policies" by S.G. Baratsas, A.M. Niziolek, O. Onel, L.R. Matthews, C.A. Floudas, D.R. Hallermann, S.M. Sorescu, E.N. Pistikopoulos, Nature Communications, 2021, Vol. 12, number 1, pp 1-12, with permission from Nature Publishing Group and Copyright Clearance Center. A summary of the work is given in Chapters 2 and 4 with additional details provided in Appendices B, C and G.

‡Reprinted from "A novel quantitative forecasting framework in energy with applications in designing energy intelligent tax policies" by S.G. Baratsas, A.M. Niziolek, O. Onel, L.R. Matthews, C.A. Floudas, D.R. Hallermann, S.M. Sorescu, E.N. Pistikopoulos, Applied Energy, 2021, with permission from Elsevier and Copyright Clearance Center. A summary of the work is given in Chapters 2 and 4 with additional details provided in Appendices C, D, and G.

end-use sectors of the US economy. The total energy demand of these products, together with their monthly prices, serve as the backbone of EPIC. However, the available data for both the key components of EPIC lag several months, so a rolling horizon model that uses information from the past so as to estimate the information that is not currently available is introduced. The initial goal is to accurately forecast the current value of EPIC and the forecasting ability of the proposed methodology is rigorously tested over a long period of 184 months, demonstrating remarkable accuracy. Ultimately, the forecasting ability of the framework is further extended providing accurate forecasts for the future values of both EPIC components. In particular, energy demands and energy prices are predicted up to 48 and 12 months in the future respectively. The high level of granularity of the framework allows also for the estimation of the average price of energy for the end-use sectors through the introduction of the energy price sub-indices.

2.3 EPIC Methodology

The two key factors comprising EPIC are the total demand of the energy products that are directed to the end-use sectors in the US along with their respective monthly prices.

2.3.1 Demand and Price Determination

Energy products consumed by the US economy originate from crude oil, natural gas, coal, nuclear, hydroelectric, geothermal, solar, wind, and several types of biomass. The exact determination of these products, their consumption, and their monthly prices is crucial. Hence, the EIA Monthly Energy Review Report is used as a reference point to determine the type and the amount of products that are consumed from each sector. The full list of these energy products and the corresponding sector that are consumed in is presented in Table 2.1.

Table 2.1: Energy Products and Sectors that are consumed in

Product No.	Product Name	Sector Consumed In
1	Distillate Fuel Oil	Residential
2	Kerosene	Residential
3	HGL (Propane)	Residential
4	Distillate Fuel Oil	Commercial
5	Kerosene	Commercial

Continued on next page

Table 2.1 – continued from previous page

Product No.	Product Name	Sector Consumed In
6	HGL (Propane)	Commercial
7	Motor Gasoline	Commercial
8	Petroleum Coke	Commercial
9	Residual Fuel Oil	Commercial
10	Asphalt and Road Oil	Industrial
11	Distillate Fuel Oil	Industrial
12	Kerosene	Industrial
13	HGL (Propane/Propylene)	Industrial
14	Lubricants	Industrial
15	Motor Gasoline	Industrial
16	Petroleum Coke	Industrial
17	Residual Fuel Oil	Industrial
18	Other Petroleum Products	Industrial
19	Aviation Gasoline	Transportation
20	Distillate Fuel Oil	Transportation
21	Jet Fuel	Transportation
22	HGL (Propane)	Transportation
23	Lubricants	Transportation
24	Motor Gasoline	Transportation
25	Residual Fuel Oil	Transportation
26	Geothermal Energy	Residential
27	Solar Energy	Residential
28	Biomass (Wood) Energy	Residential
29	Hydroelectric Power	Commercial
30	Geothermal Energy	Commercial
31	Solar Energy	Commercial
32	Wind Energy	Commercial
33	Biomass (Wood) Energy	Commercial
34	Biomass (Waste) Energy	Commercial
35	Biomass (Fuel Ethanol) Energy	Commercial
36	Hydroelectric Power	Industrial
37	Geothermal Energy	Industrial
38	Solar Energy	Industrial
39	Wind Energy	Industrial
40	Biomass (Wood) Energy	Industrial
41	Biomass (Waste) Energy	Industrial
42	Biomass (Fuel Ethanol) Energy	Industrial
43	Biomass (Losses and Co-Products) Energy	Industrial
44	Biomass (Fuel Ethanol)	Transportation
45	Biomass (Bio-Diesel)	Transportation
46	Natural Gas	Residential
47	Natural Gas	Commercial
48	Natural Gas	Industrial
49	Natural Gas	Transportation

Continued on next page

Table 2.1 – continued from previous page

Product No.	Product Name	Sector Consumed In
50	Electricity	Residential
51	Electricity	Commercial
52	Electricity	Industrial
53	Electricity	Transportation
54	Coal	Residential
55	Coal	Commercial
56	Coal	Industrial

The monthly consumption (in energy units) along with the monthly price (in \$ per energy unit) for each of these energy products are obtained from the EIA and from other sources, and are presented in Table 2.2. Please note that the proposed framework is generic and can be applied to (a) the US on a national level, (b) to US on a state-by-state basis, (c) regional level of multi-states, and (d) other countries, provided that a thorough analysis of the specific energy landscape has been conducted, the particular energy feedstocks and products have been identified, and data for their prices and demands are available.

Table 2.2: Demands & Prices of Energy Products

Product No.	Demand Data	Price Data
1	EIA MER[77]: Table 3.8a	EIA Petroleum and Other Liquids
2	EIA MER[77]: Table 3.8a	EIA MER[77]: Table 9.7
3	EIA MER[77]: Table 3.8a	EIA Petroleum and Other Liquids
4	EIA MER[77]: Table 3.8a	EIA MER[77]: Table 9.7
5	EIA MER[77]: Table 3.8a	EIA MER[77]: Table 9.7
6	EIA MER[77]: Table 3.8a	EIA MER[77]: Table 9.7
7	EIA MER[77]: Table 3.8a	EIA MER[77]: Table 9.7
8	EIA MER[77]: Table 3.8a	EIA EPM[88]: Table 4.1 & 4.2
9	EIA MER[77]: Table 3.8a	EIA MER[77]: Table 9.5
10	EIA MER[77]: Table 3.8b	EIA SEDS: Table F2[89] & BLS Database[90]
11	EIA MER[77]: Table 3.8b	EIA MER[77]: Table 9.7
12	EIA MER[77]: Table 3.8b	EIA MER[77]: Table 9.7
13	EIA MER[77]: Table 3.8b	EIA MER[77]: Table 9.7
14	EIA MER[77]: Table 3.8b	EIA SEDS: Table F10[89] & BLS Database[90]
15	EIA MER[77]: Table 3.8b	EIA MER[77]: Table 9.7
16	EIA MER[77]: Table 3.8b	EIA EPM[88]: Table 4.1 & 4.2
17	EIA MER[77]: Table 3.8b	EIA MER[77]: Table 9.5
18	EIA MER[77]: Table 3.8b	EIA SEDS: Table F15[89] & BLS Database[90]
19	EIA MER[77]: Table 3.8c	EIA MER[77]: Table 9.6 & 9.7
20	EIA MER[77]: Table 3.8c	EIA MER[77]: Table 9.7

Continued on next page

Table 2.2 – continued from previous page

Product No.	Demand Data	Price Data
21	EIA MER[77]: Table 3.8c	EIA MER[77]: Table 9.7
22	EIA MER[77]: Table 3.8c	EIA MER[77]: Table 9.7
23	EIA MER[77]: Table 3.8c	EIA SEDS: Table F10[89] & BLS Database[90]
24	EIA MER[77]: Table 3.8c	EIA MER[77]: Table 9.4
25	EIA MER[77]: Table 3.8c	EIA MER[77]: Table 9.5
26	EIA MER[77]: Table 10.2a	Lazard LCEA[91]
27	EIA MER[77]: Table 10.2a	Lazard LCEA[91]
28	EIA MER[77]: Table 10.2a	Lazard LCEA[91] and EIA AEO[81]
29	EIA MER[77]: Table 10.2a	EIA AEO[81]
30	EIA MER[77]: Table 10.2a	Lazard LCEA[91]
31	EIA MER[77]: Table 10.2a	Lazard LCEA[91]
32	EIA MER[77]: Table 10.2a	Lazard LCEA[91]
33	EIA MER[77]: Table 10.2a	Lazard LCEA[91] & EIA AEO[81]
34	EIA MER[77]: Table 10.2a	Lazard LCEA[91] & EIA AEO[81]
35	EIA MER[77]: Table 10.2a	EIA MER[77]: Table 9.7 & DOE AFPR[92]
36	EIA MER[77]: Table 10.2b	EIA AEO[81]
37	EIA MER[77]: Table 10.2b	Lazard LCEA[91]
38	EIA MER[77]: Table 10.2b	Lazard LCEA[91]
39	EIA MER[77]: Table 10.2b	Lazard LCEA[91]
40	EIA MER[77]: Table 10.2b	Lazard LCEA[91] & EIA AEO[81]
41	EIA MER[77]: Table 10.2b	Lazard LCEA[91] & EIA AEO[81]
42	EIA MER[77]: Table 10.2b	EIA MER[77]: Table 9.7 & DOE AFPR[92]
43	EIA MER[77]: Table 10.2b	Lazard LCEA[91] & EIA AEO[81]
44	EIA MER[77]: Table 10.2b	EIA MER[77]: Table 9.7 & DOE AFPR[92]
45	EIA MER[77]: Table 10.2b	EIA MER[77]: Table 9.7 & DOE AFPR[92]
46	EIA MER[77]: Table 4.3	EIA MER[77]: Table 9.10
47	EIA MER[77]: Table 4.3	EIA MER[77]: Table 9.10
48	EIA MER[77]: Table 4.3	EIA MER[77]: Table 9.10
49	EIA MER[77]: Table 4.3	EIA SEDS: Table F19[89] & Thomson Reuters Database[93]
50	EIA EPM[88]: Table 5.1	EIA EPM[88]: Table 5.3
51	EIA EPM[88]: Table 5.1	EIA EPM[88]: Table 5.3
52	EIA EPM[88]: Table 5.1	EIA EPM[88]: Table 5.3
53	EIA EPM[88]: Table 5.1	EIA EPM[88]: Table 5.3
54	EIA MER[77]: Table 6.2	EIA SEDS: Table F24[89] & BLS Database[90]
55	EIA MER[77]: Table 6.2	EIA SEDS: Table F24[89] & BLS Database[90]
56	EIA MER[77]: Table 6.2	EIA SEDS: Table F24[89] & BLS Database[90]

2.3.2 EPIC Calculation

EPIC represents the average monthly price of energy in a given month, and as such is defined as the summation of the price (in \$/MMBtu) of each product multiplied by the weight fraction of the demand of each product. The unit of EPIC is \$/MMBtu.

The real weight fraction based on the demand of each of the selected 56 energy products is calculated using Equation (2.1):

$$w_{m,p} = \frac{D_{m,p}}{\sum_p D_{m,p}} \qquad \forall (m,p) \tag{2.1}$$

where $w_{m,p}$ is the weight fraction of product *p* in month *m*, and $D_{m,p}$ is the demand of product *p* in month *m*. The mathematical formulation of EPIC is presented in Equation (2.2):

$$EPIC_m = \sum_p w_{m,p} \cdot C_{m,p} \qquad \forall m \tag{2.2}$$

where $EPIC_m$ represents the value of EPIC in month *m*, $C_{m,p}$ represents the price of product *p* in month *m*, and $w_{m,p}$ is the weight fraction of product *p* in month *m*.

2.4 Rolling Horizon Forecasting Framework

The data of the demands and the prices for some of the energy products become available with a lag of one to three months. Since both the demand and prices of the energy products enter into the EPIC calculation, a forecasting framework is required to estimate the present values for both the demand and prices of the underlying energy products. Consequently, a rolling horizon methodology is proposed as a forecasting framework to forecast the values of the required data for the time period of interest, the actual values of which will not be known until a few months later. The proposed methodology is using information from the previous three time periods, so as to forecast the values for the time period of interest.

Figure 2.1 illustrates the general concept of the rolling horizon methodology, along with its application over two stages in the future. Data from the three previous periods (T-3, T-2, T-1) are used to forecast the data of interest in the current stage T. Subsequently, data from the periods T-2, T-1, T are used for predicting the data of interest in stage T+1, and so on.

2.4.1 Forecasting of Energy Products' Demand Weights

The demand of the energy products exhibits a lag between two to three months in data availability. Thus, a rolling horizon based parameter estimation model is developed to forecast the weights

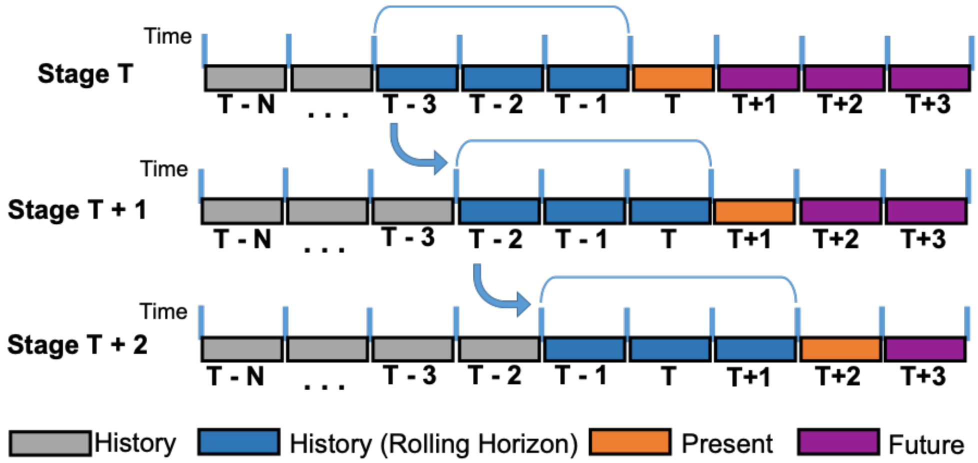

Figure 2.1: Rolling Horizon Methodology in a Multistage Problem

of the demand of each energy product up to present date using the data from the previous 3 years. The lookback period and the parameter estimation were selected considering the forecasting errors for different schemes and lookback periods, and are shown in Appendix B. It is worth mentioning that each month is trained separately since the energy demand is highly seasonal [77], as can be seen in Figure 2.2 for the case of natural gas (NG).

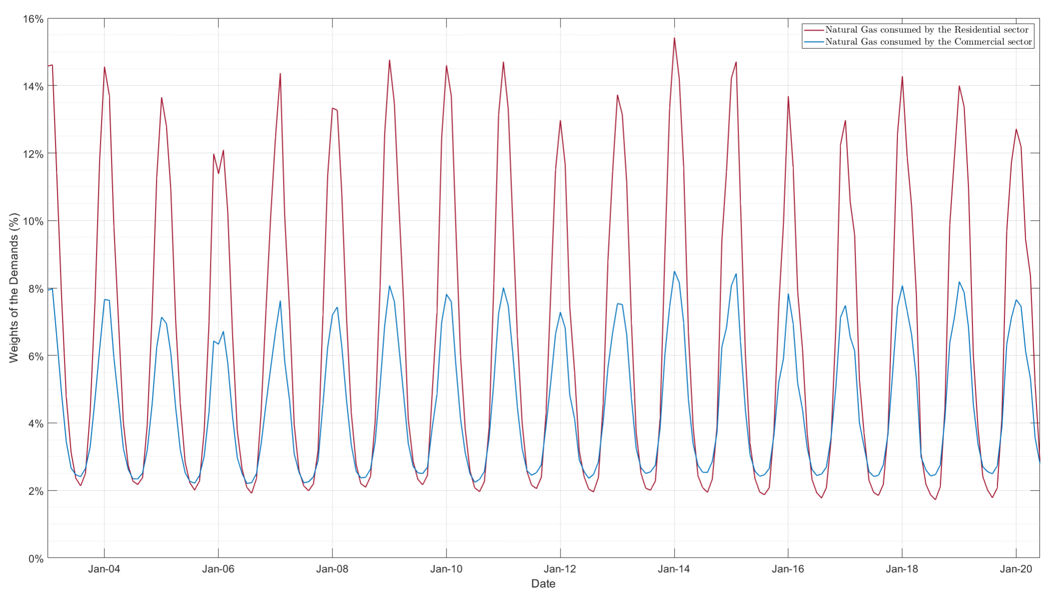

Figure 2.2: Seasonal Volatility of Natural Gas Consumption

A weight - based objective function is used to forecast the weights of the energy products. In particular, the objective function aims to minimize the squared difference between the real value of a product's weight in the past horizon and the predicted value of product's weight for the month of interest. The optimization model takes into account the data from the previous 3 years and is stated as follows:

$$
\begin{gathered}
min \sum_{m} Err_m \\
Err_m = \sum_{m',p} (w_{m',p} - \widehat{w}_{m,p})^2 \\
\sum_{p} \widehat{w}_{m,p} = 1 \\
\widehat{w}_{m,p} \geq 0 \\
\forall m' \mid (m' - m) = (-36) \quad or \quad (-24) \quad or \quad (-12)
\end{gathered} \tag{2.3}
$$

where $\widehat{w}_{m,p}$ represents the forecast weight of product *p* in month *m*.

Since the data of the energy demand has a lag between two to three months, as of August 2021, the real data until April 2021. Hence, the estimation of the weights of energy products for May 2021 requires data from May 2018, May 2019 and May 2020. Similarly, for June 2021, the data of June 2018, June 2019 and June 2020 will be used. Figure 2.3 illustrates the monthly parameter estimation for May 2021 and June 2021.

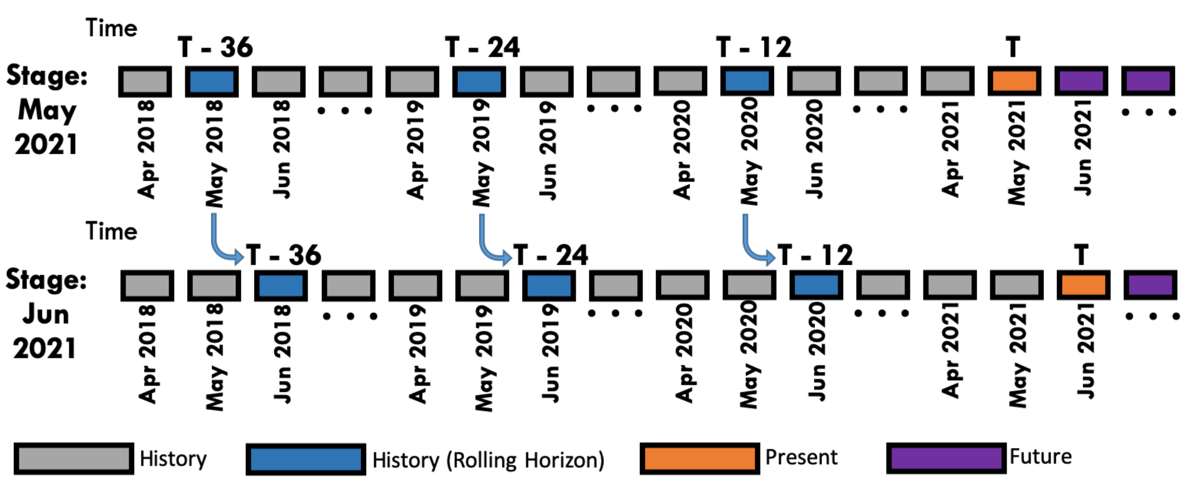

Figure 2.3: Monthly Weight Parameter Estimation

The same methodology can be extended for the following months of the year. Since at this point the real data until April 2021 is available, the weights up to April 2022 can be predicted. However, the forecasting ability of the framework is not limited to one year, but can be further extended by utilizing a combination of real and predicted data. More specifically, the forecasting methodology works as follows:

- **2nd year forecasts** require the deterministic data from the last two years along with the forecasts of the first year;
- **3rd year forecasts** require the deterministic data from the last one year along with the forecasts of the first and second years;
- **4th year forecasts** require the forecasts of the first, second and third years;

Figure 2.4 illustrates the rolling horizon framework for the first, second, third and fourth year forecasts of the weights using September 2021 as an example.

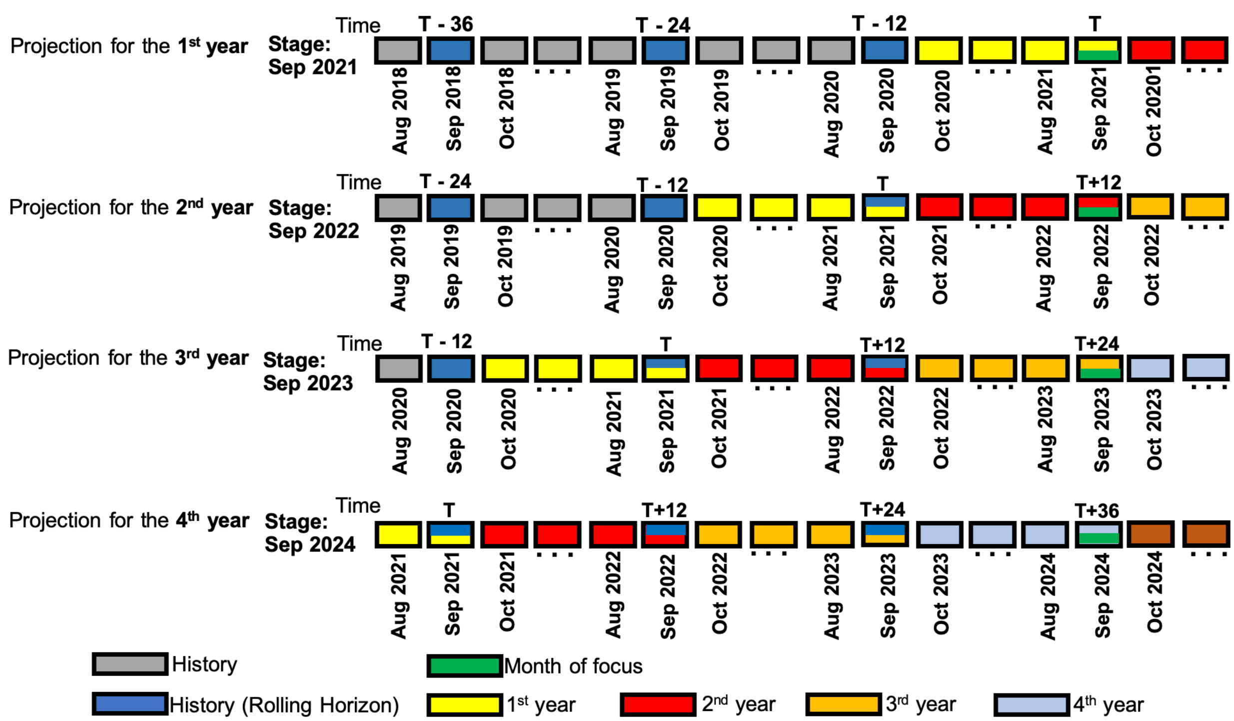

Figure 2.4: Rolling Horizon Framework up to 4 years for September 2021

2.4.2 Forecasting of Energy Products' Prices

The prices of the energy products are the second component of EPIC. As shown in Table 2.2, the required data are collected from a variety of sources. However, there is still a lag up to 3 months in data availability for some of these products. Therefore, a rolling horizon based parameter estimation model is developed so as to forecast the prices of these energy products up to the present date. As illustrated in the following figures, some of these products demonstrate high seasonality (Figure 2.5), while others demonstrate strong correlation with the spot prices of various commodities (Figure 2.6).

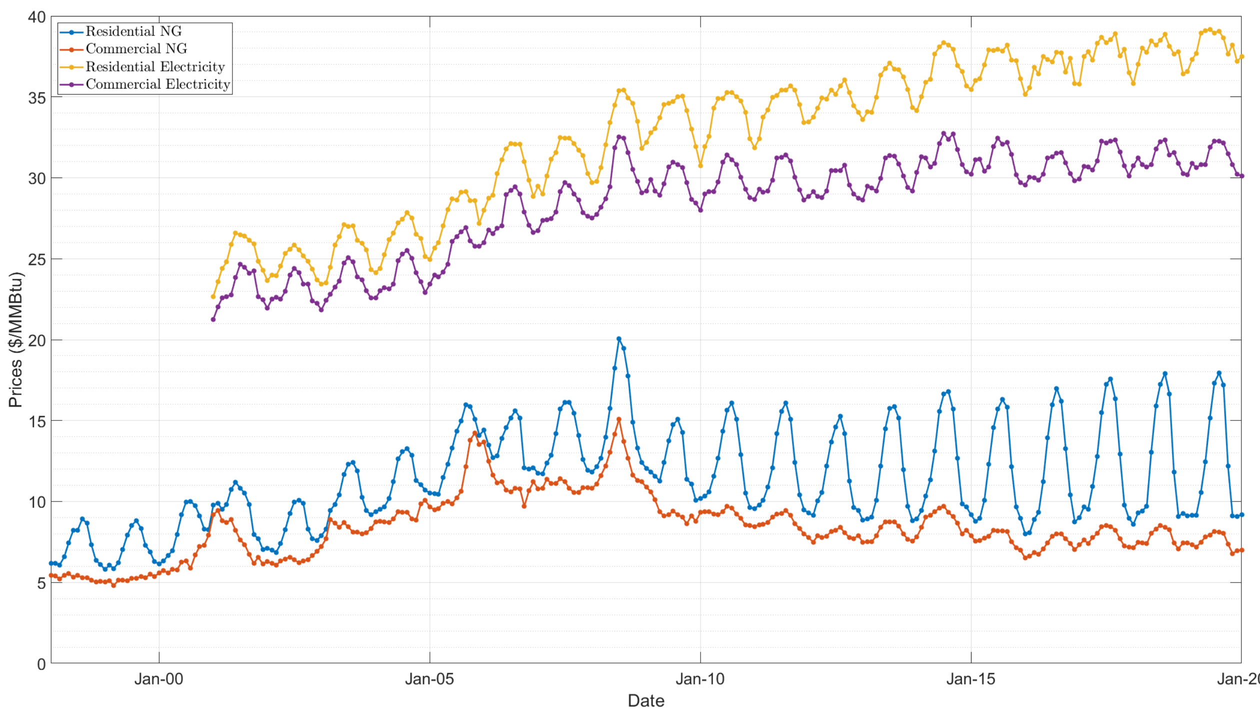

Figure 2.5: Monthly Prices of NG and Electricity - Strong Seasonality

The first step of the forecasting methodology requires the grouping of the energy products based on the lag of time until their prices become available. For the case of the US:

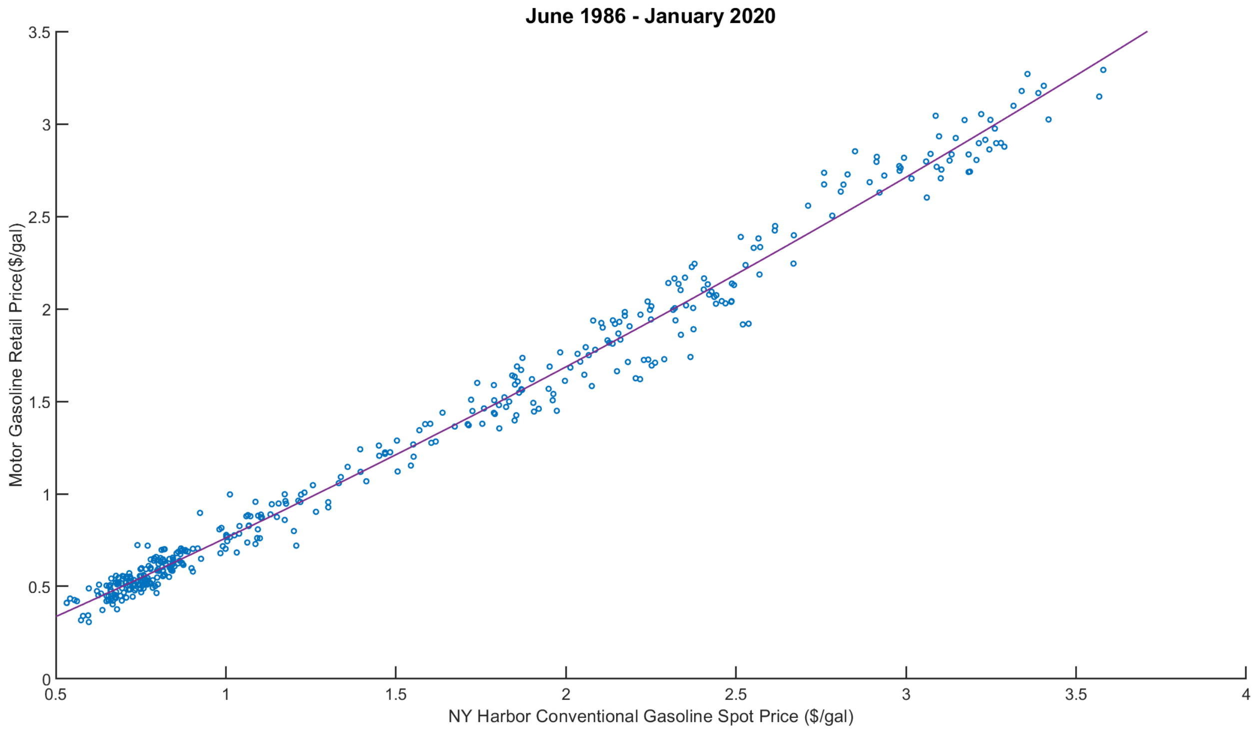

Figure 2.6: Motor Gasoline Retail Price versus NY Harbor Gasoline Spot Price - High Correlation

- 16 renewable energy products are assumed to have constant price over a year (12 months). Since their actual prices become available by the end of the year, until that point the values from the previous year are used. Thus, there is no need for forecasting for these 16 products.

- The prices of the residential distillate fuel oil and residential HGL (propane) are taken from the weekly EIA reports for the heating season (October through March), while for the rest of the year are estimated from their corresponding spot prices using linear regression. The price of NG in transportation sector is also taken from annual EIA reports and the monthly prices are estimated from the Henry Hub NG spot price using linear regression. Thus, there is no need for forecasting for these 3 products. In addition, the price of coal consumed in the residential sector has gone to zero, since no coal is consumed in the residential sector anymore.

- The prices of the industrial asphalt, lubricants that are consumed in industrial and transportation sectors, other petroleum products that are consumed in industrial sector, motor gasoline that is consumed in transportation sector, and coal in commercial and industrial sectors lag 1 month. Thus, the prices of these 7 energy products require forecast for 1 month.

- The prices of the commercial and industrial petroleum coke, and electricity for all four sectors lag 2 months. Thus, the prices of these 6 energy products require forecast for 2 months.

- The prices of the remaining 23 products require forecast for 2 or 3 months depending on the release date of the data.

Therefore, the prices of 36 energy products need to be predicted. The proposed framework takes into account the special attributes of the energy products i.e. seasonality, correlation with spot prices etc., so as to ensure the optimal forecasting ability. Specifically, the prices of 5 products (residential NG, commercial NG, residential electricity, commercial electricity, and industrial electricity) show strong seasonal pattern. Therefore, trigonometric functional form is selected to capture this pattern since it provides accurate forecasting ability for seasonal patterns over time. Moreover, the availability of the spot prices of the commodities up to the present date (without any lag) in addition to the high correlation of the price of energy products with the price of commodities, provide a great platform to accurately forecast prices up to the present date. For this purpose, three different strategies are developed:

1. A pure trigonometric function versus time is fitted for a lookback period of 12 months for the residential NG, commercial electricity, and industrial electricity;

2. A trigonometric function versus time along with a linear function versus the commodity with the largest absolute correlation coefficient is fitted for a lookback period of 12 months for commercial NG, and residential electricity;

3. The commodity with the largest absolute correlation coefficient is selected for a lookback period of 9 months for the remaining 31 products;

The following energy commodities are used within the framework:

1. Crude Oil, WTI Cushing, Oklahoma
2. Crude Oil, Brent Europe
3. Conventional Gasoline, NY Harbor, Regular
4. Conventional Gasoline, US. Gulf Coast, Regular
5. RBOB Regular Gasoline, Los Angeles
6. No.2 Heating Oil, NY Harbor
7. Ultra-Low-Sulfur No.2 Diesel Fuel, NY Harbor
8. Ultra-Low-Sulfur No.2 Diesel Fuel, US Gulf Coast
9. Ultra-Low-Sulfur No.2 Diesel Fuel, Los Angeles
10. Kerosene-Type Jet Fuel, US Gulf Coast
11. Propane, Mont Belvieu, Texas
12. Natural Gas, Henry Hub

The correlation coefficient is calculated using Equation (2.9), as follows:

$$\mu_{m,p} = \frac{\sum_{i=m-L}^{m} C_{p,i}}{L} \tag{2.4}$$

$$\mu_{m,com} = \frac{\sum_{i=m-L}^{m} C_{com,i}}{L} \tag{2.5}$$

where $\mu_{m,p}$ is the average price of product *p* in month *m*, $\mu_{m,com}$ is the average price of commodity *com* in month *m*, and L is the lookback period.

$$\sigma_{m,p} = \sqrt{\left(\frac{1}{L-1}\right) \cdot \sum_{i=m-L}^{m} \left(C_{p,i} - \mu_{m,p}\right)^2} \tag{2.6}$$

$$\sigma_{m,com} = \sqrt{\left(\frac{1}{L-1}\right) \cdot \sum_{i=m-L}^{m} \left(C_{com,i} - \mu_{m,com}\right)^2} \tag{2.7}$$

where $\sigma_{m,p}$ is the standard deviation of product *p* in month *m*, $\sigma_{m,com}$ is the standard deviation of commodity *com* in month *m*.

$$cov_{m,p,com} = \frac{\sum_{i=m-L}^{m} \left(C_{p,i} - \mu_{m,p}\right) \cdot \left(C_{com,i} - \mu_{m,com}\right)}{L-1} \tag{2.8}$$

where $cov_{m,p,com}$ is the covariance of product *p* to commodity *com* looking back from month *m*.

$$\rho_{m,p,com} = \frac{cov_{m,p,com}}{\sigma_{m,p} \cdot \sigma_{m,com}} \tag{2.9}$$

where $\rho_{m,p,com}$ is the correlation coefficient of product *p* to commodity *com* looking back from month *m*.

This procedure is recursively applied at each month for a lookback period of either 9 or 12 months to select the commodity with the most correlated price for each product. Since this calculation is over a lookback period, the commodity with the largest price correlation, *com**, is determined for each product and each month *a priori*.

The general type of the proposed fitted function for the price of each product is given in Equation (2.10):

$$\widehat{P}_{m,p} = a_{m,p,com*} \cdot C_{com*,m} + b_{m,p} + c_{m,p} \cdot sin\big(\frac{\pi}{6}m\big) + d_{m,p} \cdot cos\big(\frac{\pi}{6}m\big) \tag{2.10}$$

For the products whose prices do not show seasonality, the parameters c and d in Equation (2.10) become zero, while for those with strong seasonal prices that are explained by pure trigonometric functions, the parameter a becomes zero.

The solution of the following optimization model provides the values of the parameters a, b, c, and d of each product at each month.

$$\begin{gathered} min \sum_{p} \sum_{m} \sum_{i=m-L}^{m-1} \big(Err_{p,m,i}\big)^2 \\ Err_{p,m,i} = C_{p,i} - \Big(a_{m,p,com*} \cdot C_{com*,i} + b_{m,p} + c_{m,p} \cdot sin\big(\frac{\pi}{6}i\big) + d_{m,p} \cdot cos\big(\frac{\pi}{6}i\big)\Big) \\ \forall i : m - L \leq i < m \end{gathered} \tag{2.11}$$

The results of this optimization model provide the parameters to forecast the price of each product for the upcoming month. For the products that require forecasts for more than one month, the same parameters that are optimized for month m are used.

2.5 Forecasting Results

The accuracy of the proposed forecasting framework is demonstrated in the following sections for the weights of the demands and the prices, as well as for the overall EPIC.

2.5.1 Demand Forecasting Results

The validity of the proposed methodology for the forecasting of the weights of the demands for the energy products is tested over a period of 184 months from January 2006 to April 2021, by comparing the predicted value of the monthly weight of each product's demand with its actual, known value. For this comparison, the sum of the squared forecasting error for each month is computed over the testing period as it is shown in Equation (2.12)

$$PredErr_m = \sum_p (w_{m,p} - \widehat{w}_{m,p})^2 \qquad \forall m \tag{2.12}$$

where $w_{m,p}$ is the actual weight of product *p* in month *m*, and $\widehat{w}_{m,p}$ is the forecast of the weight of product *p* in month *m*.

Table 2.3 summarizes the results in the form of average sum of squared error, minimum sum of squared error and maximum sum of squared error. It should be noted that the number of months to be compared decreases as the year of forecasting increases. For example, the forecasts of the second year require the forecast weights of the first year so there are less actual monthly values to compare.

Table 2.3: Forecasting Results of Weights up to 4 years

Year of Forecasting	Months to Compare	Average Sum of Squares Error	Minimum Sum of Squares Error	Maximum Sum of Squares Error
1st year	184	0.000375	0.000050	0.005166
2nd year	172	0.000455	0.000075	0.005070
3rd year	160	0.000530	0.000128	0.006525
4th year	148	0.000599	0.000180	0.005886

The excellent forecasting ability of the proposed methodology is clearly shown in Table 2.3, since the reported error values are extremely low over a very long period of 184 months. This is better captured when the square root of the average sum of the squared errors is considered, which is 1.94%, 2.13%, 2.30% and 2.45% for the 1st, 2nd, 3rd and 4th year respectively. The very low forecasting error (2.45%) in the case of the 4th year where only unknown (predicted) values have been used is of significant importance. As expected, the average sum of the squared error increases as the year of prediction increases due to the decreasing number of months with known values. The robustness of the forecasting framework is evident even during the COVID-19 pandemic where unprecedented challenges in the energy sector took place. The full list of data for the sum of squared errors of weight forecasts is given in the Appendix C.1.

2.5.2 Price Forecasting Results

In this section, the accuracy of the proposed methodology for the price forecasting of the 36 energy products is evaluated. The average forecasting error for each product is defined in Equation (2.13), by comparing the predicted value of each product's price with its actual, known value over a period of 184 months from January 2006 to April 2021. For this comparison, the average absolute error for each month is computed over the testing period of 184 months.

$$Err_p = \frac{\sum_m |C_{m,p} - \widehat{P}_{m,p}|}{184} \tag{2.13}$$

where $C_{m,p}$ is the actual price of product *p* in month *m*, and $\widehat{P}_{m,p}$ is the forecast of the price of product *p* in month *m*.

Table 2.4 provides a summary of the forecasting results for the different functions and forecasting periods in the form of average absolute error ($/MMBtu). The full list of the results is shown in the Appendix C.2.

As expected, the average forecasting error always increases as the number of forecasting months increases. Hence, the one month ahead forecasting error is lower than the two and three months ahead forecasting error. Furthermore, the two months ahead forecasting error is lower than the three months ahead forecasting error. Moreover, the industrial coal always demonstrates the lowest average forecasting error with 0.069 $/MMBtu, 0.098 $/MMBtu, and 0.125 $/MMBtu respectively. On the contrary, the highest average forecasting error is always illustrated with kerosene which is consumed in the residential, commercial and industrial sectors with 1.868 \$/MMBtu, 2.472 \$/MMBtu, and 2.929 \$/MMBtu respectively.

Table 2.4: Summary of Price Forecasting Results from January 2006 to April 2021

No. of Energy Products	Forecasting Function	Average Abs. Error Ahead (\$/MMBtu)		
		1 month Ahead	2 months Ahead	3 months Ahead
3	Pure Trigonometric (12 months)	0.6587	0.7760	0.8593
2	Trigonometric & Commodity based Linear (12 months)	0.5350	0.7425	0.9170
31	Trigonometric & Commodity based Linear (9 months)	0.9146	1.2107	1.4228

Based on the above findings, the proposed methodology for the forecasting of the prices of the energy products is considered quite accurate and is utilized for the estimation of EPIC up to date. In the following sections, the forecasting framework is expanded utilizing time series forecasting methodologies such as ARIMA, exponential smoothing, as well as advanced machine learning and deep learning techniques, enabling the accurate forecast of the prices of energy products up to 12 months in the future.

Overall, the excellent forecasting ability along with the unique inherent attributes of EPIC capturing both the demands and the prices of the products over the entire energy landscape in the US, render EPIC as the ideal tool for designing, assessing and optimizing various policy decisions of public interest. Four prime, representative policy case studies are presented in the Chapter 4.

2.5.3 Releasing and Adjusting EPIC

By utilizing the accurate forecasting methodology that is presented in the previous sections, the up-to-date value of EPIC can be readily calculated. On the first day of each month, the value of EPIC for the previous month is released. Since the actual weights of the demands and the prices of the energy products are not known until a later time, the initial release of EPIC is going to be a preliminary estimate based on the forecasts of the values of both the weights and the prices. As soon as the actual data of weights and prices of the energy products become available, the value of EPIC will be re-adjusted. Since there is lag in data availability of up to three months, EPIC will be finalized after one initial release and two re-adjustments. Figure 2.7 displays this scheme through two indicative examples.

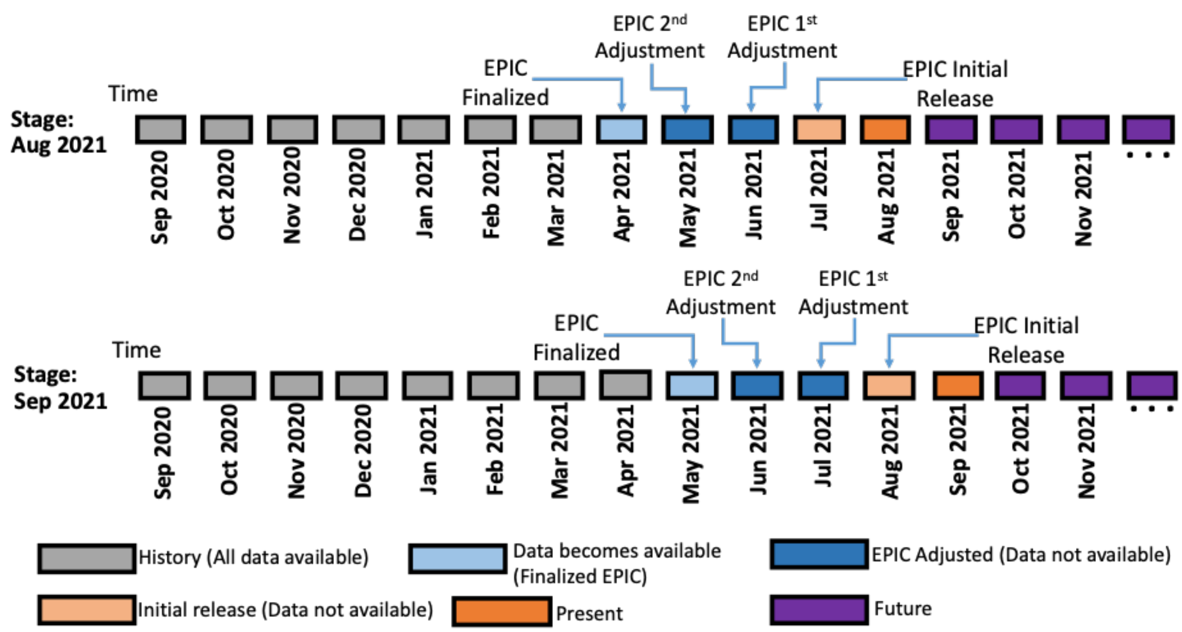

Figure 2.7: Scheme for Releasing and Adjusting EPIC

As of August 2021, EPIC of April 2021 is finalized and the initial release of EPIC for July 2021 is released. At the same time, the forecast for EPIC's value for June 2021 is re-adjusted for the first time, while EPIC's value for May 2021 is re-adjusted for the second time. The same approach is followed for the next month. In particular, having the initial release for July 2021 from the previous month and since more data has become available in the meantime, the value of EPIC for July 2021 will be re-adjusted for the first time. Similarly, the value of EPIC for June 2021 will be re-adjusted for the second time and the value of EPIC for May 2021 will be finalized. The initial release of EPIC for August 2021 will also take place. This scheme guarantees that EPIC is always accurate and up to date.

2.6 EPIC Forecasting Accuracy

The proposed forecasting framework provides accurate forecasts for both demands and prices of the energy products, enabling the up to date estimation of EPIC. Implementing the developed methodology, the EPIC is tracked for a period of 184 months, from January 2006 to April 2021. Apart from the finalized value of EPIC for each month which can be computed once the actual data become available, the initial release as well as the adjusted values of EPIC for each month are presented. The absolute differences between the actual and the predicted values of EPIC are also shown as a demonstration of the accuracy of the developed framework. Table 2.5 summarizes the mean absolute error (MAE) and the mean absolute percentage error (MAPE) of the forecasting framework over the testing period of 184 months.

Table 2.5: EPIC Forecasting Accuracy over 184 months

EPIC Forecasts	**Mean Absolute Error ($/MMBtu)**	**Mean Absolute Percentage Error (%)**
Initial EPIC Release	0.5397	2.778
1st EPIC Adjustment	0.2668	1.402
2nd EPIC Adjustment	0.1952	1.026

As expected, the error decreases once more data become available. The initial EPIC release exhibits the highest error with 0.5397 $/MMBtu and 2.778%, followed by the 1st EPIC adjustment with 0.2668 $/MMBtu and 1.402%. The 2nd EPIC adjustment shows the lowest error with 0.1952 $/MMBtu and 1.026%. It is worth mentioning that both error metrics over a long testing period of 184 months are significantly low, with the MAPE of the initial EPIC being less than 2.8%, while the 2nd EPIC adjustment is just 1.026%. Appendix D.1 demonstrates the actual EPIC values, the three forecasts along with the absolute percentage errors for each month over the testing period of 184 months.

The graphical representation of the actual EPIC along with the three forecasts is shown in Figure 2.8. The last actual EPIC value is on April 2021, and the EPIC values for the next 3 months represent forecasts. May and June 2021 are determined through the 2nd and the 1st adjusted EPIC values respectively, while the initial forecast for July 2021 is released. It can be clearly observed that the distance error between the forecast values (colored markers) and actual EPIC values (blue line) is quite small over this long testing period, and that the monthly forecasts constantly improve once more data become available. Additionally, the forecasting accuracy of the framework improves significantly over time, since more data are used to train the model.

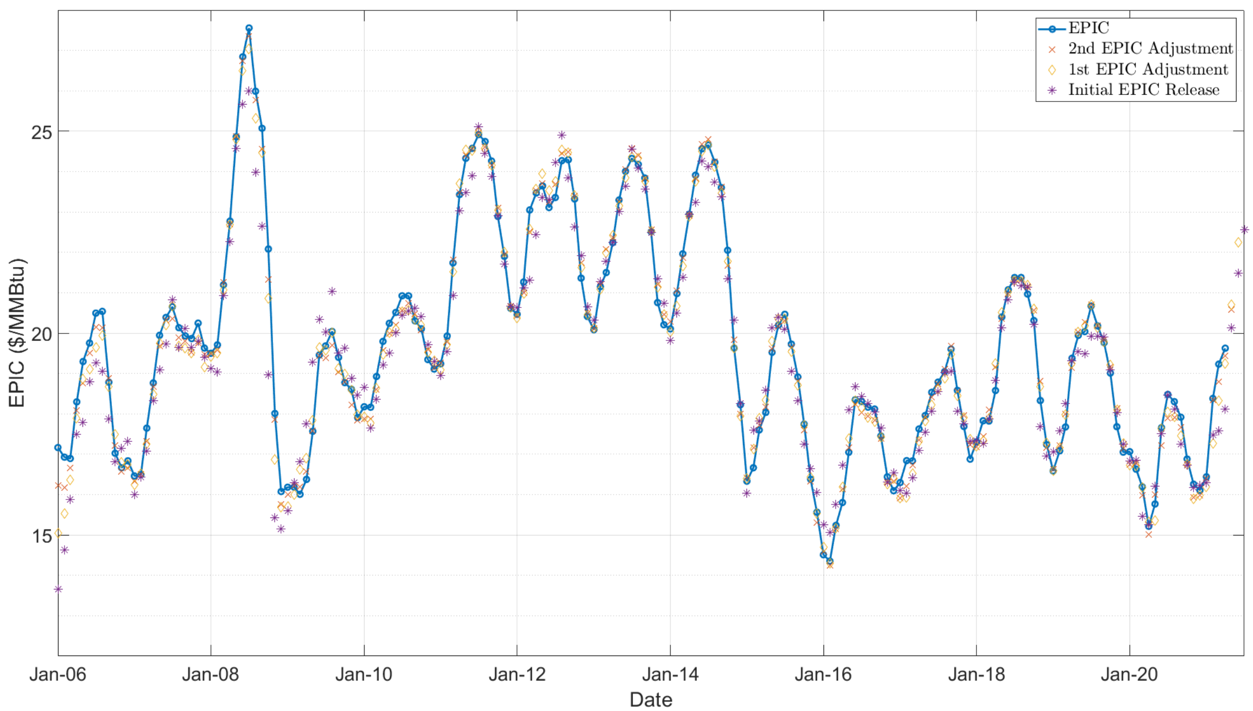

Figure 2.8: Actual EPIC versus its Forecasts

In particular, the absolute percentage error for the initial release of EPIC has been reduced to 2.07% and 2.25% for the last 120 months (May 2011 - April 2021) and 24 months (May 2019 - April 2021) respectively, indicating a substantial improvement from the 4.45% error of the first 24 months (January 2006 - December 2007). In 2020, and despite the extraordinary circumstances due to the COVID-19 pandemic, the absolute percentage error for the initial release of EPIC was just 1.50%, demonstrating the robustness of the developed framework. This forecasting ability within the energy sector is noteworthy.

Figure 2.9 illustrates the values of EPIC from January 2003 to July 2021 in $/MMBtu, with the values of the last three months being forecasts.

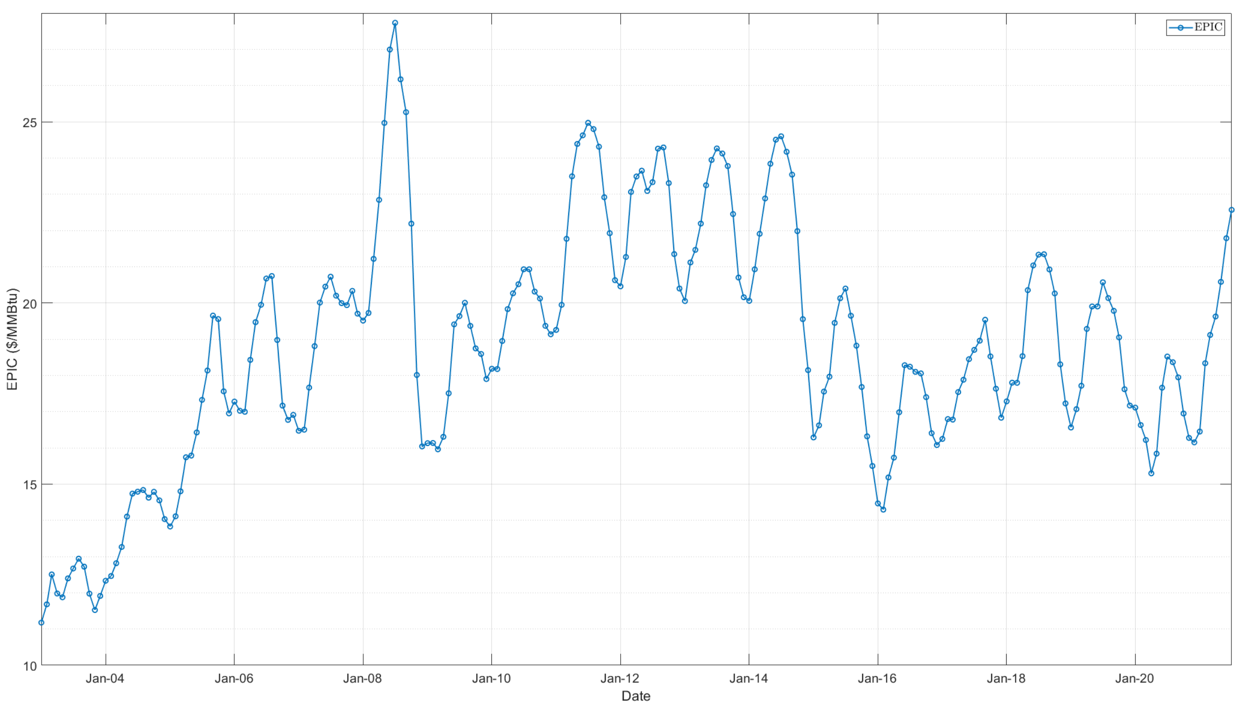

Figure 2.9: Energy Price Index - EPIC

The EPIC framework has been incorporated into a website, Energy Price Index (EPIC) - (https://parametric.tamu.edu/EPIC/), where the users are able to get information about EPIC's methodology and calculation, review historical and predicted data, as well as explore its various functionalities, including different policy case studies and comparison of EPIC and its sub-indices with various established and well accepted financial and economic metrics and benchmarks.

2.7 Expanding EPIC's Forecasting Ability - Time Series Forecasting Framework

The excellent forecasting ability of the developed framework that is presented in the previous sections allows the calculation of the current value of EPIC. The several months lag of data availability on both the key components of EPIC is tackled by the introduced rolling horizon based parameter estimation model that calculates the current value of EPIC. However, the future values of EPIC cannot be forecast under the present framework since the future prices of the energy products cannot be estimated. To this respect, the forecasting framework is expanded with the incorporation of various statistical and machine learning forecasting methods of different nature e.g. Exponential Smoothing, ARIMA, MLP, LSTM etc. Since EPIC consists of 56 different energy products with 33 unique time series data (some energy products share the same time series), the forecasting framework is applied to each one of these univariate time series individually and the forecasting model that demonstrates the most accurate forecasting results over a testing period is then utilized for the future forecasts.

The time series are monthly indexed and have a length between 161 and 425 months. The forecasting horizon is 12 months, therefore the values of EPIC up to July 2022 will be predicted. However, due to the lag in data availability for some of the energy products, the corresponding forecasting horizon for these time series will be 13 or 14 months. The large number of unique time series that needs to be predicted, each of which demonstrates different patterns, trends, cycles and forecasting horizons, introduce major challenges in the forecasting process. Figure 2.10 highlights these unique characteristics on a subset of the time series.

2.7.1 Forecasting of Energy Products' Future Prices

The expanded forecasting framework consists of 7 groups of 40 forecasting methods [94], as it is shown in Tables 2.6 and 2.7. The framework utilizes a variety of statistical and machine learning forecasting methods so as to tackle such a challenging forecasting problem.

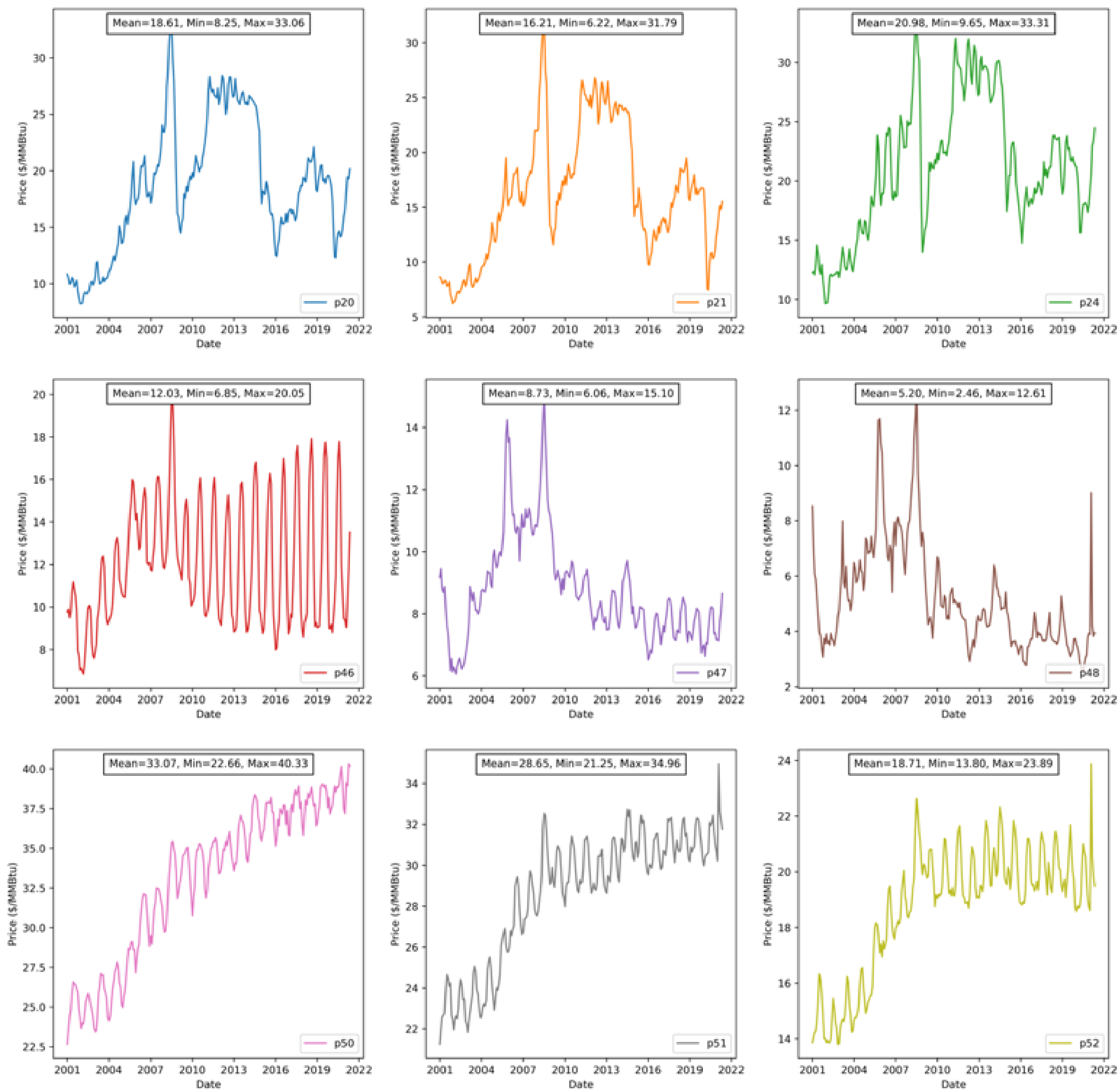

Figure 2.10: Plots of the 9 Energy Products with the Highest Energy Demand over the last 5 years

Table 2.6: Expanded Forecasting Framework for Future Prices

Forecasting Group	Forecasting Method		Description
Benchmark Forecasting	fc1a	Average [95, 96]	forecasts based on the historical mean
	fc1b	Random Walk - Naïve [95, 96]	naïve forecasts equal to the most recent observation assuming a random walk model
	fc1c	Seasonal Naïve [95, 96]	forecasts and prediction intervals from an ARIMA(0,0,0)(0,1,0)m model
	fc1d	Random Walk with Drift [95, 96]	forecasts using a random walk model with drift
	fc1e	Random Walk with Drift Transformed and Bias Adjusted [95, 96]	forecasts using a random walk model with drift, adjusted back Box-Cox transformation
Forecasting with Decom-position	fc2a	Automated STL Decomposition [95, 96, 97]	forecasts with automated STL decomposition
	fc2b	ARIMA Automated STL Decomposition [95, 96, 97]	STL decomposition with ARIMA seasonally adjusted data, returns the reseasonalized forecasts
	fc2c	Naïve Automated STL Decomposition [95, 96, 97]	STL decomposition with Naïve seasonally adjusted data, returns the reseasonalized forecasts
	fc2d	Random Walk with Drift Automated STL Decomposition [95, 96, 97]	STL decomposition with Random Walk model with drift seasonally adjusted data, & returns the reseasonalized forecasts
	fc2e	ETS Automated STL Decomposition [95, 96, 97]	STL decomposition, modeling the seasonally adjusted back Box-Cox transformed data with ETS model, & returns the reseasonalized forecasts
Exponential Smoothing	fc3a	Simple Exponential Smoothing [95, 96, 98, 99]	forecasts using simple exponential smoothing
	fc3b	Holt's Damped Trend [95, 96, 98, 100, 99]	forecasts using Holt's linear damped trend method
	fc3c	Holt-Winters' Additive [95, 96, 98, 101, 99]	forecasts using Holt-Winters' additive method
	fc3d	Holt-Winters' Multiplicative [95, 96, 98, 101, 99]	forecasts using Holt-Winters' multiplicative method
	fc3e	Holt-Winters' Damped Additive [95, 96, 98, 101, 99]	forecasts using Holt-Winters' damped additive method
	fc3f	Holt-Winters' Damped Multiplicative [95, 96, 98, 101, 99]	forecasts using Holt-Winters' damped multiplicative method
	fc3g	ETS [95, 96, 98, 99]	forecasts using Exponential smoothing state space model (Error, Trend, Seasonal)
	fc3h	ETS Transformed Bias Adjusted [95, 96, 98, 99]	forecasts using Exponential smoothing state space model (Error, Trend, Seasonal) with adjusted back Box-Cox transformation
	fc3i	Bagged ETS [95, 96, 102]	forecasts using bagged model with ETS function applied to all bootstrapped series
AutoRegressive Integrated Moving Average (ARIMA)	fc4a	Manual ARIMA [95, 96]	forecasts using manually selected non seasonal & seasonal terms in ARIMA models
	fc4b	Auto.arima Non Seasonal [95, 96]	forecasts using automated non seasonal ARIMA model
	fc4c	Auto.arima Seasonal [95, 96]	forecasts using automated seasonal ARIMA model
	fc4d	Grid Search Arima	forecasts using grid searching for all the Arima model hyperparameters
	fc4e	Grid Search arima	forecasts using grid searching for all the arima model hyperparameters

Table 2.7: Expanded Forecasting Framework for Future Prices

Forecasting Group	Forecasting Method		Description
Advanced Forecasting Methods	fc5a	Dynamic Regression model with Fourier terms [96]	forecasts using dynamic regression model with Fourier terms
	fc5b	TBATS [96, 103]	forecasts using TBATS model (Exponential smoothing state space model with Box-Cox transformation, ARMA errors, Trend and Seasonal components)
	fc5c	Bootstrapping ARIMA [96, 102]	forecasts using Box-Cox and Loess-based decomposition bootstrap ARIMA models
Neural Networks (NN)	fc6a	Feed-forward NN [95, 96]	Feed-forward neural networks with a single hidden layer and lagged inputs
	fc6b	MLP_1 [104, 105]	MLP with 5 hidden layers & 20 training reps
	fc6c	MLP_2 [104, 105]	MLP with 5 hidden layers & 50 training reps
	fc6d	MLP_3 [104, 105]	MLP with 5 hidden layers, 12 autoregressive lags, & 50 training reps
	fc6e	MLP_4 [104, 105]	MLP that uses 20% validation set for the best number of hidden nodes, max set at 8
	fc6f	ELM_1 [104, 105]	ELM with 100 hidden nodes, lasso with CV output weight estimation & 50 training reps
	fc6g	ELM_2 [104, 105]	ELM with 100 hidden nodes, stepwise regression with AIC output weight estimation & 50 training reps
	fc6h	ELM_3 [104, 105]	ELM with 100 hidden nodes, ridge regression with CV output weight estimation & 50 training reps
	fc6i	ELM_4 [104, 105]	ELM with 100 hidden nodes, linear regression output weight estimation & 50 training reps
Grid Search NN	fc7	MLP [106, 107]	MLP model with two hidden layers followed by corresponding dropout layers and a final output layer
	fc8	RNN [106, 107]	RNN model with two hidden layers followed by corresponding dropout layers and a final output layer
	fc9	LSTM [106, 107]	LSTM model with a single LSTM hidden layer, followed by a dropout layer, a dense fully connected layer followed by a dropout layer, and then a final output layer
	fc10	CNN_LSTM_DNN [106, 108, 107]	Hybrid CNN-LSTM model with two convolutional layers for 1D inputs, followed by a pooling and a flatten layer, two LSTM hidden layers, and then a final output layer

Before computing any forecasts, the time series are pre-processed so as to achieve stationarity in their mean and variance, and decomposed so as to extract time series patterns such as trend, seasonality and cycles. This is done using STL decomposition [97], Box-Cox transformation [109, 110], first order and seasonal differencing so as to remove trend and seasonality. The goal is the residuals, $(e_i = y_i - \widehat{y_i})$, to be uncorrelated and have zero mean. The data sets are split into 80% - 20% sets, with the first 80% of the data used for training/validating the models and the last 20% used for testing their forecasting accuracy. Three accuracy measures are used: the Root Mean Squared Error (RMSE), the symmetric Mean Absolute Percentage Error (sMAPE), and the Mean Absolute Error (MAE), and are defined as follows:

$$RMSE = \sqrt{\frac{1}{h}\sum_{i=1}^{h}(y_i - \widehat{y_i})^2} \tag{2.14}$$

$$sMAPE = \frac{2}{h}\sum_{i=1}^{h}\frac{|y_i - \widehat{y_i}|}{|y_i| + |\widehat{y_i}|} \cdot 100\% \tag{2.15}$$

$$MAE = \frac{1}{h}\sum_{i=1}^{h}|y_i - \widehat{y_i}| \tag{2.16}$$

where h is the forecasting horizon, y_i are the actual observations and $\widehat{y_i}$ are the forecasts produced by the model at point i.

The forecasting groups and methods are briefly discussed here. The first forecasting group "Benchmark Forecasting" consists of five methods that are rather simple but quite effective in many cases. They are used to provide a benchmark on forecasting performance against the rest of the forecasting groups which are more advanced and computationally expensive. The second forecasting group "Forecasting with Decomposition" utilizes STL decomposition [97] and then the forecasts of the STL objects are obtained by applying a non-seasonal forecasting method to the seasonally adjusted data and re-seasonalizing using the last year of the seasonal component. The third forecasting group "Exponential Smoothing" [100, 101] consists of nine forecasting methods, where forecasts are weighted averages of past observations with the weights though decaying exponentially for the older observations. A complementary approach to the exponential smoothing is the fourth forecasting group, namely "ARIMA", which combines autoregressive and moving average models, while allows differencing of the data series [111]. Seasonal and non-seasonal ARIMA models, (ARIMA(p,d,q)(P,D,Q)$_{\mathrm{m}}$), are used. Due to the large number of hyperparameters to be determined, grid search is conducted in the last two methods (fc4d, fc4e) and the configuration with the smallest AICc and AIC [96] value respectively is selected. The fifth forecasting group consists of advanced statistical forecasting methods, including dynamic regression and TBATS models [96, 103], along with bootstrapped time series that use the Box-Cox and Loess-based decomposition bootstrap [102]. The last two forecasting groups consist of machine learning methods. In the sixth forecasting group "NN", the hyperparameters of the models are pre-selected, while in the seventh forecasting group "Grid Search NN", a grid search is applied for tuning the hyperparameters. More details about the grid searches are given in Table 2.7. In the last forecasting group, each configuration is evaluated 3 times. The average of these values for each accuracy measure is considered as the final one.

Table 2.7: Hyperparameter Tuning through Grid Search

<table>
<tr><th colspan="2">Forecasting Method</th><th>Description</th><th>Hyperparameters</th></tr>
<tr><td>fc4d</td><td>Grid Search Arima</td><td>Arima function
from the forecast
package in R</td><td rowspan="2">p: order of the autoregressive part, p=[1...5]
d: degree of first differencing involved, d=1
q: order of the moving average part, q=[1...3]
P: order of the autoregressive part (seasonal), P=[1...5]
D: degree of first differencing involved (seasonal), D=[0...1]
Q: order of the moving average part (seasonal), Q=[1...3]
m: number of observations per year, m=18</td></tr>
<tr><td>fc4e</td><td>Grid Search arima</td><td>arima function
from the stats
package in R</td></tr>
<tr><td>fc7</td><td>MLP</td><td>Dense class of Keras API v2.4.3
for Python 3.9 with TensorFlow v2.5.0</td><td rowspan="3">Inputs: # of prior inputs to use as model input, inp=[h, 2h]
Nodes: # nodes to use in the hidden layer, nod=[32, 64]
Dropout rate = [0.1]
Learning rate = [1e-4]
Epochs: # of training epochs, epoch=[250]
Batches: # of samples in each mini-batch, batch=[8, 16]
Differences = [0, 1, h]
Standardization = [True, False]</td></tr>
<tr><td>fc8</td><td>RNN</td><td>SimpleRNN and Dense class of Keras API v2.4.3
for Python 3.9 with TensorFlow v2.5.0</td></tr>
<tr><td>fc9</td><td>LSTM</td><td>LSTM and Dense class of Keras API v2.4.3
for Python 3.9 with TensorFlow v2.5.0</td></tr>
<tr><td>fc10</td><td>CNN_ LSTM_ DNN</td><td>Dense class of Keras API v2.4.3
for Python 3.9 with TensorFlow v2.5.0</td><td>Nodes: # of LSTM units to use in a hidden layer, nodes=[64, 128]
Learning rate = [1e-4, 1e-6]
Epochs: # of times to expose the model to the whole training dataset, epochs=[500, 1000]
Batches: # of samples within an epoch after which the weights are updated, batches=[64]
Sequences: # of sequences within a sample, seq=[3]
Steps: # of timesteps within each subsequence, steps=[12]
Filters: # of parallel filters, filters=[128, 256]
Kernels: # of timesteps considered in each read of the input sequence, ker=[3, 6]</td></tr>
</table>

2.7.2 Future Price Forecasting Results

The first six forecasting groups of the expanded forecasting framework are implemented in R 4.1.0 and solved on an Intel 3.5GHz Quad-Core i7 Processor with 16 GB of RAM, while the last forecasting group is implemented in Python 3.9 and solved on the Atlas cluster, 60TB shared storage, 15 enrgy nodes – dual Xeon E5-2660 v2 processors, 48GB RAM. The forecasting framework is applied to each one of the 33 time series. In each case, the forecasting model with the highest forecasting accuracy based on the three accuracy measures is selected for the future forecasts. If different models result from the accuracy measures, then the following process is followed: i) if the same model results from two accuracy measures, this one is selected, ii) if a different model results from each accuracy measure, then the model that has the highest overall ranking among all three accuracy measures is selected e.g. fc3a: 1st RMSE, 2nd sMAPE, 2nd MAE. In case there is still no clear winner, the model with the lowest RMSE is selected.

Table 2.8 summarizes the forecasting results for the 33 time series, while the detailed results for the configurations of the best models for each energy products and the corresponding accuracy measures are given in Table E.1 in Appendix E. Indicative graphs of the conducted analysis with the historical data, the best selected models and the future forecasts for some of the energy products are shown in Figures E.1 to E.4 in Appendix E.

Table 2.8: Selected Forecasting Models for Future Forecasts

Energy Product	**Selected Forecasting Method**		**Energy Product**	**Selected Forecasting Method**		**Energy Product**	**Selected Forecasting Method**	
p1	fc7	MLP	**p19**	fc9	LSTM	**p45**	fc9	LSTM
p2_5_12	fc9	LSTM	**p20**	fc8	RNN	**p46**	fc8	RNN
p3	fc8	RNN	**p21**	fc9	LSTM	**p47**	fc8	RNN
p4_11	fc7	MLP	**p24**	fc9	LSTM	**p48**	fc8	RNN
p6_13_22	fc7	MLP	**p26_30_37**	fc9	LSTM	**p49**	fc9	LSTM
p7_15	fc8	RNN	**p27**	fc9	LSTM	**p50**	fc10	CNN_LSTM_ DNN
p8_16	fc9	LSTM	**p28_33_34_ 40_41_43**	fc9	LSTM	**p51**	fc4a	Manual ARIMA
p9_17_25	fc8	RNN	**p29_36**	fc7	MLP	**p52**	fc8	RNN
p10	fc9	LSTM	**p31_38**	fc7	MLP	**p53**	fc2d	RW Drift Auto STL Decomp
p14_23	fc9	LSTM	**p32_39**	fc8	RNN	**p55**	fc9	LSTM
p18	fc7	MLP	**p35_42_44**	fc9	LSTM	**p56**	fc9	LSTM

The above results clearly demonstrate the superiority of the last forecasting group "Grid Search NN" over the rest of the forecasting groups, since 31 out of the 33 energy products are modeled more accurately using one of its four forecasting methods. In particular, LSTM is the most commonly used method since it is used for 15 energy products, followed by RNN, MLP and CNN-LSTM-DNN which are used for 9, 6 and 1 energy products respectively. Just two models are modeled from forecasting with decomposition and ARIMA groups. It is worth mentioning, that even without considering the last forecasting group, the NNs of the sixth forecasting group would only be used for 5 out of 33 energy products. This finding highlights the fact that NNs require special attention and tuning before being applied to time series.

Having selected the forecasting models for the prices of the energy products, and since the forecasts of the weights of the demands of the energy products up to four years have already been specified in the previous sections, the forecast of EPIC for the next 12 months can be estimated. Figure 2.11 illustrates the historical values of EPIC from January 2003 to April 2021, along with the future forecasts until July 2022.

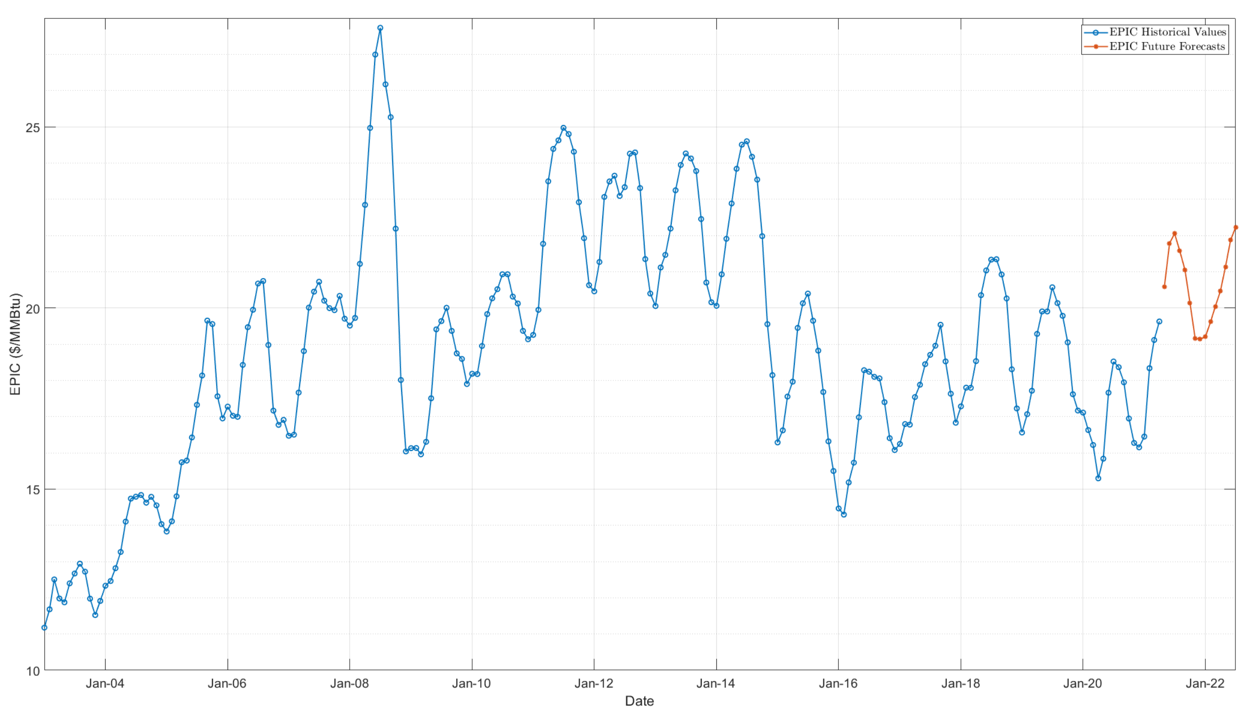

Figure 2.11: Energy Price Index - EPIC with Future Forecasts

2.8 EPIC and its Sub-Indices

Apart from EPIC that covers the whole energy landscape in the US, it would be beneficial to determine the energy prices for each of the end-use sectors. Another advantage of the proposed methodology is the ability to calculate more indices using the existing framework and data. In particular, four new sub-indices, one for each of the individual sectors, that represent the energy prices on each individual sector can be calculated i.e. residential EPIC (REPIC), commercial EPIC (CEPIC), industrial EPIC (INEPIC) and transportation EPIC (TEPIC). The weights of the demands of the energy products are re-normalized considering the products that belong to each sector.

The general formula for the re-normalization of sector S is shown in Equation (2.17):

$$w^S_{m,p'} = \frac{w_{m,p'}}{\sum_{p' \in S} w_{m,p'}} \qquad \forall (m,p) \tag{2.17}$$

where $w^S_{m,p'}$ is the weight of product *p'* in the sector S during month *m*.

As an example, the re-normalization of the residential sector is shown in Equation (2.18):

$$w^R_{m,p'} = \frac{w_{m,p'}}{\sum_{p' \in R} w_{m,p'}} \qquad \forall (m,p) \tag{2.18}$$

where $w^R_{m,p'}$ represents the weight of product *p'* in the residential sector *R* during month *m*. The rest of the sub-indices are calculated accordingly.

Figures 2.12 to 2.15 illustrate the four sub-indices of EPIC.

A couple of interesting findings can be observed from the comparison between EPIC and its sub-indices. In general, the highest prices are observed over the summer months. REPIC and CEPIC show a cyclical pattern over the years due to the seasonality of the products that make up these sectors, while EPIC, TEPIC and INEPIC do not reveal such features. The value of REPIC steadily increases over time, thus the cost of energy for the residential consumers has been increased by \$8.44/MMBtu or 46.04% (average of \$18.34/MMBtu in 2003 to \$26.79/MMBtu in 2020). The value of INEPIC is constantly lower than EPIC and the rest of the sub-indices indicating that this sector has the lowest average monthly cost of energy (about 32% on average less than EPIC). Although the price of INEPIC has been fluctuating over the period of interest, it is

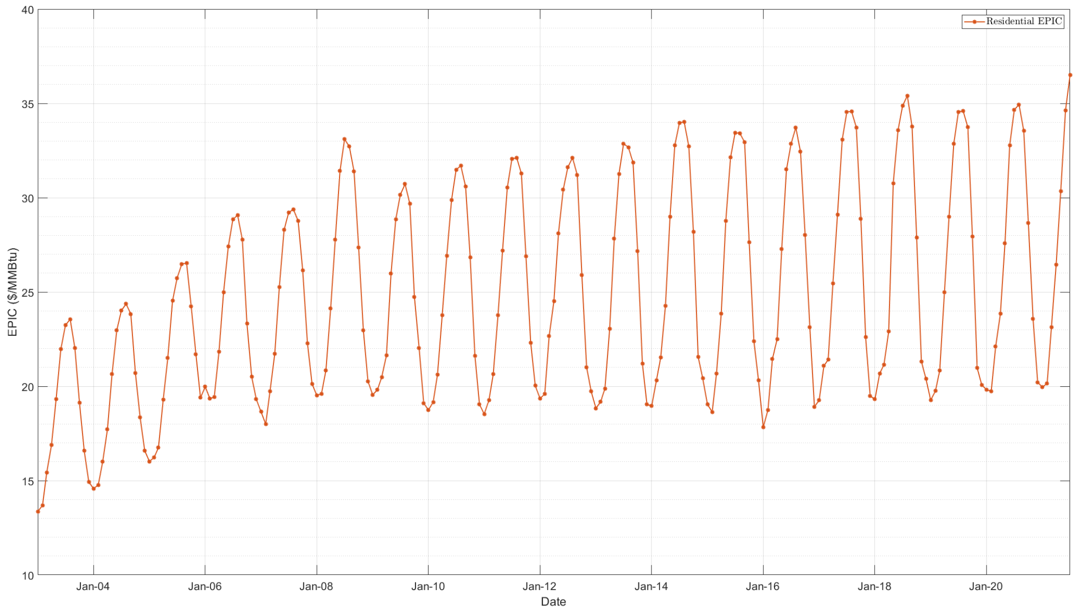

Figure 2.12: Residential Energy Price Index - REPIC

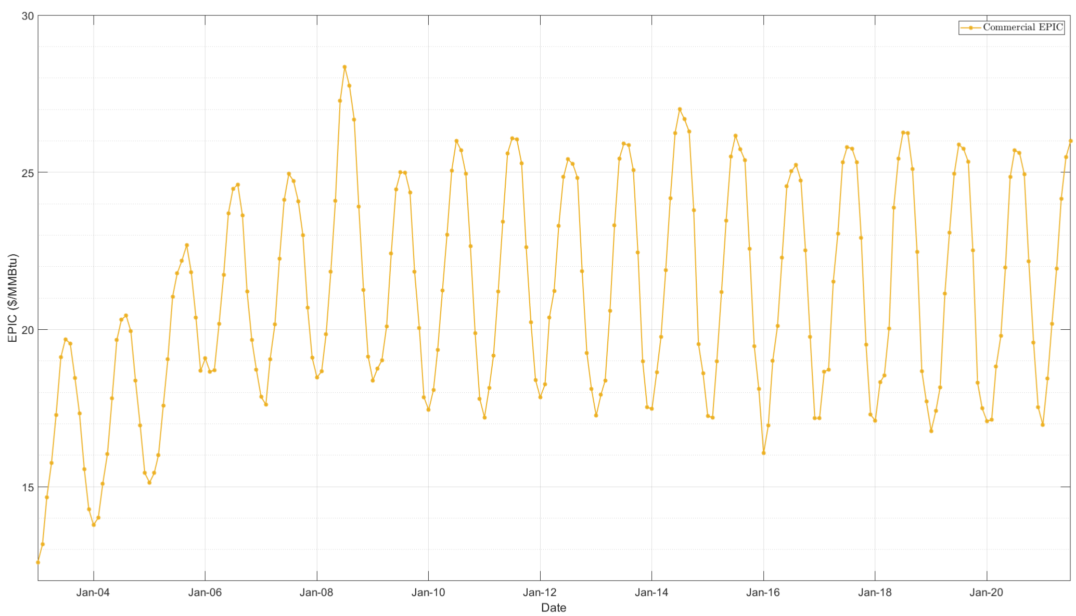

Figure 2.13: Commercial Energy Price Index - CEPIC

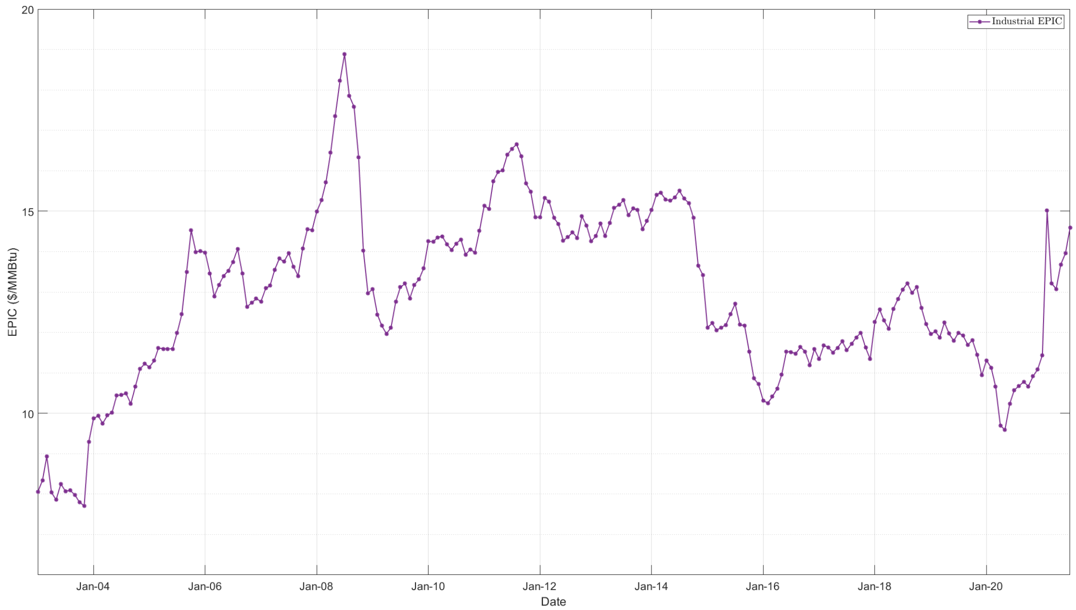

Figure 2.14: Industrial Energy Price Index - INEPIC

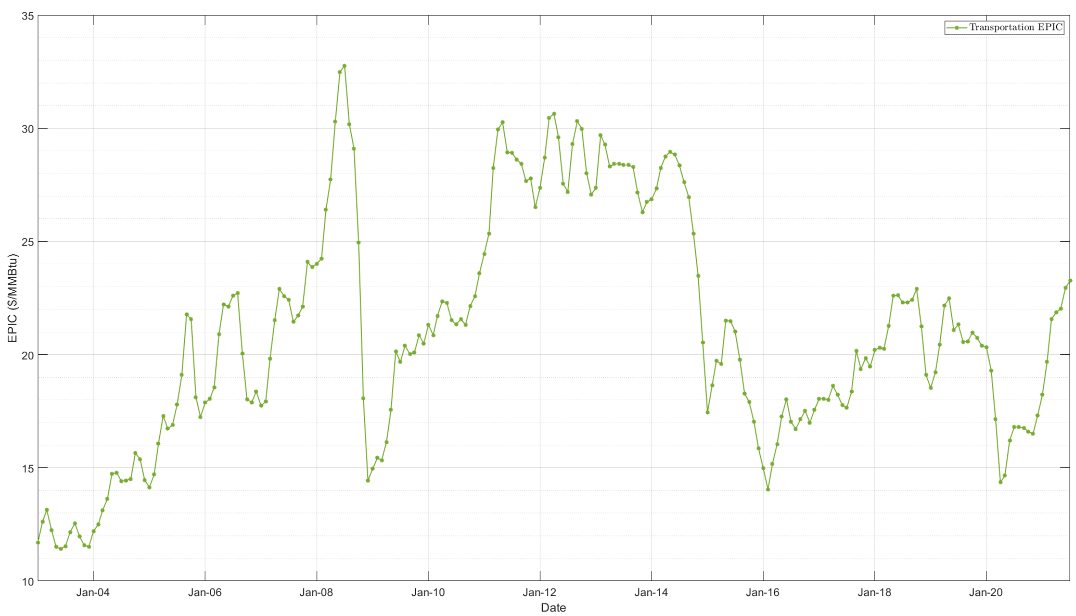

Figure 2.15: Transportation Energy Price Index - TEPIC

the only one that its price today is comparable with its price in 2003. TEPIC constitutes almost 40% of EPIC (basis on demand terms) and the indices demonstrate similar pattern and even similar price range apart from two periods in which the TEPIC was considerably higher: in 2008 due to financial crisis and from 2011 to mid 2014 due to the high oil prices. REPIC demonstrates the highest volatility over this period, followed by CEPIC, TEPIC, EPIC and INEPIC.

Figure 2.16 illustrates the EPIC and the 4 sub-indices in one graph.

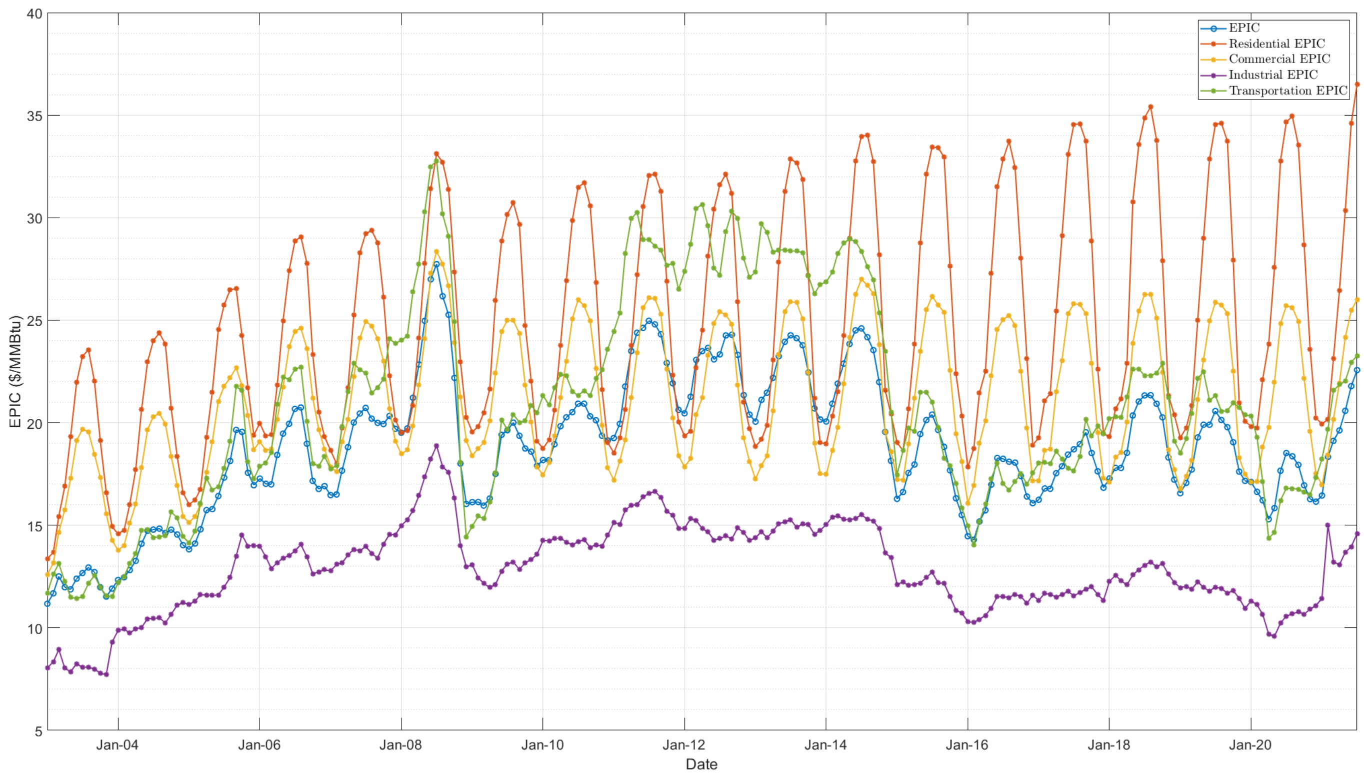

Figure 2.16: EPIC versus the 4 Sub-Indices

2.9 Comparison of EPIC with Economic and Financial Metrics

Having introduced a novel index that capture the price of energy across the energy landscape in the US, and four novel sub-indices that represent the energy prices in the corresponding end-use sector, it is beneficial to compare them against established and well accepted financial and economic metrics and benchmarks. The following figures demonstrate the normalized EPIC and its sub-indices against various normalized such metrics (min-max normalization is used).

Figures 2.17 to 2.19 present EPIC and REPIC against CPI (Consumer Price Index). The CPI represents changes in prices of all goods and services purchased for consumption by urban households [112]. CPI incorporates various energy products, however with an aggregate percentage around 6-7%. As it is clearly seen in Figure 2.17, CPI tends to increase in value over time without being significantly affected by fluctuations in energy prices in comparison to the volatile EPIC. The CPI Energy that is displayed in Figure 2.18 reflects only the changes in the price of all goods and services related to energy and reveals comparable trends and patterns with EPIC. This is particularly true during the ups and downs in 2008-2009, 2015-2016 and 2020-2021. It also seems that CPI Energy lags a couple of months versus EPIC during 2011-2014, and then 2017-2019. Figure 2.19 illustrates REPIC versus CPI Household Energy which measures the price movement of residential energy items used for heating, cooling, lighting, cooking, and other appliances and household equipment. REPIC demonstrates very strong seasonality due to the substantial changes in the weights in the winter (towards natural gas) and in the summer (towards electricity). Since the prices of natural gas and electricity are quite different, peaks are observed over the summer and valleys over the winter in REPIC. CPI Household Energy does not show any seasonality since its weights are fixed over the year, and never reaches the lows of REPIC. However, both reached their highest prices during the last months.

Figures 2.20 to 2.22 depict EPIC against financial metrics. In particular, Figure 2.20 compares EPIC versus S&P500 Energy and two related ETFs. S&P500 Energy is an index comprised of energy companies that belong to the 500 bigger listed companies based on market capitalization. As expected, the three financial indices demonstrate a very similar behavior overtime.

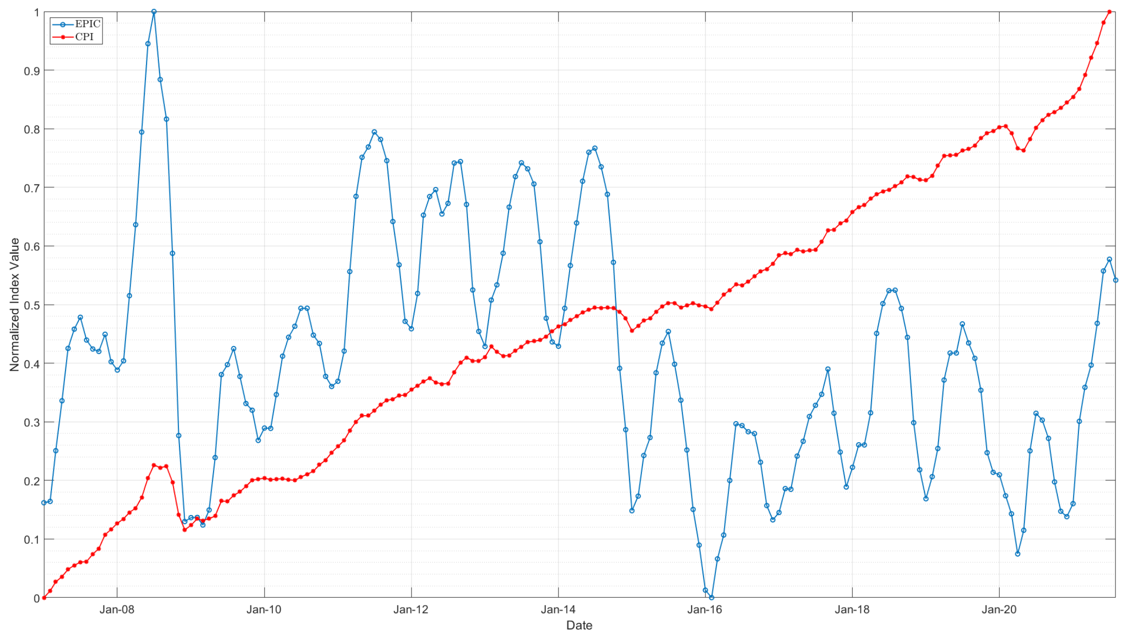

Figure 2.17: EPIC vs CPI

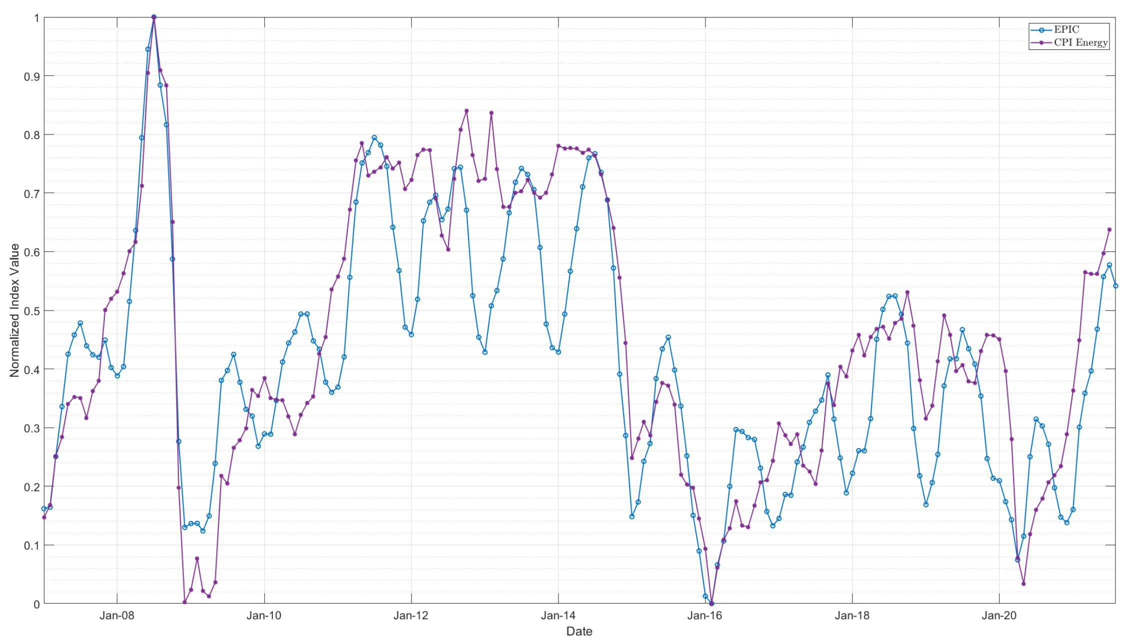

Figure 2.18: EPIC vs CPI Energy

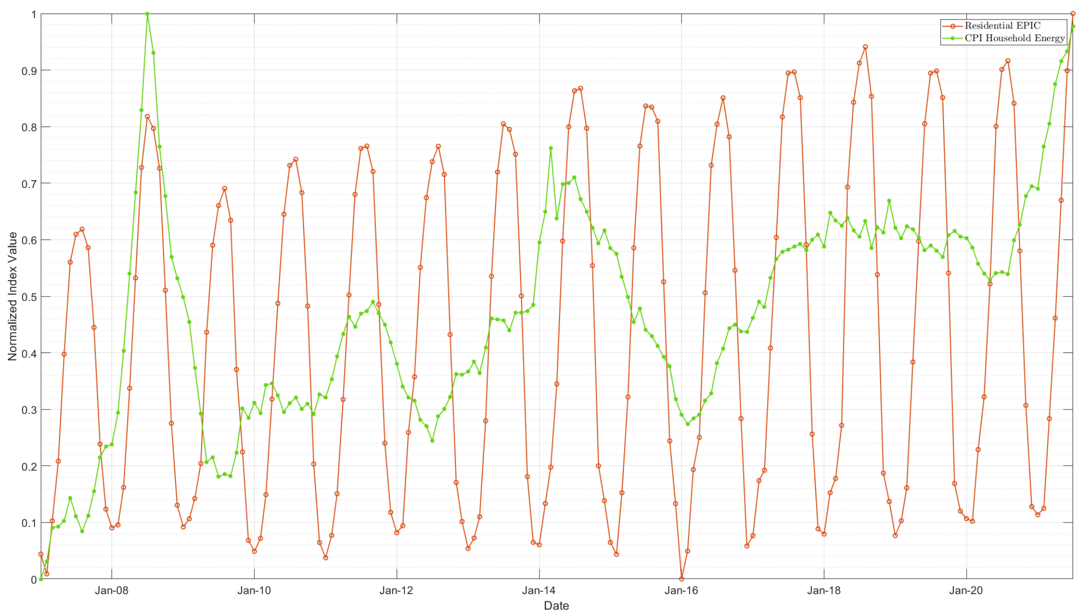

Figure 2.19: REPIC vs CPI Household Energy

In general, EPIC shows lower values than the financial indices, with the exception of its peaks in mid 2008, 2011 and 2021. Similar patterns can be observed over the years, which can be attributed to the fact the EPIC tracks the average price of all energy feedstocks and products while S&P500 Energy tracks the performance of energy companies in the stock market.

Lastly, in Figures 2.23 to 2.25, EPIC is compared against three major energy commodities (spot prices) i.e. WTI crude oil, NY Harbor Regular gasoline, Henry Hub natural gas. The spot prices of NY Harbor Regular gasoline are highly correlated to the spot prices of WTI crude oil, which is attributed to the fact that gasoline is the main product of the crude oil refining. It is clear that EPIC is greatly affected by major fluctuations in the price of oil e.g. late 2008, 2015, 2016, 2020 etc. However, the overall behavior is quite different since EPIC is affected by several other feedstocks and products. Figure 2.25 displays EPIC versus the spot prices of Henry Hub natural gas. There are no clear patterns between the two, except the first period up to 2009. After that initial close correspondence, it seems that the peaks in the price of natural gas coincide with the lows in the price of EPIC, particularly during late 2009-early 2010, early 2012, 2014, 2017, 2018 and 2019.

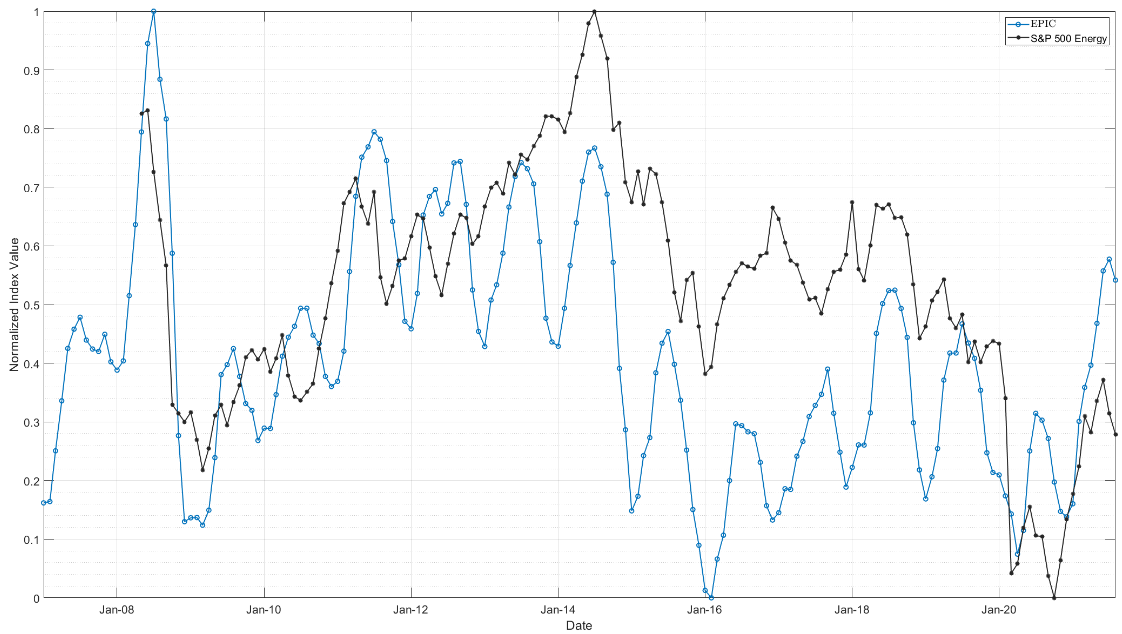

Figure 2.20: EPIC vs S&P 500 Energy

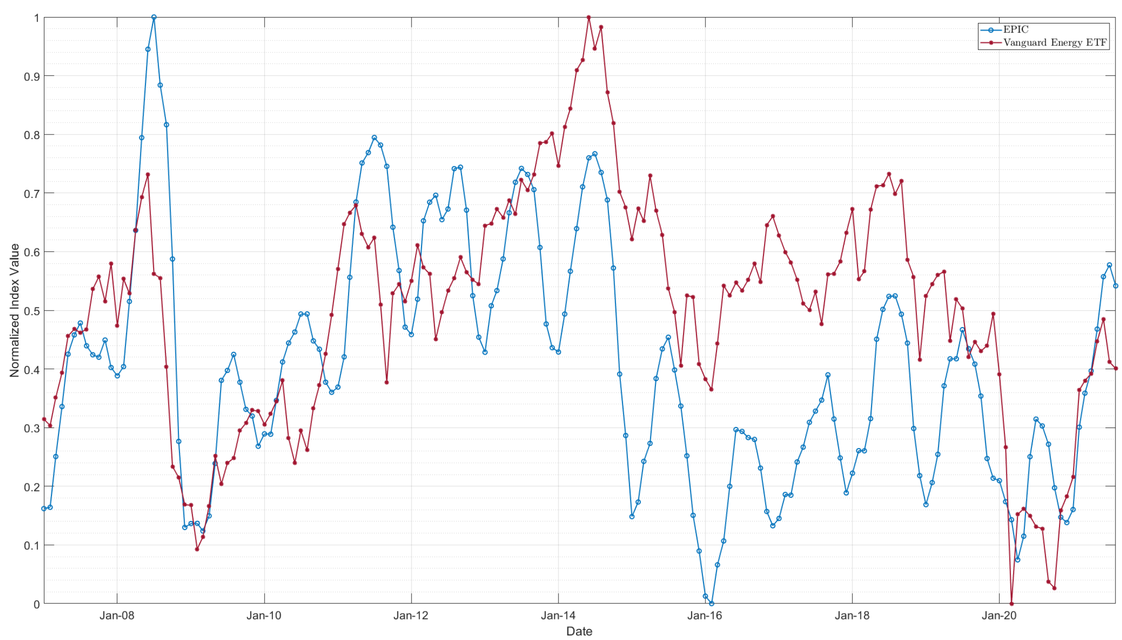

Figure 2.21: EPIC vs Vanguard Energy ETF

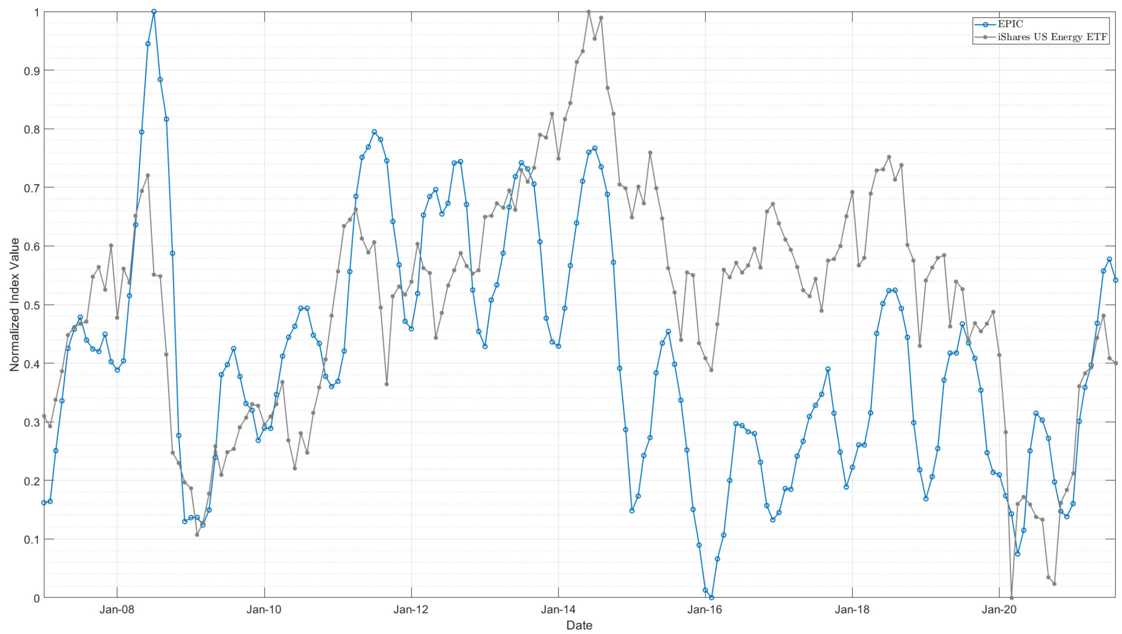

Figure 2.22: EPIC vs iShares US Energy ETF

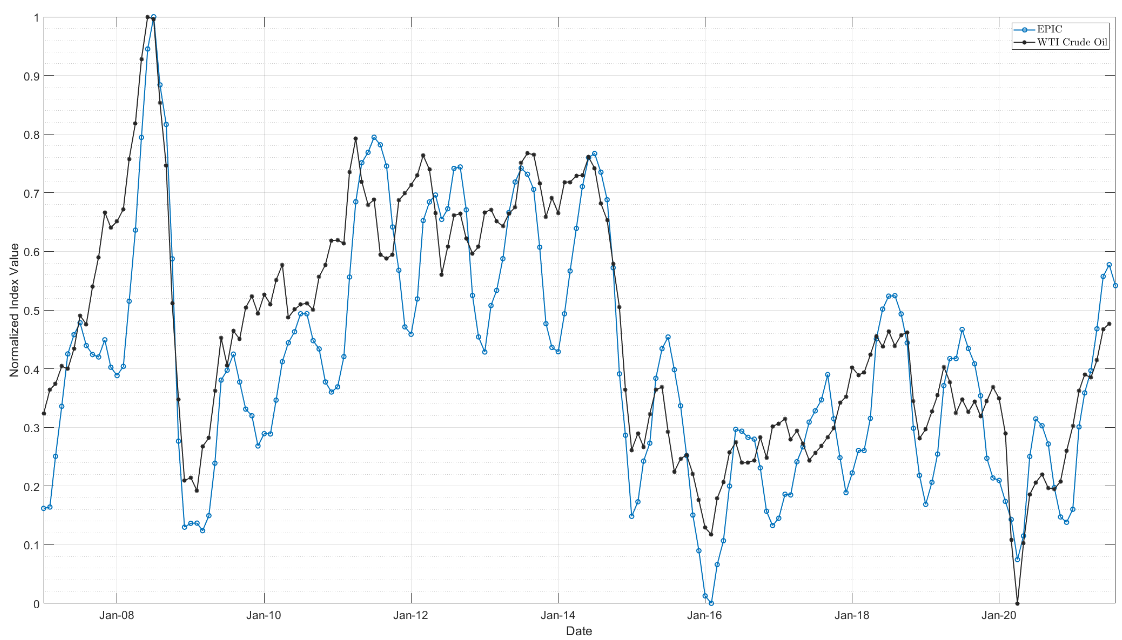

Figure 2.23: EPIC vs WTI Crude Oil

Figure 2.24: EPIC vs New York Harbor Regular Gasoline

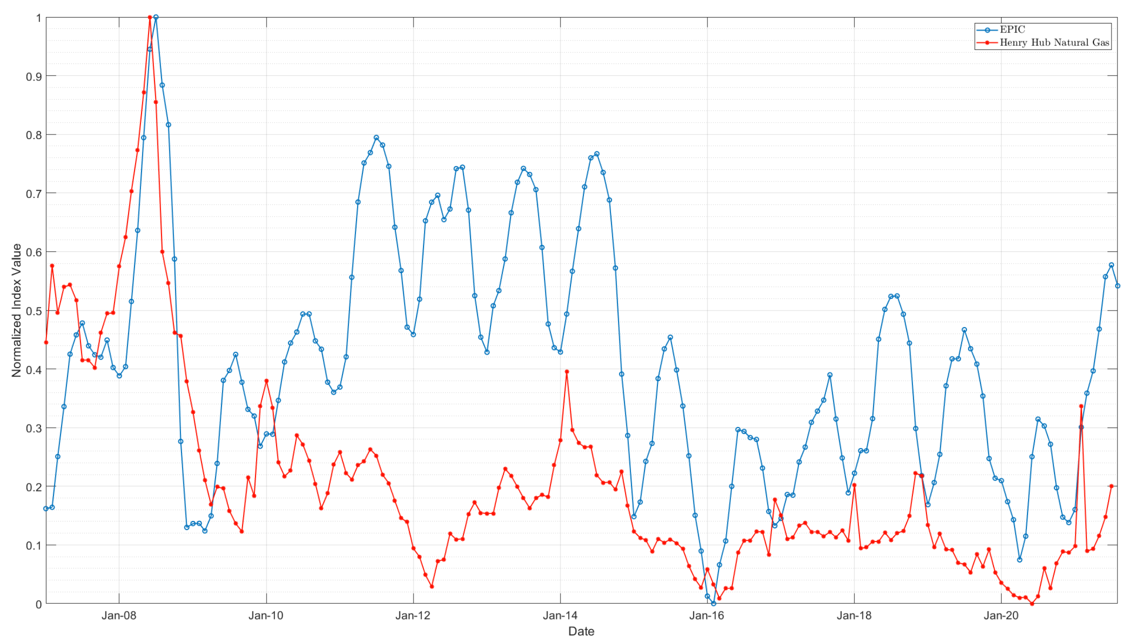

Figure 2.25: EPIC vs Henry Hub Natural Gas

2.10 Conclusion

The Energy Price Index - EPIC, a novel forecasting framework, and its unique attributes have been presented in this chapter. EPIC can be used as the benchmark to calculate the average monthly price of energy to the end-use consumers in the US in units of dollars per million Btu ($/MMBtu). For this study, the complete energy landscape of the Unites States, the four end-use sectors and the intermediate electric power sector have been thoroughly analyzed so as to identify the energy demand and the relevant prices of the energy products that serve as the backbone of EPIC. Four sub-indices are also introduced, one for each of the end-use sectors, capturing the unique characteristics of each sector.

The lag of data availability for the demands and prices of the energy products is overcome with the introduction of a rolling horizon methodology. The forecasting of the demand of the energy products is based on a rolling horizon approach that uses information from the previous three time periods for each month individually, and forecasts the values for the time period of interest. This methodology allows accurate demand forecasting not just for the lagged months, but up to the next 4 years. The validity of this methodology is demonstrated over a long period of 184 months, revealing a considerably low error between the actual and the predictive values. Likewise, a price forecasting function that is based on a time (seasonal) component and a commodity spot price component is developed to forecast the prices of energy products up to the present date. Excellent forecasting ability is also proven here over a period of 184 months, with the average forecasting error varying between $0.069 and $2.929/MMBtu. Before finalized, the monthly values of EPIC are updated three times i.e. Initial EPIC release, EPIC 1st and 2nd adjustment, based on the new information that is becoming available. As such, the mean absolute percentage error for the initial release of EPIC is just 2.778% and decreases to just 1.026% for EPIC's 2nd adjustment.

An expanded forecasting framework comprised of 7 groups and 40 forecasting methods is introduced, enabling the accurate forecast of energy prices for all energy products up to 12 months. Neural Networks, and particularly LSTMs, RNNs and MLPs are the main forecasting methods selected for conducting future forecasts based on three different accuracy measures. EPIC values are therefore predicted until July 2022. EPIC and its sub-indices are also compared against established and well accepted financial and economic metrics, revealing comparable trends and patterns as well as unique behaviors.

Overall, the developed framework allows the accurate estimation of the current and future value of EPIC, and has tremendous potential for applications in the areas of economics, finance, and policy as will be shown in the following chapters.

3. A NOVEL ENERGY FINANCIAL SECURITY: THE ENERGY SPOT PRICE INDEX

3.1 Background & Motivation

In Chapter 2, EPIC is introduced as a novel forecasting framework that accurately quantifies the average monthly price of energy in the US, considering the demand and prices of energy products across the entire energy landscape. However, EPIC cannot quantify the daily market price of energy, or capture the daily price variations of the energy products. Moreover, the available financial instruments used by investors to provide exposure to the energy markets are limited to the equity based stocks i.e. S&P 500 Energy and futures on individual energy commodities i.e. WTI Crude Oil, Henry Hub Natural Gas etc. Furthermore, these options are predominantly associated with the oil and gas sector, with almost zero emphasis placed on renewable energy. Given the lack of a financial security to effectively capture the entire US energy landscape and represent the daily average market price of energy, the Energy Spot Price Index (ESPIC) is introduced.

3.2 Introduction

Having already analyzed the complex energy landscape of the US and identified the products that are directed to the end-use sectors of the US economy in the previous chapters, the total demand of these products along with their corresponding spot prices have become known. This information is used to develop the ESPIC which is defined as the summation of the spot price of each energy product multiplied by its weight fraction as it is computed from its demand. The lag of data availability for the energy demand has been already addressed in Chapter 2, with the introduction of the EPIC predictive framework, while the spot prices of energy products are available up to date on daily basis. However, for the energy products with no spot prices, four different approaches are introduced so as to tackle this issue.

The methodology is tested over a period of 184 months to illustrate the capability of accurately determining the value of ESPIC. The proposed methodology is the first of its kind that precisely quantifies the daily average market price of energy. As such, it can be utilized as a tradable financial security tool i.e. ETF, from investors who look to get exposure to the entire energy market and hedge their investments in diversified portfolios.

3.3 ESPIC Methodology

ESPIC is comprised of the total demand of the energy products that are directed to the end-use sectors in the US along with their corresponding daily spot prices. In the following two subsections, the two key components of ESPIC are discussed in detail.

3.3.1 Demand and Price Determination

The type and the amount of energy products that are consumed from each end-use sector along with the data sources that they are collected from, have been defined in Chapter 2, and their details are provided in Tables 2.1 and 2.2. The same information and data are used to capture the demand of the energy products which is a key element of ESPIC.

The other key element of ESPIC are the spot prices of these energy products. The spot price of a commodity is the price at which it can be bought or sold for immediate delivery [113]. The selection of spot prices to capture the prices of the energy products serves two purposes: first, it provides fungible, negotiable financial instruments that are widely used to reflect the value of energy commodities, and second, the data are available on daily basis without any lag. This allows for the introduction of a tradable energy security. The list of energy commodities with at least one available spot price is shown in Table 3.1, along with the number of products in ESPIC that correspond to each commodity and the average weight of the demand of these products over a period of 220 months, from January 2003 to April 2021. The daily closing prices of the commodities are extracted from Bloomberg terminals on daily basis [114]. Appendix F.1 displays the full list of the commodities with available spot prices.

As it is illustrated in the Table 3.1, the spot prices of 33 out of 56 energy products are readily available, representing on average almost 90% of the total demand of energy. Thus, the remaining 23 energy products that constitute ESPIC cannot be associated with any spot price and are outlined in Table 3.2 along with their aggregate average weight of demand in ESPIC over the same period of 220 months.

Table 3.1: Energy Products with Available Spot Prices

Energy Product with Spot Price	Product No.	No. of Products in ESPIC	Average Weight in ESPIC
Motor Gasoline	7, 15, 24	3	24.12%
Natural Gas	46, 47, 48, 49	4	22.32%
Electricity	50, 51, 52, 53	4	18.19%
Diesel	20	1	8.74%
Kerosene	2, 5, 12, 21	4	4.60%
Distillate Fuel Oil	1, 4, 11	3	3.12%
Coal	54, 55, 56	3	2.75%
HGL (Propane)	3, 6, 13, 22	4	2.35%
Residual Fuel Oil	9, 17, 25	3	1.22%
Ethanol	35, 42, 44	3	1.28%
Bio-Diesel	45	1	0.18%
Total	-	**33**	**88.87%**

Table 3.2: Energy Products with Non-Available Spot Prices

Energy Product with No Spot Price	Product No.	No. of Products in ESPIC	Average Weight in ESPIC
Other Petroleum Products	18	1	3.91%
Asphalt and Road Oil	10	1	1.40%
Petroleum Coke	8, 16	2	1.05%
Lubricants	14, 23	2	0.40%
Aviation Gasoline	19	1	0.04%
Wood / Biomass / Waste	28, 33, 40, 34, 41, 43	6	3.98%
Solar Energy	27, 31, 38	3	0.24%
Geothermal Energy	26, 30, 37	3	0.08%
Hydroelectric Energy	29, 36	2	0.03%
Wind energy	32, 39	2	0.002%
Total	-	**23**	**11.13%**

The unavailability of spot prices for these energy products is addressed with four different approaches:

Approach 1: The weights of the demands of the 23 products with non-available spot prices are neglected, and the weights of the remaining 33 products are re-normalized to add up to 1.

Approach 2: For the 23 products with non-available spot prices, the average monthly prices from EPIC are used.

Approach 3: The 23 products with non-available spot prices are divided into two categories: the fossil fuel-based products and the renewable-based products. The average monthly prices from EPIC are used for the 7 fossil fuel-based products with non-available spot prices i.e. Petroleum Coke, Asphalt and Road oil, Lubricants, Other Petroleum Products, and Aviation Gasoline. The prices for the remaining 16 renewable products are calculated from the renewable energy certificates (RECs) [115, 116].

Approach 4: Similarly to Approach 3, the 23 products with non-available spot prices are divided into two categories: the fossil fuel-based products and the renewable-based products. The spot prices of Kerosene are used for Aviation Gasoline since there is high correlation between the two products. For the remaining 6 fossil fuel-based products, the spot prices of the most correlated commodity are used. In particular, the absolute correlation coefficients of the average monthly prices of each of these 6 fossil fuel-based products with the spot prices of each commodity are calculated, and the pair energy product - commodity with the highest absolute correlation coefficient is selected. Then, the spot prices of the commodity are assigned to its paired energy product. Table 3.3 summarizes the results of the energy product - commodity pairing, and the corresponding absolute correlation coefficients. For the 16 renewable-based products, their average monthly prices are used as per Approach 2.

Table 3.3: Energy Product - Commodity Correspondence based on Correlation of Monthly Prices

Energy Product with NO Spot Price	Commodity with Spot Price	Abs Correlation Coefficient
Other Petroleum Products	NYH Gasoline 83.5 Octane CBOB	0.96
Asphalt and Road Oil	NYH Jet Fuel 54 Prompt Spot	0.81
Petroleum Coke	Bloomberg Low Sulfur Compliance Coal/Big Sandy Barge Fob	0.69
Lubricants	Henry Hub Natural Gas	0.73

A REC is a market based instrument that represents the property rights to the environmental, social and other non-power attributes of renewable electricity generation. It is issued once one megawatt-hour (MWh) of electricity is generated and delivered to the electricity grid from a renewable energy source [116]. It is a tradable market instrument that is used in both compliance and voluntary markets so as to track and quantify the environmental and social benefits of generation and use of the renewable energy [117]. RECs can be sold either unbundled (separate from electricity) or bundled (included with the sale of electricity) [115]. RECs are not necessarily tied to the actual delivery of electricity, and can be considered as the premium of producing renewable energy. For this context in Approach 3, the overall average premium is taken at \$0.019/kWh [118], which is added on top of the price of electricity for the calculation of the price of the 16 renewable energy products, as it is shown in Equation (3.1). A representation of the electricity generation market is shown in the Figure 3.1 [119].

$$r_{renewable} = r_{elec} + r_{rec} \tag{3.1}$$

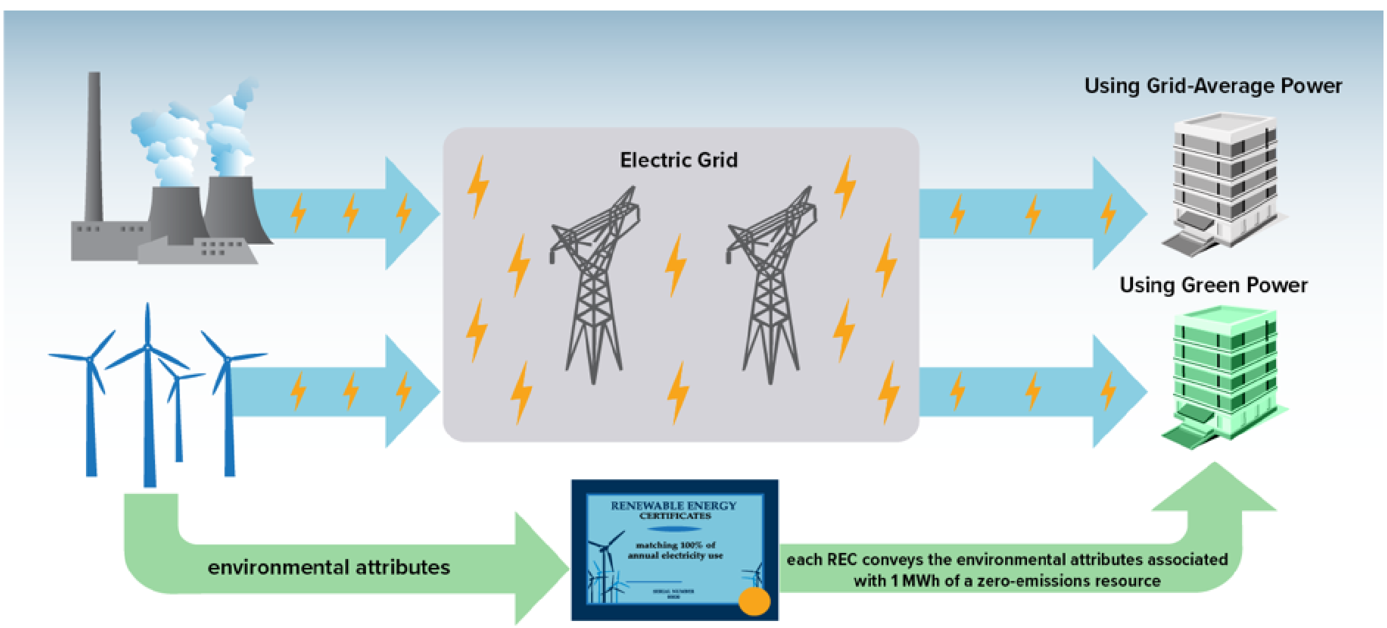

Figure 3.1: Representation of the Electricity Generation Market

3.3.2 ESPIC Calculation

ESPIC represents the daily average market price of energy in the US, and as such is defined as the summation of the spot price (in \$/MMBtu) of each product multiplied by the weight fraction of the demand of each product. The unit of ESPIC is \$/MMBtu.

Using the demands of the 56 energy products as defined in Chapter 2, the real weight fraction based on the demand of each energy product is calculated using Equation (2.1):

$$w_{m,p} = \frac{D_{m,p}}{\sum_p D_{m,p}} \qquad \forall (m, p) \tag{2.1}$$

where $w_{m,p}$ is the weight fraction of product *p* in month *m*, and $D_{m,p}$ is the demand of product *p* in month *m*.

Since by definition, ESPIC represents daily values, the daily weight fraction of each product is calculated from its monthly weight fraction, assuming that the monthly weight fraction is constant on daily basis. Thus, for a given month *m*, all daily weight fractions $w_{d,p}$ are equal.

The mathematical formulation of ESPIC is presented in Equation (3.2):

$$ESPIC_d = \sum_p w_{d,p} \cdot C_{d,p} \qquad \forall d \tag{3.2}$$

where $ESPIC_d$ represents the value of ESPIC on day *d*, and $C_{d,p}$ represents the spot price of product *p* on day *d*.

The ESPIC can also be calculated on monthly basis, using Equation (3.3):

$$ESPIC_m = \sum_p w_{m,p} \cdot C_{m,p} \qquad \forall m \tag{3.3}$$

where $ESPIC_m$ represents the value of ESPIC in month *m*, and $C_{m,p}$ represents the spot price of product *p* in month *m*.

As it has been discussed in the previous sections, the data availability of the demand of energy products normally exhibit a lag between two to three months. This is true for EPIC since the monthly value of EPIC is released on the first day of each month and refers to the previous month. For example, the value of EPIC for January is released on February 1st. But this is not the case for the daily ESPIC, since it is released on daily basis. Thus, the lag of data for the demand of energy products increases to four months. This issue is addressed by taking advantage of the excellent forecasting ability of the framework that is presented in section 2.4.1 and refers to the forecasting of the demands of energy products up to 4 years (48 months) [120]. The accuracy of the first year's forecasts that is of interest for the case of ESPIC are shown in Table 3.4.

Table 3.4: Weight Forecasting Results for the 1st Year

Year of Forecasting	Months to Compare	Average Sum of Squares Error	Minimum Sum of Squares Error	Maximum Sum of Squares Error
1st year	184	0.000375	0.000050	0.005166

3.4 ESPIC Figures

ESPIC is calculated for a period of 184 months, from January 2006 to April 2021, using the methodology with the four different approaches that is presented earlier in the chapter.

Approach 1 is used as the benchmark for comparison against the other three approaches.

Figure 3.2 demonstrates the values of ESPIC on a daily basis for all four approaches. The high spikes that are observed are caused by increases in electricity prices. These spikes are greater in the third approach where the prices of the renewables are estimated as the sum of the electricity prices and an average premium of RECs. The first approach shows the lowest prices of energy in comparison to the other three approaches over the 15-year period. On the contrary, and apart from the days with the sharp spikes, the second approach reveals higher energy prices in comparison to the other three approaches over the testing period.

The average prices of ESPIC over this period are shown in Table 3.5. It is worth mentioning that the current prices of energy are significantly reduced in comparison to those of the past 15 years. Specifically, the average value of ESPIC in 2021 (up to April 21st) is between 24.49% and 28.40% lower than the average value of ESPIC over the last 15 years (January 2006 to December 2020), depending on the selected approach.

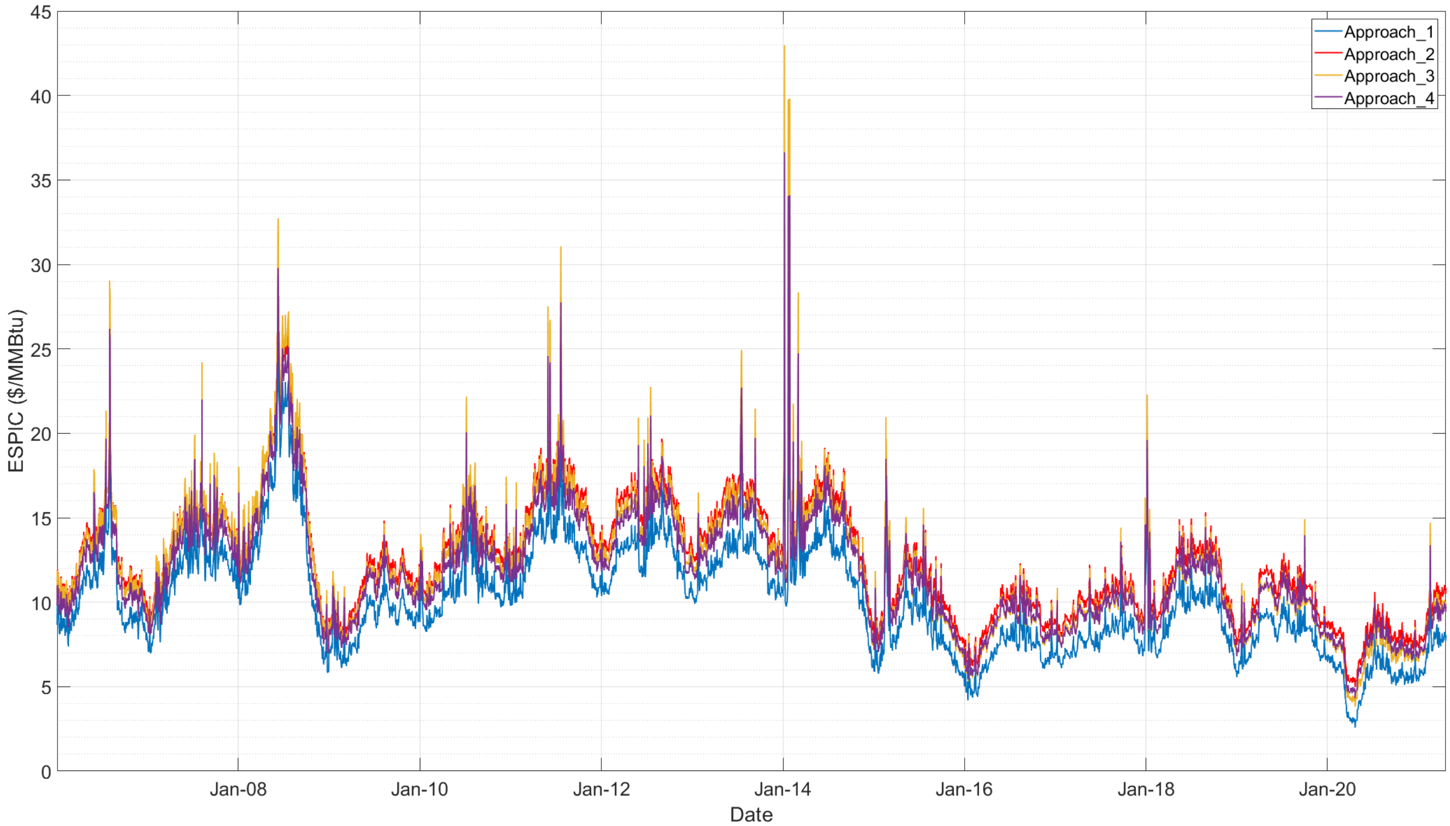

Figure 3.2: Daily Energy Spot Price Index - Daily ESPIC

Table 3.5: Comparison between Historical and Current Prices of ESPIC

Approach No.	**Average of ESPIC from 2006 to 2020 ($/MMBtu)**	**Average of ESPIC in 2021 ($/MMBtu)**	**Percentage Difference (%)**
Approach 1	10.234	7.327	-28.40
Approach 2	12.746	9.624	-24.49
Approach 3	12.263	8.953	-26.99
Approach 4	11.846	8.805	-25.67

Figures 3.3 to 3.5 present the values of ESPIC with different data indexing.

In particular, Figure 3.3 illustrates the values of ESPIC on a weekly basis for all four approaches. The high spikes are still observed, however the period is much shorter due to the weekly indexing of the data. Similarly, Approach 2 tends to have higher energy prices over the 15-year period. Approach 4 used to have lower energy prices than the other two approaches (2 & 3) until 2018. But, over the last three years the price difference between Approach 3 and 4 has been reduced. This is mainly because the electricity prices have shown a steep downward trend this period, directly affecting the REC prices of the renewables in Approach 3. On the contrary, the prices from EPIC that are used for the renewables in Approach 4 are independent of the electricity prices, and have declined moderately. Approach 1 is still the one demonstrating the lowest energy prices.

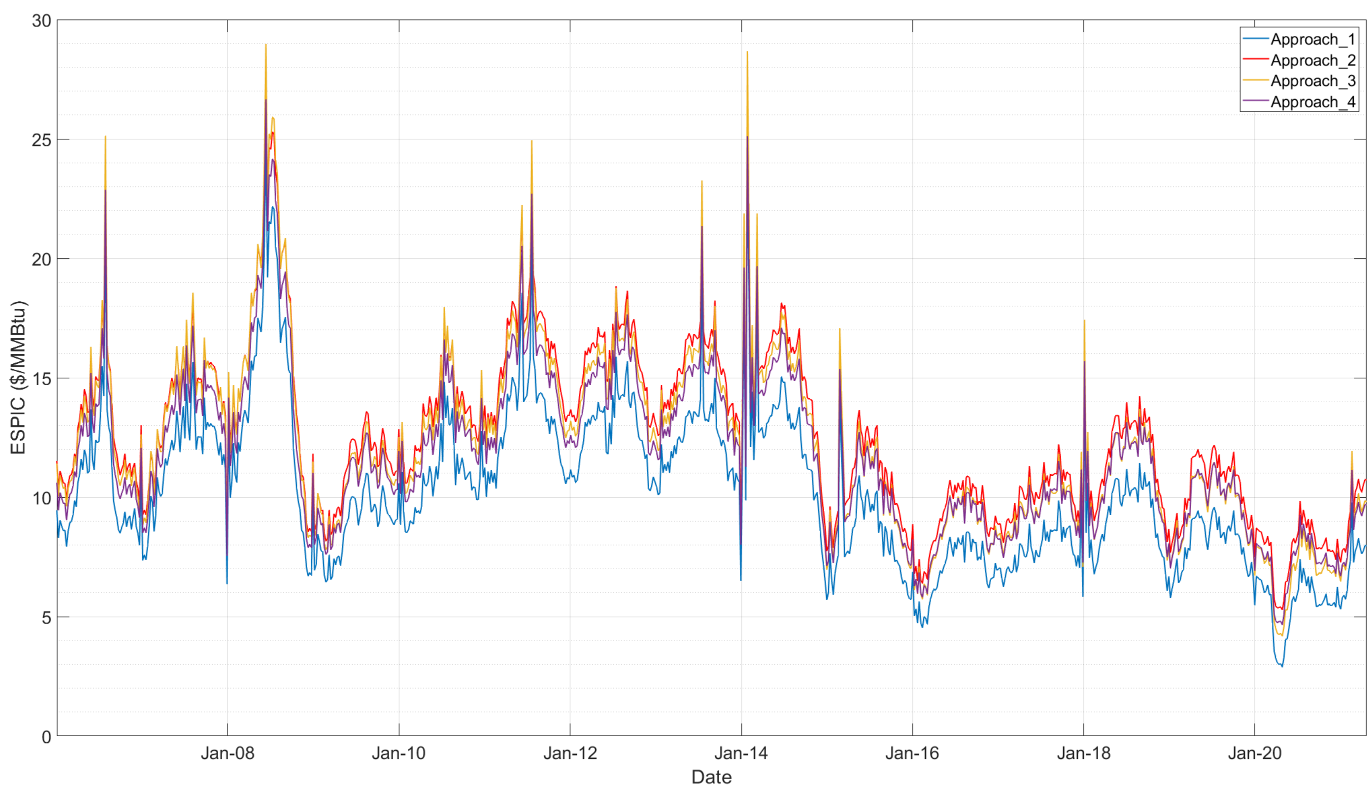

Figure 3.3: Weekly Energy Spot Price Index - Weekly ESPIC

Figure 3.4 displays the values of ESPIC on a monthly basis for all four approaches. The fluctuations become even smoother in comparison to the daily and weekly figures, due to the monthly indexing of the data. Approaches 2 and 3 result in higher energy prices due to the more expensive products (i.e. renewables). However, the drop in electricity prices the last couple of years has affected the prices of the renewables in Approach 3 (i.e. REC), decreasing the price difference between Approaches 3 and 4. Overall, Approach 2 shows the highest prices, apart from the periods of surging electricity prices which cause the spikes in the prices of Approach 3.

Figure 3.4: Monthly Energy Spot Price Index - Monthly ESPIC

Finally, Figure 3.5 depicts the values of ESPIC on an annual basis for all four approaches.

Approach 1 and 2 show the lowest and the highest prices of energy over the 15-year period respectively, while the price difference between Approach 3 and 4 decreases over time. In this figure, it is even more evident that the current energy prices are at the lowest point in the testing period. There is substantial decrease in the energy prices from 2018 on-wards, with the prices of 2020 for all four approaches being at their lowest levels.

Figure 3.5: Annual Energy Spot Price Index - Annual ESPIC

3.5 Conclusion

Energy Spot Price Index - ESPIC is a novel framework that is able to capture the entire US energy landscape and represent the daily average market price of energy, in units of dollars per million BTU ($/MMBtu). The two key factors of this framework are the total demand of the energy products that are directed to the end-use sectors along with their corresponding spot prices. The spot prices allow the estimation of the daily market price of energy without any lag, and at the same time they provide a fungible, negotiable financial reference to capture the value of energy commodities. These two features are essential in the establishment of ESPIC as a novel tradable financial security.

Taking advantage of the thorough analysis that has been conducted for the four end-use sectors and the intermediate electric power sector in the US economy, the demand of energy in the US has been carefully counted. The spot prices of the energy products are extracted from Bloomberg or estimated using four different approaches. The lag of data availability for the case of energy demand is increased to four months. This issue is overcome with the utilization of the forecasting framework that is introduced in Chapter 2 and is based on a rolling horizon approach that trains each month individually using information from the previous three time periods, to forecast the values for the time period of interest. The accuracy of the developed methodology is tested over a period of 184 months, demonstrating excellent forecasting results up to 48 months. This enables the estimation of the up-to-date value of ESPIC on daily basis.

Being composed of spot prices of commodities, ESPIC can be considered as a tradable index in the stock market and used as a tradable financial security for investors who look for exposure to the entire energy landscape, and as a benchmark for measuring the overall cost of energy in the US. Nevertheless, the future values of ESPIC cannot be calculated without the future prices of the commodities that are used within the framework. Therefore, the expanded forecasting framework that is presented in Chapter 2 can be utilized to forecast the future prices of these commodities individually as well as the future prices of ESPIC as a whole.

4. APPLICATIONS OF THE NOVEL FORECASTING FRAMEWORK † *

4.1 Background & Motivation

Energy prices in many countries do not reflect environmental degradation, notably climate change, air pollution and various health related side effects, so targeted fiscal policies should be designed and applied to address this issue [121]. In addition, there is an imbalance in the countries' fiscal objectives with excessive emphasis being put on general income, payroll and consumption taxes and limited emphasis on use of energy taxes. Nevertheless, environmental charges on fuel and energy use have a powerful incentive effect on economic behavior for different reasons [122]. First, they are the most effective at exploiting opportunities of reducing harmful health and environmental side effects. Second, they achieve environmental protection at the lowest overall cost to the economy. Third, they strike the right balance between environmental benefits and costs [122]. Moreover, by setting appropriate charges on energy use, other taxes could be cut. Thus, the environmental, health and fiscal benefits are enhanced. Therefore, a tax reform towards energy-intelligent taxes is required. These policies are designed and imposed based on quantitative, dynamic and holistic analyses, taking into account environmental, economic and social objectives. The ability to generate accurate forecasts considering various what-if scenarios is another key characteristic of energy-intelligent tax policies.

To support this argument, a recent publication from the World Bank [123] suggests that well-designed environmental tax reforms can mitigate climate change while raising well-being, having positive effects on poverty and equity, and enabling countries and firms to become more climate

*Reprinted from "A framework to predict the price of energy for the end-users with applications to monetary and energy policies" by S.G. Baratsas, A.M. Niziolek, O. Onel, L.R. Matthews, C.A. Floudas, D.R. Hallermann, S.M. Sorescu, E.N. Pistikopoulos, Nature Communications, 2021, Vol. 12, number 1, pp 1-12, with permission from Nature Publishing Group and Copyright Clearance Center. A summary of the work is given in Chapters 2 and 4 with additional details provided in Appendices B, C and G.

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resilient and productive. Consequently, fiscal and monetary policies shall be leveraged to drive climate action. Thus, it becomes crucial to accurately quantify the "price of energy" and understand the effects that fiscal and monetary policies will have in energy.

4.2 Introduction

In Chapters 2 and 3, the novelty and the uniqueness of the proposed forecasting framework are presented. In this chapter, the effectiveness of this framework in assessing, designing and optimizing various policy rules and questions is demonstrated by addressing four contemporary policy questions that have raised substantial public and governmental interest. Specifically, the effects of a gasoline tax hike (up to 25 cents per gallon) on EPIC as well as the effects of different forms of a carbon tax on EPIC are investigated [124]. Moreover, the effects of a crude oil tax (up to $25 per barrel) on EPIC are demonstrated. Finally, the effects of renewable energy production targets and subsidies on energy consumers are examined parametrically over a wide range of different weights of the energy feedstocks, as well as for tax credits ranging from 0 to 9 $/MMBtu. For all policy questions, the expected change in the price of energy along with the environmental impact under different scenarios is estimated both for the past i.e. what would have happened, as well as for the future i.e. what will happen. Also, the generated revenue or the budget required for the implementation of each scenario is calculated, taking advantage of the powerful forecasting ability and flexibility of the proposed methodology. The high level of granularity of the framework allows for the estimation of the financial burden per household for each of these policies. It is important to note that these are just four of the potential applications while several other policy questions related to energy can be investigated. At the same time the analysis of the policy questions can be further extended thanks to the capabilities of the proposed framework.

4.3 Policy Case Study for Federal Gasoline Tax

The federal gasoline tax has remained unchanged at 18.4 cents per gallon[†] since 1993. In the meantime, the construction and maintenance costs have increased significantly while the consump-

[†] 1 US liquid gallon = 0.00378541 m^3

tion has reduced due to the improvement in vehicle fuel efficiency and the popularity of hybrid and electric vehicles. As a result the purchasing power of the gasoline tax has sliced by almost two-thirds [125]. According to the American Society of Civil Engineers, one out of every five miles of highway pavement is in poor condition and the chronic underfunding of the highway systems has resulted in a $836 billion backlog of capital need [126]. The situation becomes even worse considering that the funding gap over the next 10-year in infrastructure needs totals more than $1 trillion [127]. Therefore, a sustainable and long-term funding source for the Highway Trust Fund is needed.

The US Chamber of Commerce recently proposed an increase of the gasoline tax by a total of 25 cents per gallon along with indexing the tax for inflation and for future increases in fuel economy [128]. Such a policy could generate a combination of financial and environmental benefits [129], since increases in gasoline taxes may result in significant reductions in gasoline consumption [130, 131]. However, the extent to which the gasoline taxes should be increased to result in meaningful changes in the consumption pattern over the short and long run are still debatable [132]. According to recent published studies [133, 134, 135, 136, 137, 138, 139, 140, 141], gasoline is a relatively inelastic product, meaning changes in prices have little influence on demand. This implies that the reduction in the gasoline consumption will not be important without a substantial tax hike [139]. The Congressional Budget Office reports that a 46 cents per gallon increase on federal gasoline tax would attain a 10% reduction in gasoline consumption in the long run [142].

Data of the annual household expenditure for gasoline [143], the annual household gasoline consumption [144] and the average price of gasoline [145] over the last two decades confirm the inelastic behavior of gasoline, as it is shown in Figure 4.1. Despite the fluctuations in the average price of gasoline, the consumption of gasoline remained rather constant. This is true even when the highly fluctuating annual expenditure of gasoline per household is considered; the consumption of gasoline remained stable. For instance, the price of gasoline declined by 28% and 27% between 2008-2009 and 2014-2015 respectively, but the consumption of gasoline increased by just 1% and 4% over these periods. On the contrary, the price of gasoline rose by 22% and 26% between

2004-2005 and 2010-2011 respectively, but the consumption of gasoline decreased by 2% and 4% over these periods. Such a steady gasoline consumption indicates that people's behavior does not change drastically in response to changes in gasoline prices.

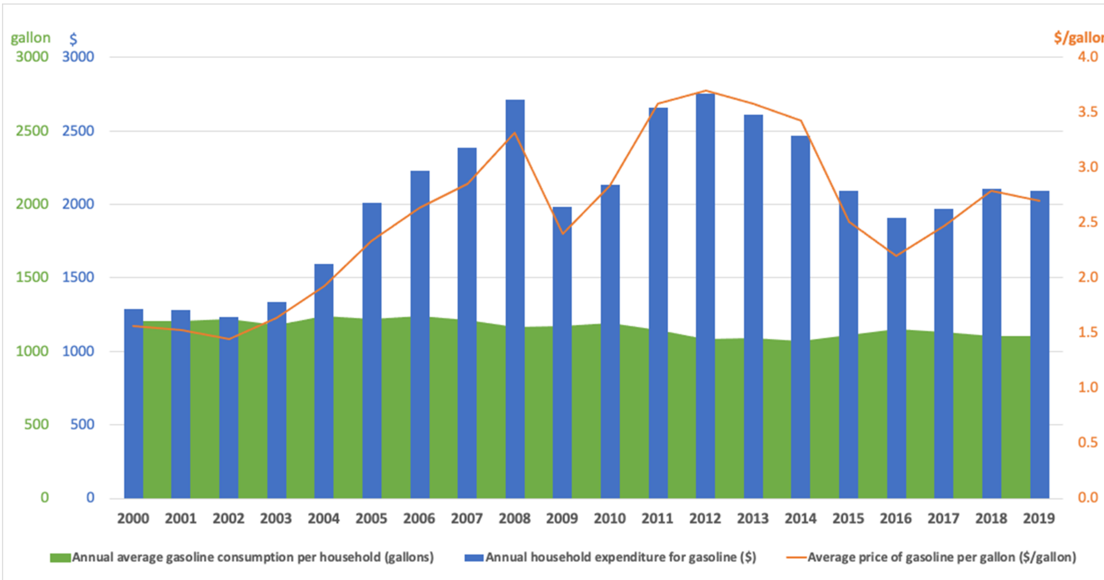

Figure 4.1: Annual Household Expenditure and Consumption for Gasoline vs Average Price of Gasoline per gallon, 2000-2019

The applicability and effectiveness of the proposed framework in designing, assessing and optimizing various policy rules is demonstrated by examining parametrically the effect an increase in the federal gasoline tax would have on the overall cost of energy (EPIC) and on the overall cost in 3 energy sectors (TEPIC, INEPIC, CEPIC). First, EPIC and its three sub-indices are recalculated for the period from January 2003 to January 2021 considering different scenarios of federal gasoline tax hikes i.e. 5, 10, 15, 20 and 25 cents per gallon. In this study as a reference approach, it is assumed that the introduction of a relatively small gasoline tax hike (i.e. 5, 10, 15 cents per gallon) does not affect the consumption of gasoline, while the introduction of a higher gasoline tax hike (i.e. 20 and 25 cents per gallon) results in a slight reduction in gasoline's consumption (i.e. 1% and 1.5% respectively).

Figure 4.2 illustrates the recalculated values of EPIC from January 2003 to January 2021. The recalculated values of the three sub-indices are presented in the Figures 4.3 to 4.5.

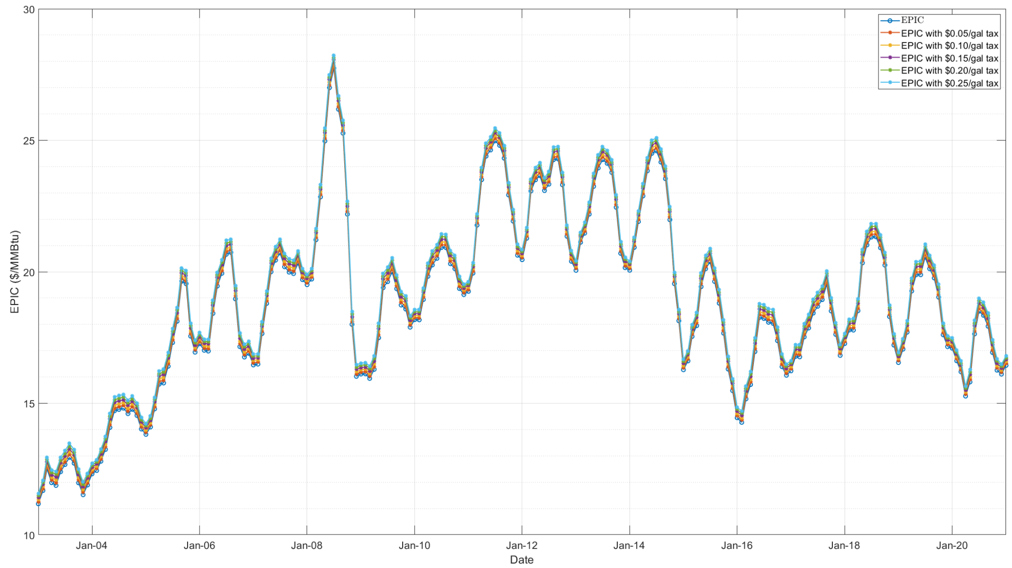

Figure 4.2: Recalculated EPIC with Parametric Gasoline Tax Hikes from January 2003 to January 2021

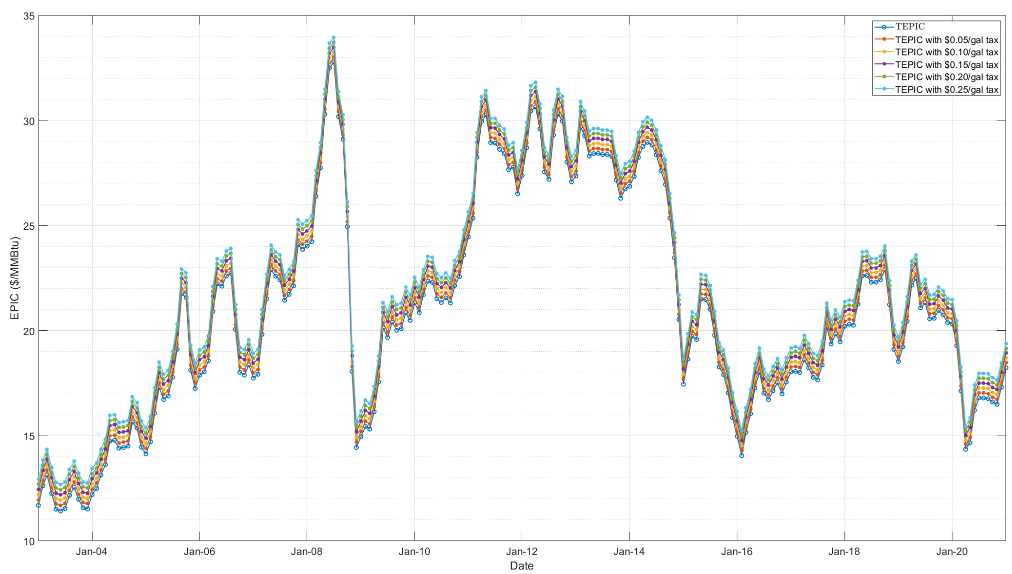

Figure 4.3: Recalculated TEPIC with Parametric Gasoline Tax Hikes from January 2003 to January 2021

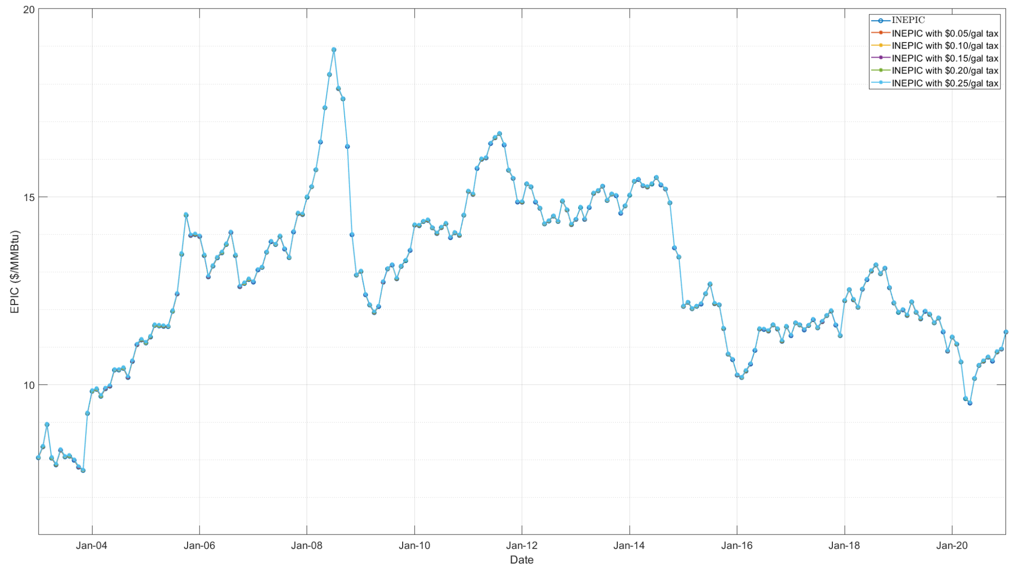

Figure 4.4: Recalculated INEPIC with Parametric Gasoline Tax Hikes from January 2003 to January 2021

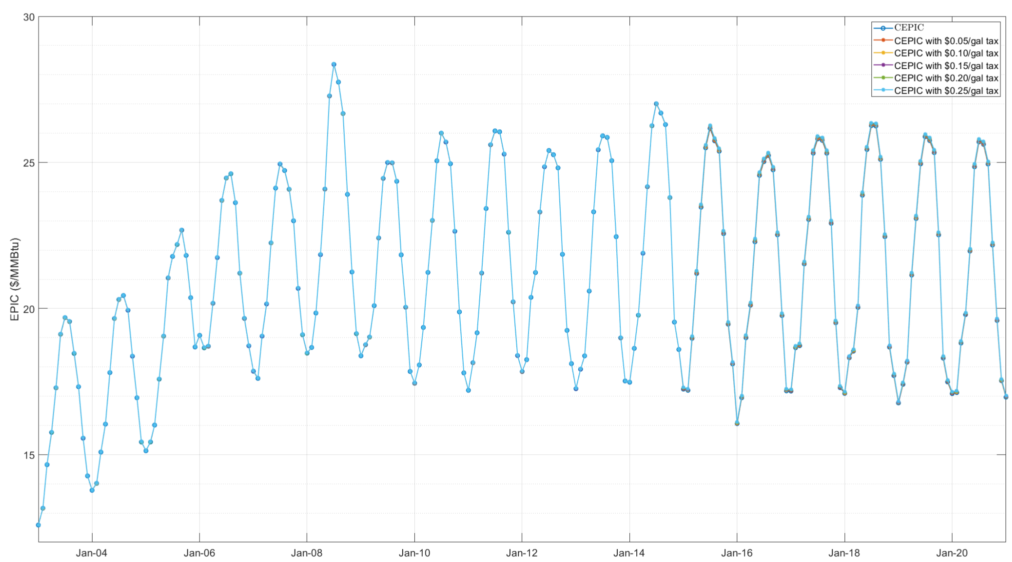

Figure 4.5: Recalculated CEPIC with Parametric Gasoline Tax Hikes from January 2003 to January 2021

The average monthly difference and percentage increase from the nominal EPIC and its sub-indices for the different taxes over the same period is presented in Table 4.1. A tax hike of 10 cents per gallon in gasoline increases EPIC by \$0.194/MMBtu or 1.067%, TEPIC by \$0.478/MMBtu or 2.446%, while the increase in INEPIC and CEPIC is negligible (just 0.081% and 0.066% respectively). Even the highest tax hike of 25 cents per gallon which results in a 1.5% reduction in the consumption of gasoline, increases EPIC and TEPIC by 2.638% and 6.080% respectively, while the increase in INEPIC and CEPIC is still negligible (just 0.200% and 0.163% respectively).

Table 4.1: Average Monthly Difference (\$/MMBtu) and Percentage (%) Increase from Nominal Indices with No Tax Hike from January 2003 to January 2021

Gasoline Tax Hike	**EPIC**		**TEPIC**		**INEPIC**		**CEPIC**	
(cents/gal)	**(\$/MMBtu)**	**(%)**	**(\$/MMBtu)**	**(%)**	**(\$/MMBtu)**	**(%)**	**(\$/MMBtu)**	**(%)**
5	0.097	0.533	0.239	1.223	0.005	0.041	0.007	0.033
10	0.194	1.067	0.478	2.446	0.010	0.081	0.014	0.066
15	0.291	1.600	0.717	3.669	0.015	0.122	0.021	0.100
20	0.386	2.118	0.953	4.873	0.020	0.161	0.028	0.131
25	0.480	2.638	1.188	6.080	0.025	0.200	0.035	0.163

The amount of revenue that would have been generated by such a tax policy over the same period in the past is displayed in Table 4.2. The average annual revenue is \$6.751 billion for every 5 cents increase in the motor gasoline tax hike, up to a tax of 15 cents per gallon. For the higher tax hikes, the average annual revenue does not increase linearly since the consumption is reduced. As such, a 20 cents per gallon tax hike generates an annual revenue of \$26.753 billion. Also, even though a 25 cents per gallon tax hike increases EPIC and TEPIC by just 2.638% and 6.080% respectively, it creates a substantial average annual revenue of \$33.250 billion.

Table 4.2: Revenue (million \$) generated with Parametric Gasoline Tax Hikes from January 2003 to January 2021

Gasoline Tax Hike	**Commercial Sector**	**Industrial Sector**	**Transportation Sector**	**Total Revenue from Jan. 2003 to October 2020**		**Annual Average**
(cents/gal)	**million \$**	**million \$**	**million \$**	**million \$**		**million \$**
5	1,116.07	2,016.69	118,952.70	122,085.45		6,751
10	2,232.14	4,033.38	237,905.39	244,170.90		13,502
15	3,348.21	6,050.07	356,858.09	366,256.36		20,253
20	4,419.64	7,986.09	471,052.67	588,815.83		26,735
25	5,496.63	9,932.19	585,842.03	601,270.85		33,250

The powerful forecasting ability of the EPIC framework can be utilized so as to determine parametrically the impact of the investigated gasoline tax hike on future energy prices. As it has been shown in Chapter 2, the weights of the demand of the energy products can be predicted with excellent accuracy of up to four years in the future. Hence, the change in EPIC and its sub-indices over the next four years can be estimated using the forecasts for the weights of the demands. The mathematical formulation for the estimation of EPIC in the future considering parametric gasoline tax hikes is shown in Equation (4.1):

$$EPIC_m^{TaxPar} = \sum_{p \in P \setminus 'gsl'} w_{m,p} \cdot C_{m,p} + w_{m,'gsl'} \cdot (C_{m,'gsl'} + TaxPar) \tag{4.1}$$

where $w_{m,'gsl'}$ stands for the weight of gasoline "gsl" in month *m*, $C_{m,'gsl'}$ stands for the price of gasoline 'gsl' products in month *m*, and $TaxPar$ stands for the parametric gasoline tax.

The change in EPIC in the future is calculated as shown in Equation (4.2):

$$\Delta EPIC_m = TaxPar \cdot w_{m,'gsl'} \tag{4.2}$$

where $TaxPar$ stands for the parametric gasoline tax and $w_{m,'gsl'}$ stands for the weight of gasoline "gsl" in month *m*.

Following the retrospective calculations, it is assumed that the introduction of a relatively small gasoline tax (i.e. 5, 10, 15 cents per gallon) will not affect the consumption of gasoline in the future. However, higher gasoline tax hikes (i.e. 20 and 25 cents per gallon) will marginally reduce the predicted consumption of gasoline in the future (in comparison to the original forecasting scenarios without tax hikes) by 1% and 1.5% respectively.

Figure 4.6 and 4.7 illustrate the change in EPIC and TEPIC over the next four years (February 2021 to January 2025) respectively by taking into account the proposed motor gasoline tax hikes parametrically.

A 25 cents per gallon increase in the gasoline tax will raise EPIC between \$0.3833/MMBtu and \$0.5186/MMBtu, while TEPIC will rise even more (up to \$1.1765/MMBtu). It is worth noting that the change in TEPIC is rather steady for each tax hike. Even with the highest tax hike, TEPIC rises

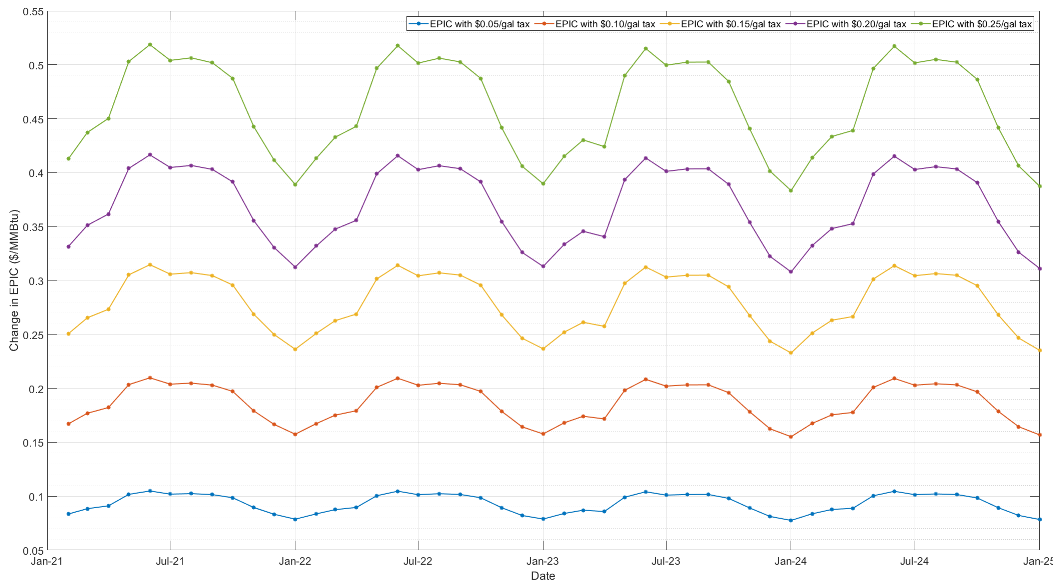

Figure 4.6: Change in EPIC with Parametric Gasoline Tax Hike from February 2021 to January 2025

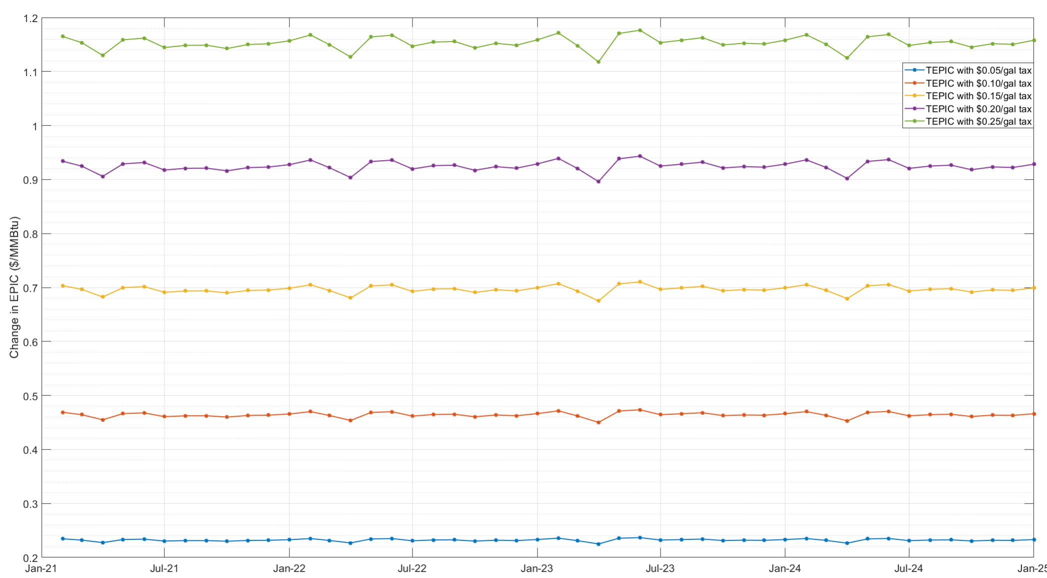

Figure 4.7: Change in TEPIC with Parametric Gasoline Tax Hike from February 2021 to January 2025

between \$1.1177/MMBtu and \$1.1765/MMBtu, due to the relatively constant percentage (around 60%) of motor gasoline in the transportation sector. Assuming that the future monthly values of EPIC and TEPIC are equal to the average monthly known values of the last four years (February 2017 to January 2021), the average monthly percentage increase over the next four years (from February 2021 to January 2025) are shown in Table 4.3. For a motor gasoline tax increase of 15 cents per gallon, EPIC increases roughly 1.662% while TEPIC increases approximately 4.165%.

Table 4.3: Average Monthly Percentage (%) Increase from Nominal indices with No Tax Hike from February 2021 to January 2025

Gasoline Tax Hike (cents/gal)	**EPIC (%)**	**TEPIC (%)**
5	0.554	1.388
10	1.108	2.777
15	1.662	4.165
20	2.199	5.532
25	2.738	6.901

The future revenue that will be generated by this gasoline taxation policy over the next four years can also be calculated using the demands of the gasoline energy products that have been estimated from the EPIC framework along with the projections for the total annual energy demand from the EIA Annual Energy Outlook 2021 - Reference case [81]. The average annual revenue generated for every 5 cents per gallon increase (up to 15 cents per gallon) in the gasoline tax hike is \$6.837 billion. The revenue does not increase linearly for the higher tax hikes, resulting in \$27.138 and \$33.790 billion average annual revenue for the tax hikes of 20 and 25 cents per gallon respectively.

The average US household expenditure on gasoline in 2019 was estimated to be about \$2,094 according to the US Bureau of Labor Statistics [143]. By using the recalculated values of TEPIC for the new gasoline tax, the annual increase in the average US household expenditure is calculated. In particular, for 2019 the estimated average US household expenditure would have been \$2,117 (or 1.12% higher) for the case of 5 cents per gallon tax hike, and \$2,209 (or 5.50% higher) for the case of 25 cents per gallon increase in a gasoline tax.

4.4 Policy Case Study for the Carbon Tax

The second policy case study for the design of energy-intelligent taxes investigates the effects on the price of energy as well as on the energy consumption from the implementation of a carbon tax. The Intergovernmental Panel on Climate Change (IPCC) and the International Monetary Fund (IMF) in recent reports [146, 147] argue that carbon taxes are the most powerful and efficient tools to mitigate climate change. In particular, a carbon tax scheme allows customers to identify the most effective ways of reducing energy consumption by shifting to more environmentally friendly alternatives while it generates a significant amount of revenue that can be used to offset the affected macroeconomic variables e.g. unemployment, or fund initiatives such as those described in the United Nations Sustainable Development Goals [148]. Carbon taxes can also generate substantial domestic environmental benefits and at the same time are straightforward to administer. However, the effects of a carbon tax in the economy are subject to the utilization of the generated revenues since the actual impacts can vary significantly depending on the selected policies. For instance, revenues can be directed towards reducing budget deficits, decreasing current marginal tax rates or offsetting the burden from the imposed tax on taxpayers [149].

A review of the current status of global carbon pricing initiatives reveals a mixed picture with regards to the type and stage of carbon pricing initiatives as well as to the level of pricing of these initiatives. Although there is a rising number of jurisdictions that are implementing or planning to implement a carbon tax or an emission trading system (ETS), only 22% of global greenhouses gas emissions are covered by a carbon price. Most notably, less than 5% of those initiatives are priced at levels consistent with achieving the temperature goals that have been set in the Paris Agreement [2]. In the US currently there is no federal carbon tax, with only twelve states (California and eleven Northeast states) having active carbon pricing schemes [150]. Even though numerous federal carbon pricing plans were proposed over the last few years, none has become law [151]. Therefore, strategic and long-term action plans for carbon pricing must be established from all jurisdictions across the globe as part of their climate policies.

An overview of the global carbon pricing initiatives is shown in the Appendix G (Figures G.1, G.2). Only 61 carbon pricing initiatives have been implemented or scheduled for implementation globally, with an extremely wide range of pricing in existing initiatives from \$1/tCO_2e to \$119/tCO_2e [2]. Thus, a parametric approach is needed to quantitatively evaluate and optimize the carbon pricing initiatives. The EPIC framework offers this functionality along with an agile platform that can incorporate different dynamic models for capturing the impacts of the subject policies realistically. A federal carbon tax policy is investigated, addressing the key questions of what would have happened (retrospective analysis) and what will happen (prospective analysis) by the introduction of a federal carbon tax. In particular, the effects of an incremental carbon tax in the price of energy as well as in the reduction of the CO_2 emissions are estimated, along with the generated revenue from such a taxation policy.

Figure 4.8 highlights the effects of an incremental carbon tax in the price of energy as well as in the reduction of the annual CO_2 emissions from January 2007 until April 2021. The same effects are assessed for the next 10 years (May 2021-April 2031) in Figure 4.9. Both scenarios involve an incremental annual rise of \$5 per metric ton of CO_2 emitted starting from year 1, along with two sub-scenarios each demonstrating the impact of this escalating taxation policy on the annual CO_2 emissions. Since there are no actual data on the effects that a carbon tax could have on the CO_2 emissions on a federal level in the US, a rather moderate case study based on the findings in the literature is considered [149, 152, 153, 154]. This is also in line with similar studies from other countries such as Canada, and China [155, 156]. Nevertheless, the key outcome is that EPIC is a versatile tool that can analyze different policy scenarios and quantitatively evaluate their effects in energy and economy. It is also worth noting that regardless of the sub-scenario that is selected, the increase of the values of EPIC remain similar.

The difference between the two sub-scenarios lies in the estimation of the revised CO_2 emissions upon the introduction of the taxation policy. In sub-scenario A the CO_2 emissions are calculated as an adjustment on their historical monthly values, while in sub-scenario B the CO_2 emissions are calculated independently of their historical monthly prices having only the CO_2 emissions of year 0 as a reference point. Specifically, in sub-scenario A, it is assumed that the

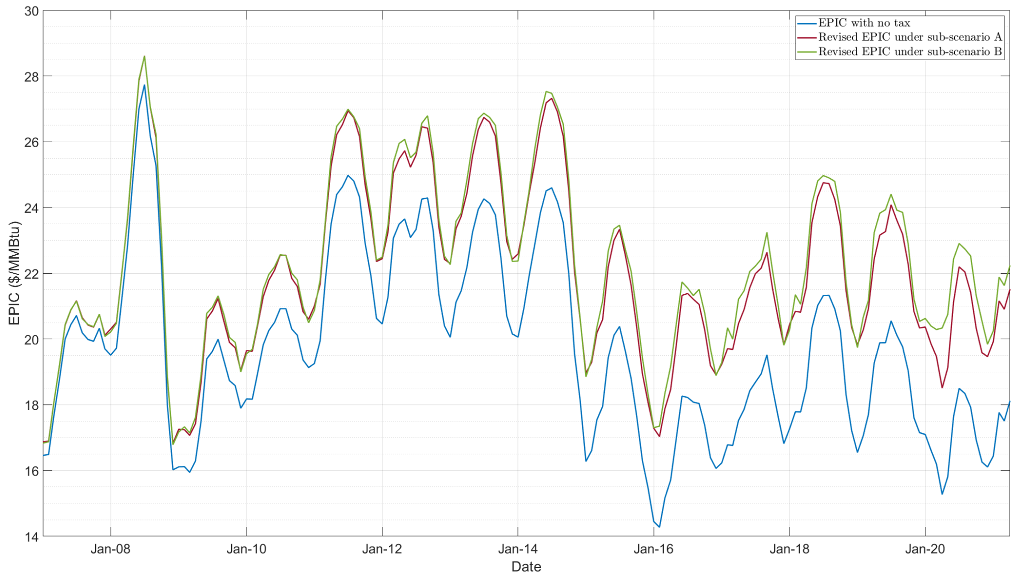

Figure 4.8: Effects of an Incremental Carbon Tax in EPIC ($/MMBtu) and CO_2 emissions from January 2007 to April 2021

historical monthly CO_2 emissions would have decreased by 3% starting from year 1 and continue to decrease by 3% compounded annually for the next years. For the first scenario that covers the period from January 2007 to April 2021, the hypothetical CO_2 emissions of 2007 would have been 3% less than their historical ones, while the CO_2 emissions until April 2021 would have reduced by approximately 36.7% from their historical values (red line in Figure 4.8). In sub-scenario B, it is assumed that the introduction of the $5 per metric ton of CO_2 emitted taxation in year 1 would have caused an immediate decrease of 3% on the historical CO_2 emissions of year 0. So, for the first scenario again (January 2007-April 2021), the hypothetical CO_2 emissions of 2007 would have been 3% less than those of 2006, the hypothetical CO_2 emissions of 2008 would have been 3% less than the hypothetical ones of 2007 and so on (green line in Figure 4.8).

As a result of this policy, the price of energy from January 2007 to April 2021 would have increased on average about 11.90% and 13.37% for sub-scenario A and B respectively. Over the same period, the total revenue generated from this incremental carbon increase is $2,2682 billion and $2,528 billion for sub-scenario A and B respectively, while the average annual revenue over this period is \$158.25 billion and \$176.38 billion respectively. The total amount of CO_2 reduced over this period is 16,028 million metric tons, or an annual average decrease of 1,118 million metric tons for sub-scenario A. For sub-scenario B, the total reduction of CO_2 emissions from the atmosphere is 10,499 million metric tons or 733 million metric tons on average annually. Therefore, if this policy was implemented, the reduction that would have been achieved represents a 19.74% decrease from historical CO_2 emissions for sub-scenario A and 12.93% decrease for sub-scenario B.

The effects of an incremental carbon tax in the future are also investigated using the same principles over the next 10 years. Figure 4.9 demonstrates the change of EPIC in \$/MMBtu over this period. The projected CO_2 emissions as well as the projected annual energy demand for the reference case from the EIA's Annual Energy Outlook of 2021 are used [81]. The incremental annual increase of \$5 per metric ton of CO_2 emitted in the carbon tax starts in May 2021 and escalates up to \$55 per metric ton by April 2031. The same sub-scenarios A and B are also considered. In sub-scenario A, the hypothetical CO_2 emissions of 2021 will be 3% less than their projected values in the outlook report, while the CO_2 emissions of 2031 will be reduced by approximately 28.5% (compounded annually) from their projected values in the outlook report (blue dots in Figure 4.9). In sub-scenario B, the hypothetical CO_2 emissions of 2021 will be 3% less than the actual CO_2 emissions of 2020, the hypothetical CO_2 emissions of 2022 will be 3% less than the hypothetical ones of 2021 and so on. Thus, the projected CO_2 emissions from the outlook report are not considered in sub-scenario B (red dots in Figure 4.9). The average increase in EPIC's values over the next 10 years is around \$1.5/MMBtu regardless of the selected sub-scenario. The increasing annual tax has a stronger effect on EPIC in comparison to the reduced CO_2 emissions, causing only positive changes in EPIC's values.

The total revenue generated from this incremental carbon increase over the next 10 years is calculated to be \$1,1877 billion and \$1,1472 billion for sub-scenario A and B respectively. The total amount of CO_2 reduced over the next 10 years is 8,081 million metric tons and 9,794 million metric tons for sub-scenario A and sub-scenario B respectively. Therefore, the implementation

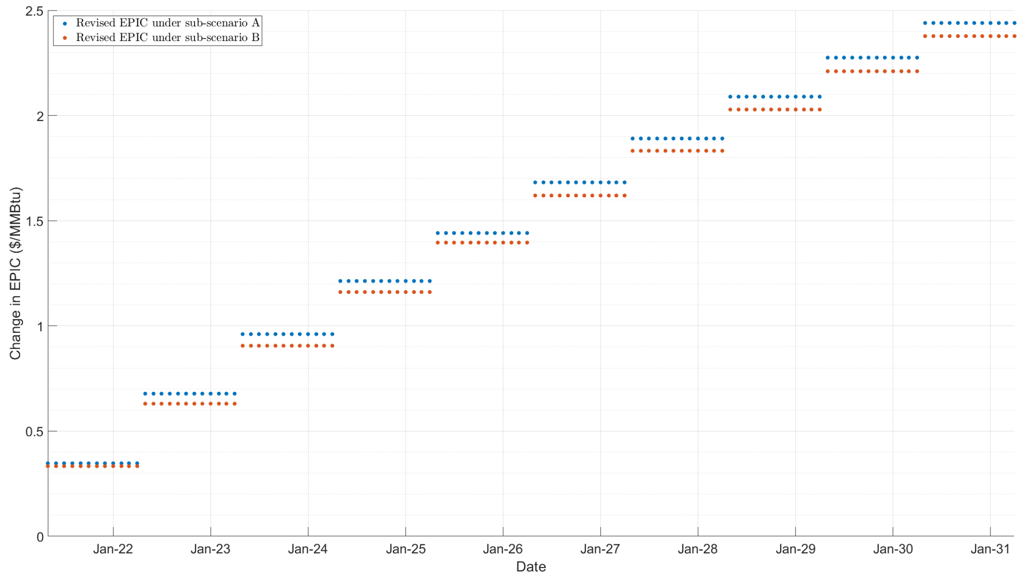

Figure 4.9: Change in EPIC ($/MMBtu) due to the Proposed Incremental Carbon Tax and CO_2 Emissions Reduction over the next 10 Years

of this policy from May 2021 and for the next 10 years is estimated to decrease CO_2 emissions by approximately 15.86% for sub-scenario A and by approximately 19.23% for sub-scenario B in comparison to the projected CO_2 emissions without any tax.

4.5 Policy Case Study for Crude Oil Tax

A potential tax in crude oil is investigated as an alternative policy for mitigating climate change and concurrently generating substantial revenue that is required for climate finance. Such a policy of $ 10.25 per barrel tax on crude oil was also proposed by US President Barack Obama back in 2016 to support new transportation systems designed to reduce carbon emissions and congestion [157].

The effects of a crude oil tax ranging from $2.5 per barrel up to $25 per barrel in EPIC are parametrically examined. The amount of revenue that could be generated by such a policy from January 2003 until June 2020 is also calculated. Taking advantage of the excellent predictive ability of the proposed EPIC framework, the changes in EPIC in the next four years along with the future revenue that will be generated by such a policy are estimated. It is assumed that crude oil has a heating content of 5.721 MMBtu per barrel [77] and a petroleum refinery efficiency of 90%. Moreover, the amount of petroleum and petroleum products being sent for electricity generation is assumed to be negligible ($\approx$ 0.57% over the last year). Crude oil demand is considered as inelastic in the short-run, with long-run values of elasticity being generally higher in absolute values but still well below 1 [158, 159, 160, 161].

The average monthly difference (in $/MMBtu) and the average monthly percentage increase of EPIC in comparison to its reference values from January 2003 to June 2020 are presented in Table 4.4 for the different values of crude oil tax. Since crude oil is inelastic, the investigated crude oil tax has not affected the historical values of crude oil consumption. As can be seen, a $10.25 per barrel of crude oil tax increases EPIC by $1.019 per MMBtu or 5.60%, while a $25 per barrel of crude oil tax rises EPIC by $2.484 per MMBtu or 13.66%. Table 4.4 also summarises the amount of revenue generated from the investigated crude oil tax scenario over the same period (January 2003 - June 2020). The average annual revenue from a $10.25 per barrel of crude oil tax is estimated to be $70.962 billion or $17.308 billion for every $2.5 per barrel rise of crude oil tax. Figure G.3 in appendix G illustrates the recalculated EPIC for the above-mentioned values of crude oil tax along with the reference value of EPIC without tax for easy comparison, over the same period (January 2003 to June 2020). As expected, the higher the crude oil taxes, the greater the increase in EPIC values.

The average increase in energy related expenses per household as a result of the proposed increase in crude oil tax are calculated, using data from the relevant survey published by EIA [162] in conjunction with the EPIC findings from our previous analysis. According to the 2015 survey data, the annual energy consumption per household is 77.1 MMBtu while in 2015 the average value of EPIC is $18.01/MMBtu. Using this information, the average annual energy related expenses per household for 2015 are estimated to be $1,389.06. Taking into consideration the effects on EPIC from the increase in the crude oil taxation, a $2.5 per barrel increase in crude oil tax would have led to an average rise of $0.2432/MMBtu or 1.35% in EPIC for 2015. Therefore, the projected average annual energy related expenses per household would have increased by $18.76, up to a total of $1,407.82. Similarly, an increase of $10.25 per barrel in crude oil tax would have burdened the average energy related expenses per household by $76.90 or 5.54%, up to a total of $1,465.95.

Table 4.4: Average Monthly Difference ($/MMBtu), Percentage Increase (%) and Revenue Generated ($ billion) from January 2003 - June 2020

Crude Oil	**Average monthly EPIC difference**	**Average monthly EPIC percentage increase**	**Total revenue**	**Average annual revenue**
($/barrel)	**($/MMBtu)**	**(%)**	**($ billion)**	**($ billion)**
2.5	0.248	1.37	302.886	17.308
5.0	0.497	2.73	605.772	34.616
7.5	0.745	4.10	908.658	51.923
10.0	0.994	5.46	1211.545	69.231
10.25	1.019	5.60	1,241.833	70.962
12.5	1.242	6.83	1,514.431	86.539
15.0	1.491	8.19	1,817.317	103.847
17.5	1.739	9.56	2,120.203	121.154
20.0	1.987	10.92	2,423.089	138.462
22.5	2.236	12.29	2,725.975	155.770
25.0	2.484	13.66	3,028.862	173.078

The effects on EPIC from the investigated policy during the next four years is demonstrated in Figure 4.10, using the predictive weights of demand of the energy products for this period. Similarly, with the results for the past period, the increase of EPIC in the future is investigated parametrically for different values of the crude oil tax.

According to Figure 4.10, a $10.25 per barrel of crude oil tax raises EPIC over the next four years by $0.977/MMBtu on average, whereas a $25 per barrel of crude oil tax surges EPIC by $2.384/MMBtu on average in the same period. Using the weights of the demand of the petroleum energy products that have been estimated from the EPIC framework along with the projections for the total annual energy demand from the EIA Annual Energy Outlook 2021 - Reference case [163], the future revenue that will be generated by the crude oil taxation policy over the next four years can be estimated. As a result, a total of $147.882 billion revenue is generated for every $5 per barrel increase in the crude oil tax over the next four years.

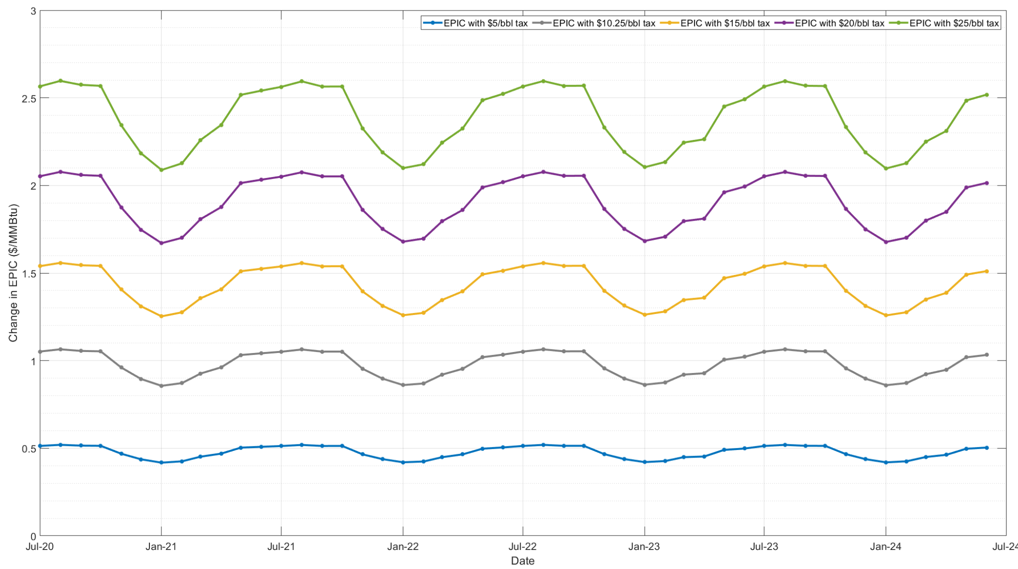

Figure 4.10: Change in EPIC with Parametric Crude Oil Tax over the next 4 years (July 2020 to June 2024)

4.6 Policy Case Study for Renewable Energy Production Targets and Subsidies

The renewable energy has been selected as the fourth policy case study since it plays a growing role in the global energy mix. The electric power sector is heavily dominated (around 67%) by fossil fuels (coal, natural gas, petroleum, and other gases), while nuclear and renewable energy sources contribute about 17% and 16% of the remaining electricity generation respectively [164] (see Table G.1). As a result, the electric power sector emits about 31.5% of the total US energy-related CO_2 emissions [77]. Thus, coordinated efforts for new policies and technologies are required so as to lessen the dependence on fossil fuels and subsequently reduce CO_2 emissions. To accomplish such reduction, the share of renewable energy within the electric power sector should be increased. This can be achieved either by setting a target renewable energy share for each power feedstock (analogous to the State based Renewable Portfolio Standards) and/or by providing subsidies to the renewable energy generation (analogous to the Public Benefits Funds for Renewable Energy).

As of 2020, 30 US states, Washington D.C., and three US territories have adopted a Renewable Portfolio Standard (RPS), while seven US states and one US territory have set renewable energy goals for electricity generation [165]. The National Renewable Energy Laboratory (NREL) indicates that these standards are most successful drivers of renewable energy projects when combined with tax credits [166]. However, the impact of these standards on the ratepayer are not clear and should be carefully evaluated. Although some reports claim that the benefits outweigh the costs of these standards [167, 168], EPIC is an excellent tool to quantitatively analyze the costs of different renewable standards to the government and to the end-use consumers.

Therefore, in this policy case study, six non-fossil fuel feedstocks that are used in the electric power sector (nuclear, hydroelectric power, biomass, geothermal, solar and wind) are investigated over a range of different target weights with tax credits/subsidies ranging from 0 to $9/MMBtu. The main assumptions for this policy case study are:

- The effect of the policy is investigated independently for each feedstock.
- The production targets/subsidies affect only the electric power sector, so only the relative weights within the electric power sector change.
- The target weights are attainable with the existing resources and at the current production costs.
- When a specific target weight is enforced on an electricity energy feedstock, the remaining feedstock weights are normalized to add up to 1.
- The levelized cost of the energy feedstocks is taken from Lazard's Levelized Cost of Energy Analysis report for the period 2008 to 2013 [169, 170, 171, 172, 173, 174] and the EIA Annual Energy Outlook for period 2014 to 2020 [175, 176, 177, 178, 179, 180, 181], with the exception of data for the petroleum liquids, which are also taken from Lazard's Levelized Cost of Energy Analysis reports. The data from 2008 are used for the period from 2003 to 2007 (Table G.1).

- The future effects (up to 2024) are assessed using the predicted values for the weights of the electricity products applying the methodology that is described in the Chapter 2.
- The future annual demand as well as the future nominal weights within the electric power sector are estimated using data from the EIA Annual Energy Outlook 2020 - Reference case[163].

Once a target weight for a renewable feedstock has been set, all other weights within the electric power sector are re-normalized as follows:

$$w_{norm,f} = w_f^{old} \cdot \frac{1 - w_{f'}^{target}}{1 - w_{f'}^{old}} \tag{4.3}$$

where f' represents the feedstock investigated and f represents all other feedstocks.

The change in EPIC due to the new target weight is then calculated as follows:

$$\Delta EPIC_1 = w_{elec} \cdot [\sum_f Cost_f * (w_{norm,f} - w_f^{old}) + Cost_{f'} \cdot (w_{f'}^{target} - w_{f'}^{old})] \tag{4.4}$$

where w_{elec} stands for the aggregate weight of electricity (i.e. products 50-53) while $Cost_{f'}$ and $Cost_f$ stand for the levelized cost of electricity production from feedstock f' and f respectively. When this delta term becomes positive, meaning that the value of EPIC increases, the cost of the targeted feedstock is higher than the average cost of the displaced feedstocks. On the contrary, when this delta term becomes negative, the cost of the targeted feedstock is lower than the average cost of the displaced feedstocks, and so the value of EPIC decreases.

The change in EPIC due to subsidies is calculated as follows:

$$\Delta EPIC_2 = w_{elec} \cdot w_{f'}^{target} \cdot Tax_{cred} \tag{4.5}$$

where Tax_{cred} represents the subsidy in \$/MMBtu.

The revised EPIC from the subject policy case study is estimated for the past as well as for the future as follows:

$$Past: \ EPIC_{policy} = EPIC + \Delta EPIC_1 + \Delta EPIC_2 \tag{4.6}$$

$$Future: \Delta EPIC_{policy} = \Delta EPIC_1 + \Delta EPIC_2 \tag{4.7}$$

Table 4.5 illustrates the grid of investigated target weights for each of the non-fossil feedstocks based on their nominal weights within the electric power sector.

Table 4.5: Investigated Weights for the Non-Fossil Fuel Feedstocks within the Electric Power Sector

Feedstock	**Minimum weight (%)**	**Increment increase (%)**	**Maximum weight (%)**
Nuclear	18.0	3.0	30.0
Hydroelectric Power	8.0	2.0	16.0
Wind	5.0	2.0	13.0
Biomass	0.5	0.25	1.5
Solar	1.0	1.0	5.0
Geothermal	0.3	0.1	0.7

Table 4.6 summarises the results of this policy case study in terms of percentage change in EPIC at the maximum weight target for each non-fossil fuel feedstock in the past period (January 2003 to June 2020). It can be observed that nuclear energy causes a minor increase to EPIC at no tax credit, but as the tax credit increases, EPIC decreases significantly, for a maximum decline of -2,549% corresponding to a tax credit of \$9/MMBtu. Also, solar energy requires a subsidy of at least \$6/MMBtu in order to lower the value of EPIC. It is also worth noting that increases either in the weights or in the tax credits of wind, hydroelectric, biomass and geothermal energy always lead to a reduction in EPIC. This is also true even without a tax credit. For example, wind energy decreases EPIC from 0.177% up to 0.929% as the weight target increases with no tax credit, and from 0.621% up to 2.085% depending on the targeted weight with \$9/MMBtu tax credit.

In Table 4.6, the average annual budget (\$ million) required to provide subsidies at the maximum weight target for each non-fossil fuel feedstock in the same period (January 2003 to June

2020) is also presented. Clearly, the target weight and the tax credit are the key factors, affecting the annual budget. As either the target weight of each feedstock or the tax credit rises, the annual budget required to provide the relevant subsidy rises. Nuclear energy requires the highest subsidy budget (due to its maximum weight of 30%), but the corresponding decline in EPIC is also substantial (-2.549%) at the maximum level of tax credit.

Table 4.6: Average % Change in the EPIC and Average Annual Budget ($ million) at the Maximum Weight Target from January 2003 to June 2020

Tax Credit	nuclear (0.30)		hydroelectric (0.16)		biomass (0.015)		geothermal (0.007)		solar (0.05)		wind (0.13)	
($/MMBtu)	(%)	($ mil)	(%)	($ mil)	(%)	($ mil)	(%)	($ mil)	(%)	($ mil)	(%)	($ mil)
0	0.118%	0	-0.602%	0	-0.026%	0	-0.032%	0	0.257%	0	-0.929%	0
1	-0.178%	3,787	-0.760%	2,020	-0.041%	189	-0.039%	88	0.208%	631	-1.058%	1,641
2	-0.475%	7,573	-0.918%	4,039	-0.056%	379	-0.046%	177	0.158%	1,262	-1.186%	3,282
3	-0.771%	11,360	-1.076%	6,059	-0.071%	568	-0.053%	265	0.109%	1,893	-1.315%	4,923
4	-1.067%	15,147	-1.234%	8,078	-0.086%	757	-0.060%	353	0.059%	2,524	-1.443%	6,564
5	-1.364%	18,933	-1.392%	10,098	-0.100%	947	-0.067%	442	0.010%	3,156	-1.572%	8,204
6	-1.660%	22,720	-1.550%	12,117	-0.115%	1,136	-0.073%	530	-0.039%	3,787	-1.700%	9,845
7	-1.956%	26,507	-1.708%	14,137	-0.130%	1,325	-0.080%	618	-0.089%	4,418	-1.828%	11,486
8	-2.253%	30,293	-1.866%	16,156	-0.145%	1,515	-0.087%	707	-0.138%	5,049	-1.957%	13,127
9	-2.549%	34,080	-2.024%	18,176	-0.160%	1,704	-0.094%	795	-0.187%	5,680	-2.085%	14,768

Taking advantage of the excellent predictive ability of EPIC, the previous analysis can be extended to the future. As such, Figure 4.11 demonstrates the effect on EPIC of various levels of tax credit applied to wind energy, for various weight levels of wind. The results for the remaining non-fossil feedstocks at different target weights and tax credits are presented in Figures G.4 to G.8.

At the lower end of tax credit (0 or 1$/MMBtu), the weight of the wind energy needs to be at least 11% so as to decrease the EPIC value, whereas at the higher end of tax credit (8 or 9$/MMBtu), the EPIC value decreases even when weight contribution of wind energy is minimum (5%). Interestingly, as the percentage weight of wind energy increases within the electric power sector, EPIC decreases since the levelized cost of wind energy is rather low. As an example, even without any tax credit, EPIC decreases by 0.143% when wind energy provides 13% of the electric power. Moreover, at the higher end of tax credit, the average decrease in EPIC exceeds $0.23/MMBtu.

Table 4.7 summarises the average percentage change in EPIC and the average annual budget ($

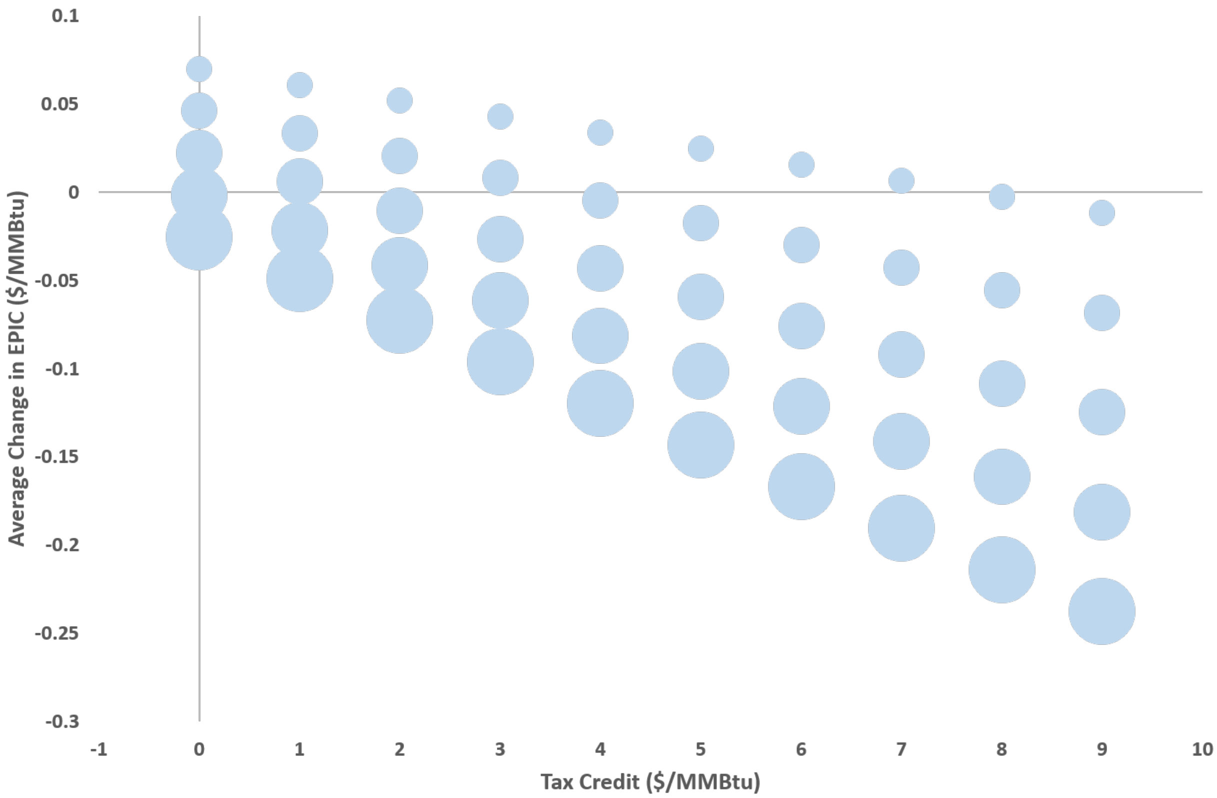

Figure 4.11: Wind Power at different Target Weights (size of the bubble) and Tax Credits (x-axis), 2020-2024. At maximum weight (13%) and without tax credit, EPIC decreases by 0.143% with no budget required, whereas at maximum weight (13%) and maximum tax credit ($9/MMBtu), EPIC decreases by 1.341% requiring around $16.5 billion annually from the government's budget.

million) required to provide the relevant subsidies in the future period from July 2020 to June 2024. The results are analogous with those from past period. More specifically, hydroelectric, wind, solar and geothermal power cause a drop of 0.198%, 0.143%, 0.090% and 0.019% respectively in EPIC prices even with no tax credit. On the contrary, nuclear and biomass require a tax credit of at least $3/MMBtu and $4/MMBtu respectively so as reduce the value of EPIC. The most significant declines in EPIC are associated with potential subsidies of $9/MMBtu in the nuclear, hydroelectric and wind power, resulting in a decline of 2.107%, 1.672% and 1.341% respectively. Nuclear energy is again expected to need the highest budget to provide the required subsidy, due to its maximum weight of 30%.

Table 4.7: Average % Change in the EPIC and Average Annual Budget ($ million) at the maximum weight target from July 2020 to June 2024

Tax Credit	nuclear (0.30)		hydroelectric (0.16)		biomass (0.015)		geothermal (0.007)		solar (0.05)		wind (0.13)	
($/MMBtu)	(%)	($ mil)	(%)	($ mil)	(%)	($ mil)	(%)	($ mil)	(%)	($ mil)	(%)	($ mil)
0	0.657%	0	-0.198%	0	0.054%	0	-0.019%	0	-0.090%	0	-0.143%	0
1	0.350%	4,223	-0.362%	2,252	0.039%	211	-0.026%	99	-0.141%	704	-0.276%	1,830
2	0.043%	8,445	-0.525%	4,504	0.023%	422	-0.033%	197	-0.192%	1,408	-0.409%	3,660
3	-0.265%	12,668	-0.689%	6,756	0.008%	633	-0.040%	296	-0.244%	2,111	-0.542%	5,489
4	-0.572%	16,891	-0.853%	9,008	-0.007%	845	-0.047%	394	-0.295%	2,815	-0.675%	7,319
5	-0.879%	21,113	-1.017%	11,260	-0.023%	1,056	-0.055%	493	-0.346%	3,519	-0.808%	9,149
6	-1.186%	25,336	-1.181%	13,513	-0.038%	1,267	-0.062%	591	-0.397%	4,223	-0.941%	10,979
7	-1.493%	29,559	-1.344%	15,765	-0.053%	1,478	-0.069%	690	-0.448%	4,926	-1.075%	12,809
8	-1.800%	33,781	-1.508%	18,017	-0.069%	1,689	-0.076%	788	-0.500%	5,630	-1.208%	14,639
9	-2.107%	38,004	-1.672%	20,269	-0.084%	1,900	-0.083%	887	-0.551%	6,334	-1.341%	16,468

4.7 Conclusion

Four of the potential applications of the proposed forecasting framework are presented in this chapter, demonstrating the effectiveness of the framework as an excellent tool to design, assess and optimize contemporary governmental policies with a focus on energy-intelligent taxes. In particular, the effects of various gasoline tax hikes, the effects of different carbon taxes, the effects of a crude oil tax and the effects from the implementation of subsidies and production targets on renewable energy on the price of energy are examined. Retrospective as well as prospective analyses are conducted under different scenarios where apart from the change of the price of energy and the tax burden in a household, the generated revenue and the environmental impacts are estimated.

As expected, the transportation EPIC is affected greatly by potential increases in the gasoline taxes, much more so than the other indices (the percentage increase is more than double of that in EPIC). An estimated annual revenue of $6.751 billion will be generated for a gasoline tax hike of just 5 cents. A more aggressive tax hike of 25 cents per gallon is expected to generate an annual revenue of $33.250 billion, providing financial sources to tackle the chronic underfunding of the highway systems. For this analysis, the historic gasoline consumption is considered unchanged after the introduction of low and moderate taxes. The introduction of higher taxes though, results in a reduction in the consumption of gasoline. Additionally, the framework is flexible enough to incorporate different dynamic models that describe the relation between the gasoline consumption and tax rates, providing a quantitative platform for various policy analyses. The framework can also be used as a quantitative policy tool to estimate the optimum tax rate given a specific target of annual revenue.

Similarly, the introduction of an incremental carbon tax that would result in a reduction of CO_2 emissions is estimated to increase on average the price of energy by $1.5/MMBtu over the next 10 years. It will also generate more than $110 billion in annual revenue and will decrease the emitted CO_2 by 8,081-9,794 million metric tons over the same period. Since EPIC can quantitatively estimate the impacts of different policy scenarios in the energy and economy sectors, it can be used as a tool for sensitivity analysis and identification of the optimum combination of economic (carbon tax) and environmental (CO_2 emissions) variables. Having accurate estimations for different policy case studies allows the government to make quantitative based decisions regarding course of action with respects to socioeconomic aspects.

Additionally, an increase of $10.25 per barrel in crude oil tax would have burdened the average energy related expenses per household by 5.54% in 2015, while $10.25 per barrel of crude oil tax will raise EPIC over the next four years by $0.997/MMBtu on average and will generate more than $300 billion over the same period. Increasing the percentage share of nuclear and renewable energy in the electric power sector will also assist towards tackling policy issues related to climate change. Moreover, the design of the policy case study using the EPIC framework has proved the unique ability of EPIC to determine the trade-offs among different energy sources within the electric power sector. The results have shown that hydroelectric, wind, solar and geothermal power will cause a drop in energy prices even with no tax credit. Hydroelectric and wind power should be the main areas of interest due to their higher impact in reducing the cost of electrical energy without requiring any subsidies.

Living in an era where the mitigation of climate change with sustainable solutions has become a key target globally, the developed framework provides a mathematical tool to accurately quantify and evaluate different policies.

5. UTILIZING PROCESS SYSTEMS ENGINEERING TOWARDS CIRCULAR ECONOMY*

5.1 Background & Motivation

Natural resources, the environmental impact of manufacturing, and the economics of production play critical roles in the development and wealth of societies. Preservation, impact reduction, and economic efficiency are vital for the provision of manufactured goods, energy, food, shelter, transport, and – more generally – almost all basic functions of society. Population growth, economic growth, and increasing requirements for the standard of living mean that more and better goods are in demand, which in turn require more natural resources and manufacturing activity. Such developments, if not carefully designed, can lead to resource depletion/degradation, more landfill waste, higher levels of pollutants, and increased environmental impacts, such as climate change.

The concept of "Sustainability" has been gaining traction as climate change, resource depletion and biodiversity loss are becoming more and more evident. Even though this term is highly used by businesses, governments and the research community, it lucks implementation specificity as it is open to a wide interpretation. This has lead to vagueness of the term, while Circular Economy (CE) can be viewed as an operational tool with specific goals, aimed for businesses as a means to achieve economic, environmental and social sustainability.

5.2 Introduction

CE aims to solve resource, waste, and emission challenges confronting society by creating a production-to-consumption total supply chain that is restorative, regenerative, and environmentally benign. It does this by keeping products, components, and materials at their highest utility and value with minimal to non-existent waste at all times.

The transition towards CE requires four areas of system improvements: reuse, repair, re-

*Reprinted from "Circular Economy-A challenge and an opportunity for Process Systems Engineering" by S. Avraamidou, S.G. Baratsas, Y. Tian, E.N. Pistikopoulos, Computers & Chemical Engineering, 2020, 133, p.106629, with permission from Elsevier and Copyright Clearance Center. A summary of the work is given in this chapter, with additional details provided in Appendix H.

manufacturing, and recycling. Although these actions help close loops and connect discrete stages of the supply chain, interconnections among the diverse supply chain elements, stakeholders, and regulatory environments, they also pose significant challenges for decision making. In addition to these strategic actions and goals, there is still a lack of quantitative metrics to define the targets of CE. For example, what is considered as a proper baseline metric for waste recovery rate achieved via CE? Also, how is the assessment of waste recovery rate defined, e.g. based on available wastes or their re-usability factor? Thus, it is clear that a holistic systems engineering approach is needed to quantitatively navigate and fully consider the multi-scale, multi-faceted and interconnected CE supply chain, to identify opportunities for beneficial improvement, to systematically explore interactions and trade-offs, as well as to assist quantitative assessment and decision making.

Process engineering could play a crucial role in providing the required tools and methods for the transition towards CE. There is a large overlap between the objectives widely explored by the Process Systems Engineering (PSE) community and the CE reported goals [182, 183], which are presented in the following sections and Appendix H. Additionally, a systems engineering framework for the optimization of food supply chains under circular economy considerations is demonstrated in Chapter 6.

5.3 Literature Review Process Systems Engineering and Circular Economy

Since a holistic systems engineering approach is required for the transition towards a CE, PSE could provide many of the necessary tools and methods assisting to this direction. Therefore, a literature review on PSE tools and research areas focusing on achieving the objectives of CE is presented in this section and in Appendix H.4 .

Figure 5.1 illustrates the large overlap between the objectives widely explored by the PSE community and the CE reported goals, showing that most of the CE reported goals have been explored by the PSE community. Even though these objectives have not been tackled holistically, or at the scale to be directly applicable for CE, the methodologies and tools developed by the PSE community (Figure H.1) have the potential to assist decision-makers in the transition towards a CE.

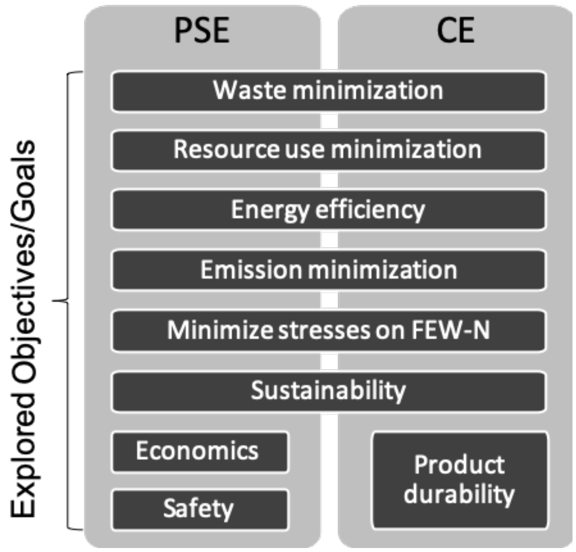

Figure 5.1: Explored Objectives in Process Systems Engineering and Set Goals of Circular Economy

Tables 5.1 includes indicative contributions by the PSE community for the achievement of different CE goals as reported in [182] and [183]. From this table, it is clear that different PSE approaches have already been applied for decision making regarding most of the goals of CE. It is also evident that the PSE community has a lot of expertise in some areas and goals of CE, even though these were not addressed holistically and their original intent was not explicitly for CE. But, at least to my knowledge, no effort or developments have been reported by the PSE community for the maximization of the durability and reliability of the products, which is a key goal of CE - even though many PSE tools can have the potential to include this consideration (Figure H.1). This indicates an obvious gap in PSE research and exploring this can have a high impact towards the transition to a CE.

Appendix H.5 provides a selection of some of the most important PSE tools and methods that can be utilized towards a CE.

However, PSE faces several challenges and scientific needs towards this transition to a CE. Appendix H.6 highlights these challenges and presents some of them in detail.

Table 5.1: Indicative PSE Contributions for Achieving Different CE Goals

PSE Field	Circular Economy Goal				
	1	2	3	4	5
Multi-Objective Optimization	[184] [185]	[186] [184] [187] [185] [188] [189] [190]	[184] [191] [185] [189] [190]	[186] [192] [193] [194] [184] [195] [188] [196] [190]	
Multi-Scale Modeling and Optimization	[197]	[198]	[198]		
Supply Chain Optimization	[199] [200] [59]	[186] [187] [201] [188]	[199] [202]	[186] [192] [199] [202] [193] [194] [188] [196]	
Optimization under Uncertainty	[203]	[204] [205] [201]	[206]	[195] [206]	
Mixed-Integer Optimization	[199] [207] [208] [200] [209] [184] [210] [59]	[186] [199] [207] [184] [187] [188] [189]	[199] [184] [189] [211] [210]	[186] [192] [199] [193] [207] [194] [184] [188] [196] [210]	
Resource Management	[207] [212] [213]	[207] [212]		[207]	
Food-Energy-Water Nexus	[207] [214] [184]	[207] [215] [184] [187] [189]	[215] [184] [189]	[207] [184]	
Process Integration and Intensification	[216] [210] [217] [218] [219]	[216] [217]	[211] [210] [220] [218] [219]	[216] [221] [210] [222] [223] [218] [219]	
Sustainable Process Synthesis and Design	[216] [199]	[216] [199]	[199] [202]	[199] [202] [194] [224]	
Life Cycle Assessment	[216] [225] [199] [226]	[216] [225] [186] [199] [190]	[225] [199] [190]	[225] [186] [199] [193] [196] [190]	

1 - Reduce Material Losses/Residuals, 2 - Reduce Input and Use of Natural Resources, 3 - Increase Energy Efficiency and the Share of Renewable, 4 - Reduce Emission Levels, 5 - Increase the Value Durability of Products

5.4 Motivating Case Study - The Supply Chain of Coffee

The aforementioned challenges and opportunities of PSE transitioning to a CE are illustrated through the supply chain of coffee. The coffee supply chain is selected since it produces a lot of waste and uses a lot of resources, thus it is highly relevant and easily understandable for the transition towards a CE. More details about the efficient transition towards a CE coffee supply chain are illustrated in the next chapter, where the newly developed systems engineering framework for the optimization of food supply chains under CE considerations is applied into the coffee supply chain.

Coffee is one of the most popular beverages worldwide with more than 167 million 60-kg bags of coffee being consumed yearly worldwide [227, 228]. The global coffee supply chain creates an estimated 23 million tons of organic coffee waste per year [229]. In fact, just one cup of coffee (containing about 10g dry coffee), produces through its entire supply chain about 49g of CO_2 emissions [230], 9.9g of dry spend coffee waste, 6.9g of dry coffee pulp, husk and skin waste [3] and plastic used for packaging, cups, straws and stirrers. Furthermore, just for one cup, 140 liters of water (mainly for irrigation) [7] and 0.13 kWh of energy [230] are needed.

The following subsections and Appendix H.7 present the linear and circular coffee supply chain, discuss the challenges that arise from the transition and the opportunities for PSE to assist in this transition.

5.4.1 The Transition from a Linear to a Circular Coffee Supply Chain

The produced wastes and the used resources can be minimized when linear coffee supply chain evolves into a CE structure. Figure 5.2 illustrates a simplified coffee supply chain. Energy, mainly from fossil fuels, is used for every process in the supply chain, while water is used and contaminated in many processes (highly based on the coffee processing methods).

Moreover, waste is created at every stage; **W1** corresponds to the wastes and emissions created when fossil fuels are used for the generation of energy, **W2** corresponds to the water contaminated with fertilizers during irrigation processes, **W3** are bad coffee berries collected during harvesting, **W4** are berry parts (the coffee pulp, coffee husk, and silver skin) that are discarded during processing, **W5** corresponds to spillages and degradation during packaging, **W6** corresponds to plastic waste, **W7** corresponds to expired and degraded packaged coffee, **W8** corresponds to expired coffee, spent coffee and plastic packaging and **W9** corresponds to the plastic cups, straws, and stirrers.

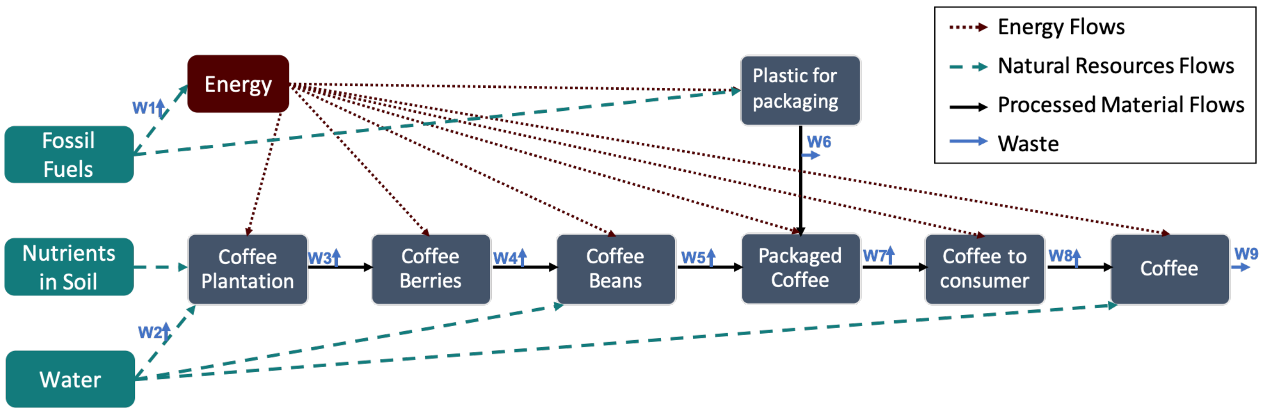

Figure 5.2: Supply Chain of Coffee in a Linear Economy

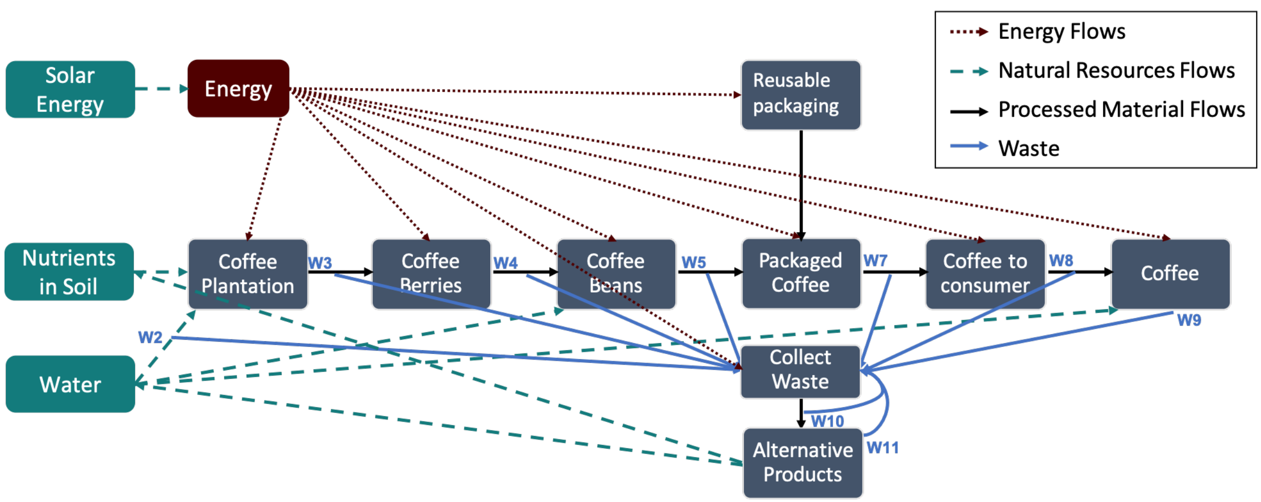

Figure 5.3: Supply Chain of Coffee in a Circular Economy

The transition towards a CE coffee supply chain (Figure 5.3) would require the transition to renewable energy resources and reusable packaging solutions. Processes that are more energy efficient, produce less waste and contaminate less water, will need to be chosen. It would also require the collection of all created waste and their processing to produce alternative products.

In addition, natural resources (water and nutrients) need to be returned to their source, thereby, closing the loops and creating a CE that is closed in terms of material flows and open in terms of energy flows.

5.4.1.1 Coffee Organic Wastes and Alternative Waste Management Pathways

Coffee production generates waste from the coffee berries responsible for more than 50% of the fruit mass [231], while spent coffee (the residue obtained during the brewing process) constitutes about 99% of the dried roasted coffee bean. In most of the soluble coffee producing industries, the waste is collected at a cost and disposed or, in limited cases, it is used as a raw material for different purposes. A selection of the different products that can be produced form organic coffee waste is illustrated in Figure H.3. These different pathways can reduce not only the economic and environmental costs of disposal but also to generate revenue from an undervalued material.

5.4.1.2 Challenges and Opportunities for PSE towards a Circular Coffee Supply Chain

The transition of the coffee supply chain from a linear to a CE consists of many challenges but at the same time many opportunities for PSE. Advanced modeling and novel optimization techniques can be used for the assessment and identification of multiple and alternative pathways, while process integration and intensification could lead to more efficient processes. Therefore, a methodology that combines CE assessment metrics along with superstructure optimization shall be developed, enabling the evaluation of the different supply chain pathways and their technologies. The coffee supply chain also involves multiple stakeholders at multiple levels. Hence, hierarchical modeling and multi-objective optimization is needed for such a complex supply chain. Additionally, the multi-spacial and multi-temporal nature of the coffee supply chain complicates even more the situation, requiring new multi-scale modeling approaches and effective decomposition methods for a supply chain of such scale.

Appendix H.7.1 summarizes some of these challenges and the corresponding research opportunities for PSE.

5.5 Conclusion

Circular economy (CE) is considered as an approach that effectively matches the economic growth with sustainable economic, environmental and social development, providing an alternative, cyclical flow model to the conventional linear economy models [28]. A systems engineering approach can have a big impact on the understanding, analysis, and optimization of the multi-scale, multi-spacial and multi-temporal interconnected CE supply chains that are governed by multiple stakeholders with conflicting objectives, under uncertain and dynamic conditions. The goal remains the convergence of different disciplines towards a common vision of CE. The move towards such an economy model can result in many challenges but also many opportunities for PSE due to the inherent complexities of this model. Thus, this work serves as a first step for the identification of these challenges and a review of the literature gaps on the necessary methodologies, which along the existing techniques will allow the transition towards a CE.

In the next two chapters, two such frameworks that utilize PSE methodologies towards the CE transition are presented. The first one refers to a systems engineering framework for the optimization of food supply chains under CE considerations, with a detailed case study on the coffee supply chain. The second one demonstrates a quantitative and robust CE assessment framework that holistically assess circularity at the micro level.

6. A SYSTEMS ENGINEERING FRAMEWORK FOR THE OPTIMIZATION OF FOOD SUPPLY CHAINS UNDER CIRCULAR ECONOMY CONSIDERATIONS*

6.1 Background & Motivation

Rising populations across the world [232] seek to improve their standards of living, placing huge stresses on natural resources and supply chains [233]. Energy and operational efficiency, improvement in manufacturing processes, quantitative management of food-energy-water nexus [234, 235, 184], and economic growth are vital to fulfill the increasing demand for goods, food and services [120], however they still lead to natural resource degradation [236], substantial waste generation [237], water contamination [238], and surging greenhouse gas emissions [239, 240, 241, 242]. Thus, economic expansion shall be combined with sustainable development, ensuring the advancement of our societies while preserving the environment [243, 244, 245]. This requires a fundamental transformation of our economic model [246] that promotes the "take-make-use-dispose-pollute" concept to a more "sustainable" one [247, 248].

Circular Economy (CE) has emerged as a potential solution for such a transition, with extreme emphasis being put towards improvement in reuse, remake, repair and recycling [249]. [250] defines CE as a combination of production-consumption systems that maximizes the output services in a sustainable manner, without violating the natural reproduction rates, while utilizing cyclical material flows, and renewable energy sources and flows. CE aims to solve resource, waste, and emission challenges confronting society by creating a production - to - consumption total supply chain that is restorative, regenerative, and environmentally benign [28]. Eco-effectiveness, through a holistic optimization of all components, along with a great emphasis on the design and systems thinking, is the main focus of CE [249, 27]. As it has been been highlighted in the previous chapter and Appendix H, the goals and key characteristics of CE [182] are summarized as follows:

*Reprinted from "A systems engineering framework for the optimization of food supply chains under circular economy considerations" by S.G. Baratsas, E.N. Pistikopoulos, S. Avraamidou, Science of Total Environment, 2021, Vol. 794, pp 148726, with permission from Elsevier and Copyright Clearance Center. A summary of the work is given in this chapter, with additional details provided in Appendix I.

1. Reduction of material losses/residuals: Waste and pollutants minimization through the recovery and recycle of materials and products.

2. Reduction of input and use of natural resources: The reduction of the stresses posed on natural resources through the efficient use of natural resources (e.g. water, land, and raw materials).

3. Increase in the share of renewable resources and energy: Replacement of non-renewable resources with renewable ones, limiting the use of virgin materials.

4. Reduction of emission levels: The reduction in direct and indirect emissions/pollutants.

5. Increase the value durability of products: Extension of product lifetime through the redesign of products and high-quality recycling.

CE can contribute to all dimensions of sustainable development, but it should not be confused with sustainability since they have different goals, motivations, prioritizations, institutionalizations, beneficiaries, time-frames, and sense of responsibilities [251]. The successful and inclusive economic, environmental, and social integration is fundamental for sustainability and sustainable development. Although, the term is quite ambiguous and lacks implementation specificity, it refers and applies to a variety of contexts and time horizons. On the contrary, CE is viewed as an operational tool to enforce sustainability [252] through economic prosperity, environmental quality and social equity considering earth as a closed and circular system where economy and environment coexist in equilibrium. Even though the CE concept is still relatively new, with little scientific guidance regarding its successful implementation and its effective evaluation [253, 254], the economic, environmental and social aims are evident from its adoption into national laws at international and regional levels (macro and meso systems), as well as at the level of private corporations and businesses (micro system). However, the extensive and universal nature of CE introduces significant challenges for the decision-making which are exacerbated from the interconnections among the diverse supply chain elements, stakeholders, and regulatory environments. Therefore, a holistic systems engineering approach is required to quantitatively navigate and thoroughly address the multi-scale, multi-faceted and interconnected CE supply chains [255].

6.2 Introduction

Food loss and waste throughout the supply chains represent about one-third of the food that is produced, although more than 820 million people remain chronically undernourished [256]. The annual economic costs of this food waste are estimated at $ 1 trillion, skyrocketing to $ 2.6 trillion on annual basis when environmental and social costs are accounted for [257]. Likewise, the contributions of food loss and waste to climate change are also significant, accounting for about 8% of global greenhouse gas (GHG) emissions [258].

Innovative, collaborative and drastic approaches must be deployed to tackle such a challenging issue. The 2030 Agenda for Sustainable Development from the United Nations has identified and promoted two Sustainable Development Goals (SDGs), particularly SDG 2 and SDG 12 for targeting a Zero Hunger world and ensuring sustainable production and consumption patterns respectively [148]. The implementation of sustainable agriculture will assist towards food security and enhanced nutrition while reducing food loss and waste would result to more efficient land use and improved water resource management with beneficial effects on climate change and livelihoods. Thus, intergovernmental and international collaborations to promote such transformations and advocate new policies are required. Moreover, coordination among the various stakeholders of the food supply chains (FSCs) with parallel switch of the shopping and consumption habits will accelerate this transition [259].

6.2.1 CE Food Supply Chains - (CE FSCs)

The concept of CE is of extreme importance in this direction since by definition it is associated with optimization of resources and energy utilization while preserving the environment. CE-FSCs imply minimization of the waste and GHG emissions generated at the various stages of the supply chain. This can be achieved through recovery and recycle, valorization of food waste and by-products as well as by re-using food and recycling nutrients through behavioral change of the consumers, integration of renewables and efficient use of natural resources. Moreover, advanced preservation techniques and reliable storage shall be utilized to increase the lifetime and quality of products. The loop of the nutrients and other materials shall be closed; while the loop of energy shall be open. This "zero-waste" approach is a key differentiating factor between CE and the other sustainability thinking approaches [260].

Governments, industry and academia have demonstrated a growing interest towards CE over the recent years, however it is still at an early stage. Fassio and Tecco [261] conducted a thorough analysis in 40 case studies evaluating the effectiveness of various CE actions towards integration of SDGs into the food systems. Although, the concepts of optimization performance and efficiency along with regenerative and loop actions have emerged, however the practical implementation of CE into the food systems is still missing, while socio-economic and environmental considerations are often omitted. Innovation for circularity and sustainability have become not only a necessity due to climate change and economic environment, but a fundamental for all involved parties to maintain and/or improve their competitive advantage in the 21st century. The intrinsic complexity and comprehensive nature of CE mandates multidisciplinary and collaborative efforts. Process systems engineering (PSE) accompanied by environmental engineering and horticultural sciences could play a crucial role in providing the required tools towards the transition to CE-FSCs [255].

To this respect, the foundations of a systems engineering framework and quantitative decision-making tool for the analysis and trade-off optimization of interconnected FSCs, governed by the CE principles are presented [262]. The explicit incorporation of CE goals and objectives into the design and operation of FSCs is a key contribution of the proposed framework. FSCs demonstrate unique characteristics, restrictions, objectives and challenges in comparison to the other product or service supply chains. In particular, FSCs consist of several interdependent steps such as farming, processing, distribution, retailing, in a domino type transition. Humans ingest food for nourishment, and as such issues related with perishability, preservation requirements, quality decay, short shelf life and delivery restrictions, necessitate the highest standards of safety and quality for the delivered products [263]. FSCs are also confronted with soaring consumer demand, leading to huge stresses on natural resources and the environment, significant energy requirements as well as substantial waste generation at the various stages. The recent movements towards improved food quality, increased food shipping traceability, along with the emerging ethical dilemmas such as the utilization of biomass for food or fuel and the rising sustainability concerns, set a new scene around the globe, calling for transformational changes across the multi-spacial and multi-temporal FSCs.

The proposed CE-FSC framework combines data and information from the academic and industrial literature, along with mixed-integer modeling to establish the interconnections among different stages of the circular FSCs as well as multi-objective optimization to consider all CE objectives and analyze trade-offs. It is flexible since the set of resources and tasks, as well as the supply and demand information can be constantly updated, reflecting recent trends and developments. Apart from systematically capturing the extensive, up-to-date set of production, processing and valorization pathways, the proposed CE-FSC framework contributes to the literature in a dual manner. First, it enables the identification and selection of the optimal tasks from the list of all alternative processes based on certain CE objectives. On top of that, it allows the identification of the least efficient processes or even sections of the network, which introduce potential bottlenecks within the supply chain. This is a key feature that refocuses the interest and promotes the research and development on the less developed sections of the supply chain. Furthermore, users from a variety of backgrounds can benefit from the proposed framework. Academics and experimentalists could concentrate on the improvement of existing processes or on the creation of completely new ones, while private corporations could evaluate the circularity of parts or their entire supply chains. Governmental policymakers could determine areas that require improvement, and thus promote legislative actions and allocate funding towards these areas.

The supply chain of coffee is used as a case study to illustrate the effectiveness and applicability of the proposed framework. The current linear coffee supply chain is transformed into a circular one under different supply and demand scenarios. Due to the competing nature of CE objectives and supply chain's stakeholders, a multi-objective optimization approach is developed, and solved to optimality by generating different pareto fronts. Therefore, the case study highlights the usefulness of the framework as a decision-making tool that incorporates all sets of tasks and resources under various design and operational criteria and conditions.

6.3 Circular Economy Food Supply Chain Framework

The necessity of the transition to a sustainable food system through the application of CE principles has been recognized and discussed in the literature [259]. Potential barriers and promising solutions have been considered, including economic and environmental [264, 265], regulatory [266], technological [267], and sector specific [268] obstacles. In addition, theoretical and practical insights along with strategic aspects of the CE supply chains in general have also been reviewed [269]. Business and governmental leaders have initiated collective efforts to accelerate the transition towards CE for the food system and FSCs, by setting objectives, identifying barriers and proposing solution strategies [270]. The interest though is focused on the theoretical and qualitative analysis of this transition, primarily for individual supply chains, without providing a holistic, quantitative framework.

The developed framework comes to address this gap through a holistic systems engineering approach, enabling the navigation and fully consideration of any multi-scale, multi-faceted and interconnected CE-FSC. It provides a systematic way to identify opportunities for beneficial improvement, and exhaustively explore interactions and trade-offs. Specifically, it addresses the following problem:

"Given a specific food supply chain, the framework determines the optimal production and processing network based on all CE criteria and different supply and demand scenarios."

The proposed CE systems engineering framework for FSCs consists of five steps. 1) Production and Processing Pathways. This step is used to model all the stages for the production and processing of the existing supply chain, and then identify and assess all the alternative pathways for the production of the desired product. 2) Waste, Loss and By-Products Valorization Pathways.

This step involves the identification and assessment of all the alternative pathways for the waste valorization and food losses minimization. 3) Resource-Task-Network (RTN). In this step, a RTN superstructure representation that includes all the various alternative pathways shall be designed. 4) Mixed-Integer Linear Programming (MILP) Model. This step involves the formulation of the MILP model that captures the entire FSC, its objectives and its constraints into a mathematical modeling representation. 5) Single or Multi-Objective MILP Optimization and Assessment. This last step translates the decision-making process into a single or multi-objective MILP optimization problem, allowing for simultaneous consideration of economic, energy efficiency and environmental criteria. The framework is summarized in Figure 6.1. Each step is discussed in detail in the following sections.

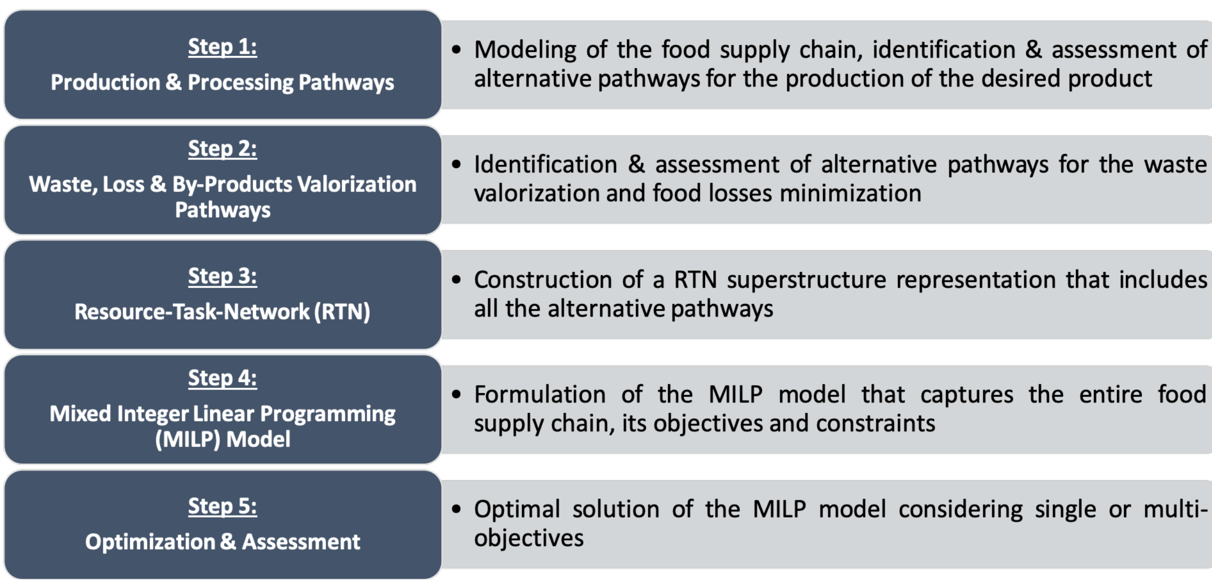

Figure 6.1: CE-FSC Framework

6.3.1 Step 1: Production and Processing Pathways

Agricultural commodities such as crops and livestock are produced when farmers, fishers, and ranchers combine their land, water and labor resources with capital, machinery and manufactured inputs [271]. Then, food can be sold either directly to the end-consumers, or is handled and processed by other sectors before being consumed. The optimization of any FSC considering CE goals and objectives, requires the detailed identification and assessment of all possible stages of the supply chain, including any alternative pathways along with the involved resources. The initial step requires the identification of the input, intermediate, and output resources. Then, a superstructure representation of the FSC must be developed that involves all the stages from harvesting and processing to production and distribution of the final desired product(s), including the conversion factors among these stages. Having determined the resources and processes that are required to produce, process and distribute the final product(s), then any alternative pathways that improve circularity have to be identified and incorporated within the supply chain. The exacerbated nutrients and water imbalances among supply chains and countries driven by the increasing demand for nutrients, especially phosphorus, the massive nutrient losses, the water scarcity and pollution, and the globalized structural development of industrialized agriculture [272] must be thoroughly investigated. Under the current linear FSCs, the majority of the waste generated at the different stages are sent to landfills, while the CE-FSC has a zero-waste vision. The goals and key characteristics of CE as described above, should be the guide for this transition towards CE. As such, minimization of the usage of new materials and valorization of wastes through recycling and recovering as well as improving the efficiency of processes or introducing new more efficient ones, should be the priority. New technologies and processes that promote a restorative and regenerative design of FSCs taking advantage of renewable resources and energy must be considered. Having a thorough and inclusive perception of the production and processing pathways of a particular FSC along with the state-of-the-art new developments require a comprehensive literature and business review.

6.3.2 Step 2: Waste, Losses and By-Products Valorization Pathways

In continuation to the previous step, the superstructure representation is extended to capture all the waste, losses and by-products pathways. CE aims to close the material loops and turn the outputs of one supply chain or a manufacturer into inputs for another [273], treating waste as a secondary resource [27]. To this direction, it is necessary to have a clear and unambiguous hierarchy of the food waste (FW), surplus (FS) and losses (FL), which will allow the selection of the most environmentally-efficient end-of-life treatment.

The prevention of FS should be the top priority, followed by reuse of food for human consumption and then reuse for animal feed, before considering material recycling, nutrient and energy recovery and having as the last step the food disposal only if it is unavoidable [274]. However, and despite the efforts, a certain amount of food will end up as waste and/or loss. Thus, it is important to incorporate into the CE-FSC framework the concepts of edibility and possibility of avoidance, which eventually leads to six distinct categories for FS, FW and FL, as proposed by Teigiserova et al. [274]: i) edible - (FS), ii) naturally inedible - (FW), iii) industrial residue - (FW), iv) inedible due to natural causes - (FW), v) inedible due to ineffective management - (FW) and vi) not accounted for - (FL).

Treating waste, losses and by-products as a resource into the CE-FSCs, enables an indefinite use of natural materials and resources [266]. An extensive literature and technological review needs to be conducted for the identification and assessment of alternative pathways for the waste and by-products valorization across the supply chain. Technological innovations, superior processes, optimized sequences for the design, processing, packaging, distribution of food products, must be integrated into the original FSCs to ensure the successful implementation of the "zero-waste" goal. By determining the input - output relationships and the conversion factors among the processes, the energy and material footprints of the FSCs are modeled and calculated. Equally important is the extent of utilization of model approximations within the framework which is directly related to the data availability, data acquisition and handling as well as the degree of acceptance of approximate representations [275]. Various sources could provide significantly different or even contradicting technological, environmental and economic information, thus minimum and maximum limitations are taken into consideration. Ideally, the CE-FSCs would demonstrate alternative pathways that will utilize any waste and by-products for the production of high added value products, such as energy and new materials.

6.3.3 Step 3: Resource-Task-Network (RTN) formulation

Having completed the identification of the alternative pathways for production, energy and waste valorization, the next step of the CE-FSC framework involves the construction of a Resource-Task-Network (RTN) representation. The RTN representation is a generic and simple mathematical formulation of the interactions between tasks and resources that lead to a bipartite directed graph. Resources include equipment, materials, energy, utilities, manpower, warehouses, distribution locations etc., and are represented as a circle in the RTN, and can be classified as renewable and non-renewable. As non-renewable resources are considered all kinds of materials, utilities, manpower etc., whereas as renewable resources are considered any technological resources in the supply chain network such as production facilities, warehouses, distribution centers, transportation vehicles. Resources are also characterized by their location, enabling the identification of distances between units, which is essential for the modeling of the material transfers within the supply chain network. Therefore, a facility that involves multiple tasks is modeled implicitly, not explicitly, through its associated equipment and technologies at a particular location. A task, represented as a rectangle, is actually an abstract operation that can produce, transform, transport, store, and/or supply resources, with the resources being treated uniformly. As such, tasks may purchase, sell, or store resources, transform one set of resources into another, produce or consume resources at any point of time etc. [276]. Figure 6.2 provides an example of the RTN representation. In this case, Resource1 and Resource3 are consumed in Task 1 for the production of Resource4. Similarly, Task2 consumes Resource1 and Resource4 for the production of Resource6 and so on.

Such a representation enables the modeling of the supply chain resources and tasks as an optimization model, integrating all the design and planning characteristics of the particular supply chain. The resources and tasks along with their interrelationships need to be identified from the postulated set of alternative options. Processing equipment units are treated explicitly, which means that units in different conditions e.g. "clean" or "dirty" shall be treated as different resources, although in general, the defining attributes of a resource type depend on the content and the detail of modeling [276, 277]. This superstructure representation provides a generic design methodology that can be applied to any type of FSCs.

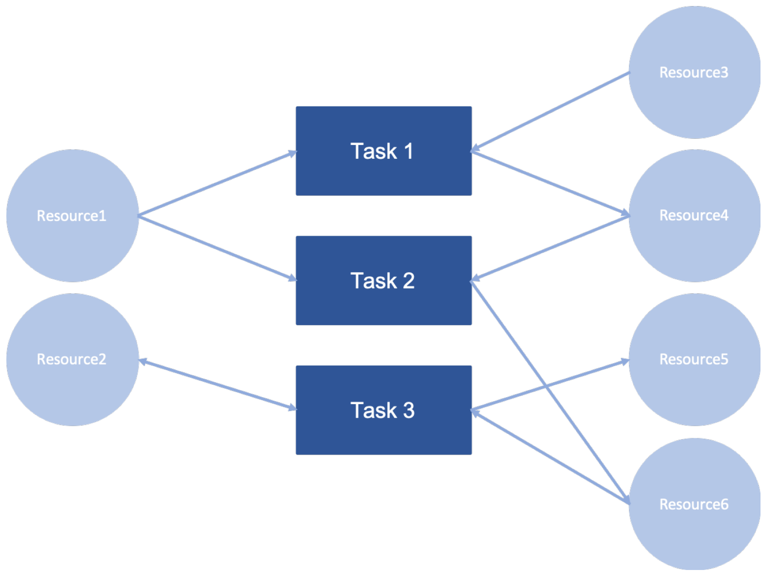

Figure 6.2: Resource-Task-Network (RTN) representation [1]

6.3.4 Step 4: Mixed-Integer Linear Programming (MILP) model formulation

Taking advantage of the previous step where the FSC is represented as a RTN superstructure, here this information is translated into a mathematical model of the supply chain. The mathematical model consists of variables, parameters, constraints and mathematical relationships. Variables can take different values reflecting different states of the supply chain. These values can be continuous, integer, or a mixed set of continuous and integers. On the contrary, the parameters have specific, one or multiple, fixed values with each one of those representing different models of the system. Restrictions and limitations of the supply chain are expressed through constraints. The logical conditions among the variables, along with the equality and inequality expressions define the mathematical relationships of the system [278].

Based on the RTN superstructure representation both continuous and integer variables are required to capture the entire FSC, economic and environmental objectives and constraints. The selection (or not) of any task, meaning any process, technology and/or equipment, within the mathematical model is governed by a binary variable. The same applies for the selection (or not) of a resource, i.e. material, energy etc. Therefore, a binary variable y_j is introduced in the model to represent the selection (or not) of a task (process, technology or equipment) and a binary variable y_i is introduced for the selection (or not) of a resource (material, energy etc.) as follows:

$$y_j = \begin{cases} 1, & \text{if the corresponding task (process, technology or equipment) is selected} \\ 0, & \text{otherwise} \end{cases}$$

$$y_i = \begin{cases} 1, & \text{if the corresponding resource (material, energy etc.) is selected} \\ 0, & \text{otherwise} \end{cases}$$

Then, continuous variables are used to reflect the design and operational decisions that need to be made. For example, the amount of material that is used as input or output of a process, or the amount of material that is consumed during a process are modeled through continuous variables. All the mass and energy characteristics of the tasks that arise from the mass and energy balances are governed by linear relationships with respect to the inputs / outputs and conversion rates.

The various constraints that govern a FSC are also captured through the introduction of equality and inequality constraints. Typically, these constraints are imposed by the conservation of mass or energy (mass and energy balances) within the supply chain, the conversion rates of a task/process, raw material availability, and/or capacity and technological limitations. For example, limited supply of resources for a production process leads to constraints derived from the relationship between this supply and its possible utilization by different tasks. Constraints may be also introduced from externalities such as governmental policies, market restrictions etc., in a form of limitations in the supply of resources and/or demand of products. Finally, big-M constraints are used to ensure that a process is not operational unless it is built. If it is built, then certain limitations are enforced to the model e.g. operating levels of a process may not exceed an upper bound of M.

The existence of both continuous and integer variables in approximated linear forms lead to the formulation of the FSC model as a mixed-integer linear programming (MILP) problem. The performance criterion is denoted as objective function, and can involve economic, energy efficiency and/or environmental features. Here, the objective functions are matched with the aforementioned goals and characteristics of CE as can be seen in Table 6.1. Therefore, the reduction of material losses and residuals is explored through the minimization of the generated waste, and the like. In case non-linear terms are required either in the objective function and/or in the constraints to represent the involved phenomena, then the model is classified as mixed-integer nonlinear programming (MINLP) problem. This implies a number of difficulties associated with the modeling and the solution of such problems, which must be carefully addressed [278, 279], and are beyond the scope of the proposed framework.

Table 6.1: Formulating the Objective Functions based on the CE Goals

#	CE Goals & Key Characteristics		Objective Functions
1	Reduction of material losses/residuals: Waste and pollutants minimization through the recovery and recycle of materials and products.	↔	Minimization of generated waste, Maximization of recycling
2	Reduction of input and use of natural resources: The reduction of the stresses posed on natural resources through the efficient use of natural resources.	↔	Minimization of consumed raw materials and natural resources
3	Increase in the share of renewable resources and energy: Replacement of non-renewable resources with renewable ones, limiting the use of virgin materials.	↔	Maximization of total energy and/or renewable energy output
4	Reduction of emission levels: The reduction in direct and indirect emissions / pollutants.	↔	Minimization of GHG emissions
5	Increase the value durability of products: Extension of product lifetime through the redesign of products and high-quality recycling.	↔	Maximization of product, equipment and packaging durability

6.3.5 Step 5: Single or Multi-Objective Optimization and Assessment

The final step of the CE-FSC framework involves the optimization of the model developed in the previous steps, considering single or multi-objectives. In case of a single objective, the optimal solution is easily determined against other solutions by comparing their objective function values. When more than one objective function is involved and must be optimized systematically and simultaneously, then the problem is called multi-objective optimization. In general, there is no single global solution for this type of problems but rather a set of solutions that define the best trade-off among the competing objectives. The set of these non-dominated solutions over the entire feasible space is called pareto-optimal set, and a pareto efficient front is generated from the boundary of this set.

The most commonly used methods for solving multi-objective optimization problems are the weighted sum method and the ϵ-constraint method [280, 281]. In the first method, the multi-objective problem is transformed into a single objective one by adding weighted objectives. The weights used reflect the relative importance of each objective. The second method involves the optimization of one of the objective functions using the rest of the objective functions as constraints of the problem [282, 283]. In the developed CE-FSC framework the ϵ-constraint method is used, ensuring that the pareto solutions are evenly distributed over the solution space, while attaining a precise representation of the efficient set. The user can even specify the number of the generated efficient solutions by adjusting the number of intervals on the feasible region.

6.4 Case Study: Circular Economy Supply Chain of Coffee

In continuation to the motivating case study that is presented in the previous chapter, the supply chain of coffee is selected for demonstrating the applicability and effectiveness of the proposed CE-FSC framework, as a tool for designing and optimizing the transition from the current linear supply chain of coffee to a circular one. Coffee has been selected here since it is one of the most popular beverages globally with more than 167 million 60-kg bags of coffee being consumed yearly worldwide [284]. This is translated into over 2 billion cups of coffee being consumed on daily basis [228, 285]. As a result, the global coffee supply chain creates an estimated 23 million tons of organic coffee waste per year [229], while it requires a considerable amount of resources such as energy and water. Coffee industry has also an enormous impact in the economy, representing approximately 1.6% of the total US GDP [286]. Therefore, such as global supply chain that produces a lot of waste and uses a lot of resources, is ideal for the demonstration and application of the proposed framework towards CE.

A typical coffee supply chain is shown in Figure 6.3. Coffee cherries are harvested and then processed in two different ways, the dry and the wet process, resulting in different coffee products and by-products as well as products of different quality. In the dry process, the cherries are dried for a period up to three weeks (i.e. Drying) and then the outer and the inner shells are mechanically removed (i.e. Hulling), producing the desirable green coffee beans along with the husk as a by-product [287]. Conversely, the wet process requires excessive amount of water and is conducted in multiple stages. The process start with the removal of the outer skin that covers the beans (i.e. Pulping), and then continues with the complete removal of the mucilage from the parchment (i.e. Fermentation & Washing). Then, the parchment is dried either naturally under the sun or technically in a dryer (i.e. Drying) until its moisture level reaches about 10%. Finally, the parchment is removed mechanically (i.e. Peeling & Polishing), producing the desirable green coffee beans [3, 15, 287]. Green coffee beans require further processing before become available for consumption. As such, the green coffee beans must be roasted (i.e. Roasting), acquiring a characteristic flavor and aroma, and becoming available for consumption as whole beans. The roasted coffee is then grounded and can be consumed either as a brew beverage (i.e. Coffee Beverage), after brewing, or further treated by extraction, evaporation/concentration, and drying and consumed as Soluble/Instant Coffee [287]. Caffeine is responsible for the stimulating effect of coffee, and so decaffeination is an extra step that must be taken before roasting the green coffee beans, so as to remove caffeine from the beans.

Apart from the desirable products, wastes and by-products, namely, husk, pulp, mucilage, parchment, silverskin etc. are generated during the coffee supply chain, while significant amounts of resources such as energy and water are also consumed. The overall life cycle burdens of even just one cup of spray dried soluble coffee, equivalent to 4.44 g of green coffee, are significant, with approximately 1 MJ of primary non-renewable energy and up to 400 ltr of water consumed, 70 g of CO_2eq released [6], 3 g of spent coffee and 12 g of coffee by products (pulp, mucilage, parchment) generated [3]. Moreover, plastics are used in various stages of the coffee supply chain introducing another substantial environmental burden.

With the current linear supply chain model (see Figure I.1 in Appendix I), only a small fraction of these burdens are reused or recycled even though there are plenty of studies demonstrating sustainable alternatives [3, 20, 288]. Hence, as the coffee consumption increases, so does the amount of organic coffee waste and the amount of resources used, aggravating both the waste, water and energy management problems.

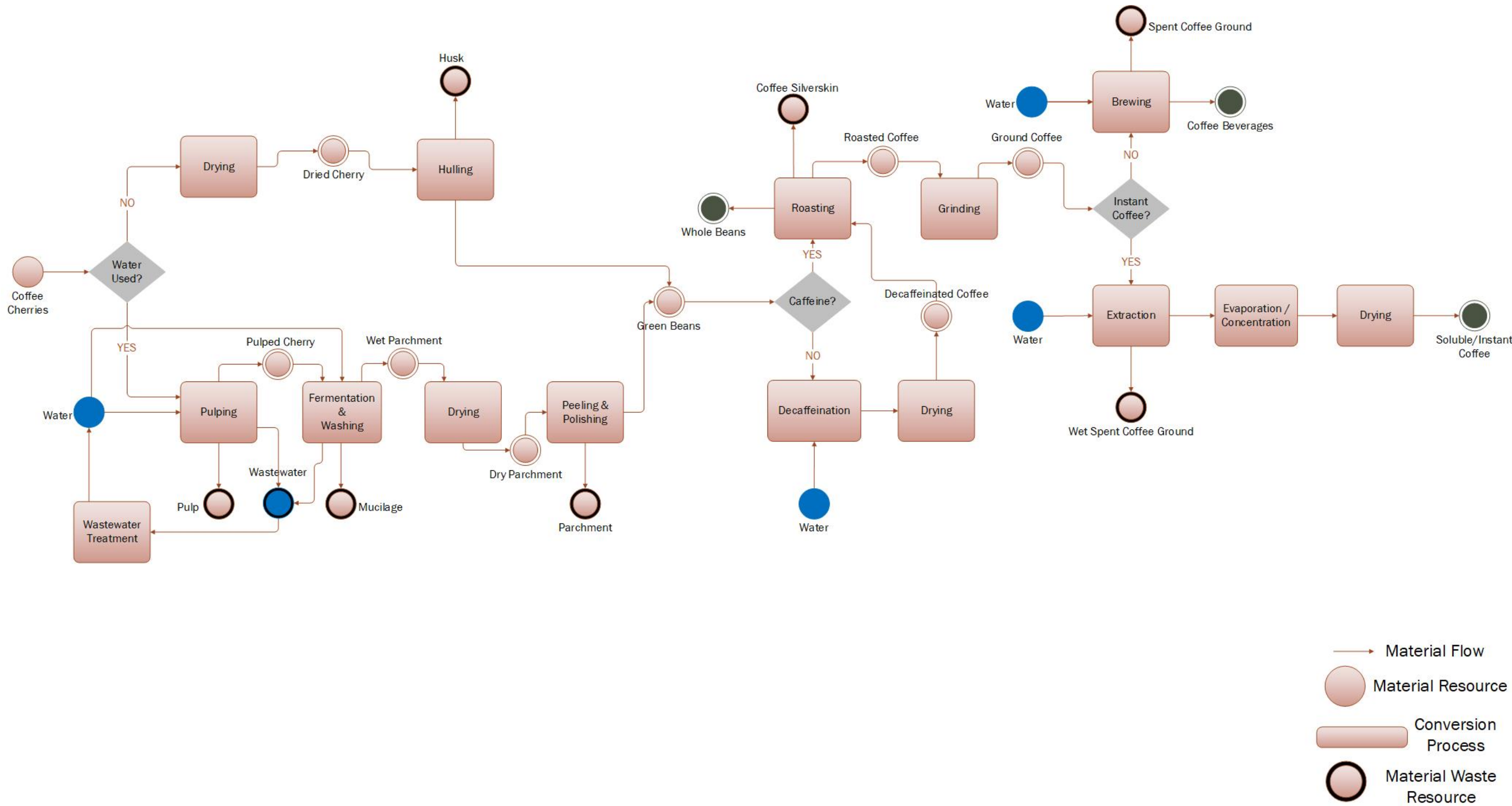

Figure 6.3: Supply Chain of Coffee

A solution to this problem would be the transition to a circular supply chain (see Figure I.2 in Appendix I), where renewable energy resources and more efficient processes will be utilized; water consumption will be reduced and wastewater treatment will be applied; waste generation will be minimized, and all wastes will be collected and utilized for the production of alternative products. The material flows ultimately shall be closed, while the energy flows shall be opened. However, it is evident that the transition to a CE model while tackling the challenges from the multi-scale and multi-faceted coffee supply chain require a holistic systems engineering approach. Therefore, the proposed CE-FSC framework can be utilized in this direction, ensuring an effective and efficient transition. The following sections demonstrate step by step the application of the framework in the supply chain of coffee.

6.4.1 Step 1: Production & Processing Pathways

As an initial step, the coffee supply chain is modeled by identifying the inputs and outputs along with the processes that take place so as to produce the desirable end-products. In this supply chain, three are the desirable end-products i.e. the whole beans, the coffee beverages and the soluble/instant coffee (Figure 6.3), while coffee cherries and water are considered as the main inputs. Moreover, the alternative pathways for the production of the desired product have to be identified and assessed, i.e. wet or dry method for the production of green beans [20], decaffeinated or caffeinated coffee. As it is shown in the following steps, the selected pathway(s) might be different each time, depending on the objective(s) of the optimization problem. This complexity requires extra care during the modeling process.

6.4.2 Step 2: Waste, Loss & By-Products Valorization Pathways

As a second step, the waste, losses and by-products of the coffee supply chain must be identified. Coffee husk is the main pre-roasting by-product from the dry processing method, while coffee pulp, mucilage and parchment are the by-products of the wet processing method. Silver skin is the by-product from roasting the green beans, and spent coffee grounds (SCG) are the final by-products from either brewing or extraction processes. The majority of the wastewater is generated during pulping and fermentation. Thus, a waste waste-treatment facility is considered so as to properly treat this water either for re-use in in the coffee supply chain or for safe discharge back to the environment. Similarly, to the previous step, the alternative pathways for the valorization of the wastes have to be identified and assessed. Thus, an extensive literature review shall be conducted. The following tables highlight such alternative pathways for the valorization of the coffee wastes and by-products for the production of energy (Table 6.2), as well as for the production of value added products (Table 6.3). This analysis, in conjunction with feedback from experimentalists, can help towards the identification of sustainable CE coffee supply chain alternatives.

Table 6.2: Valorization of Coffee By-Products & Wastes for the Production of Bio-Energy

Coffee By-Products & Wastes	Bio-Energy Production						
	Biodiesel	**Bioethanol**	**Biogas**	**Bio-oil**	**Fatty Acid Methyl Ester (FAME)**	**Fuel Pellet**	**Hydrogen**
Coffee Husk		[18]	[288] [20] [3] [11]			[288]	
Coffee Pulp		[288] [289]	[288] [20] [290]			[288]	
Coffee Mucilage		[291]	[20]				[292]
Coffee Parchment			[20]				
Coffee Silverskin		[288] [290]					
Spent Coffee Grounds	[288] [293] [8] [4] [3] [294] [295] [9] [296] [21] [297]	[288] [8] [4] [290] [3] [294] [297]	[8] [4] [290] [298] [299] [300]	[8] [4] [290] [298] [21]	[8] [4] [299]	[288] [8] [4] [290] [301] [296]	[8] [4]

Table 6.3: Valorization of Coffee By-Products & Wastes for the Production of Value-Added Products

Coffee By-Products & Wastes	Value-Added Product Recovery									
	Antioxidants	**Biochar**	**Biopigments**	**Biopolymers**	**Biosorbents**	**Caffeine**	**Carbon Material**	**Composting**	**Enzymes**	**Food ingredients**
Coffee Husk				[290]	[288]	[302]		[288] [290] [3]	[3] [16]	[288] [290] [3]
Coffee Pulp				[3] [302]	[3]	[302]		[288] [3]	[288] [3]	[288] [3]
Coffee Mucilage										
Coffee Parchment										
Coffee Silverskin	[290] [303]					[302]		[302]		[288]
Spent Coffee Grounds	[288] [293] [8] [4] [290] [3] [295] [304] [302] [297]	[8] [4] [301] [298] [295] [21]	[293] [8] [4] [290]	[288] [293] [8] [4] [290] [301]	[288] [8] [4] [290] [3]	[293] [8]	[293] [8] [4] [3]	[288] [293] [290] [301] [297]	[301]	[288] [293] [4] [3] [301]

6.4.3 Step 3: Resource-Task-Network (RTN)

In the previous steps the main along with the alternative pathways of the coffee supply chain have been identified, and so the next step involves the generation of a Resource-Task-Network (RTN) representation that incorporates all these pathways. Here, and for demonstrating purposes, only the alternative pathways for the production of bio-energy are considered. Figure 6.4 illustrates such a RTN representation of the supply chain of coffee, capturing the sections in the production as well as in the consumption countries, the conversion coefficients of the various processes, along with waste valorization alternatives for the production of energy.

The part of the supply chain from the plantation of the coffee cherries, to the production of green coffee beans through the dry or wet processing methods, typically takes place in the production countries, while the rest of the supply chain, that includes the production of the final products, takes place in the consuming countries. The coffee producing countries consume significant resources in the form of raw materials, energy, and water while the generated wastes and by-products constitute a source of severe contamination and environmental threat. The consuming countries face similar problems, with the most challenging being related with the waste management of the coffee by-products and wastes.

The conversion coefficients of the various processes are another crucial factor within the coffee supply chain. On average, just 190 kg of green coffee are produced per ton of coffee cherries [11, 12, 15], due to the mass reduction that occurs during the drying process as a result of the high moisture of coffee beans, along with the considerable waste that is generated during the dry or wet processes [5, 17]. Moreover, on average one ton of green coffee generates 370 kg of coffee beverages or 370kg of soluble/instant coffee [14, 13], and about 650 kg of SCG or about 2 kg of wet SCG from each kg of soluble/instant coffee produced [8, 3, 10].

About 23 kg of CO_2eq per ton coffee cherries and 76 kg of CO_2eq per ton coffee cherries are released during the dry and wet processes respectively, while substantial is also the environmental burden during the brewing and extraction processes, with 1.38 ton of CO_2eq per ton of roasted coffee and 3.28 ton of CO_2eq per ton of roasted coffee respectively [6]. It is worth mentioning, that no CO_2 emissions are released to the atmosphere during any of the waste valorization processes. Similarly, wet method requires substantial more power consumption (2.735 MWh per ton of coffee cherries) in comparison to the dry method (0.103 MWh per ton of coffee cherries). Minimal is the energy requirement for the roasting process (0.042 MWh per ton of green coffee) [19], while coffee extraction process [19] is more energy intensive (4.68 MWh/ton instant coffee) than brewing process (1.87 MWh/ton coffee beverages) [6]. Finally, the water conversion coefficients are estimated based on [7], with 10.5 cubic meters of water per ton of roasted coffee been used during brewing process, and 11.67 cubic meters of water per ton of roasted coffee been used during the extraction process. As expected, zero water is consumed during the dry process, while 9.7 cubic meters of water per ton of coffee cherries is consumed during the wet process.

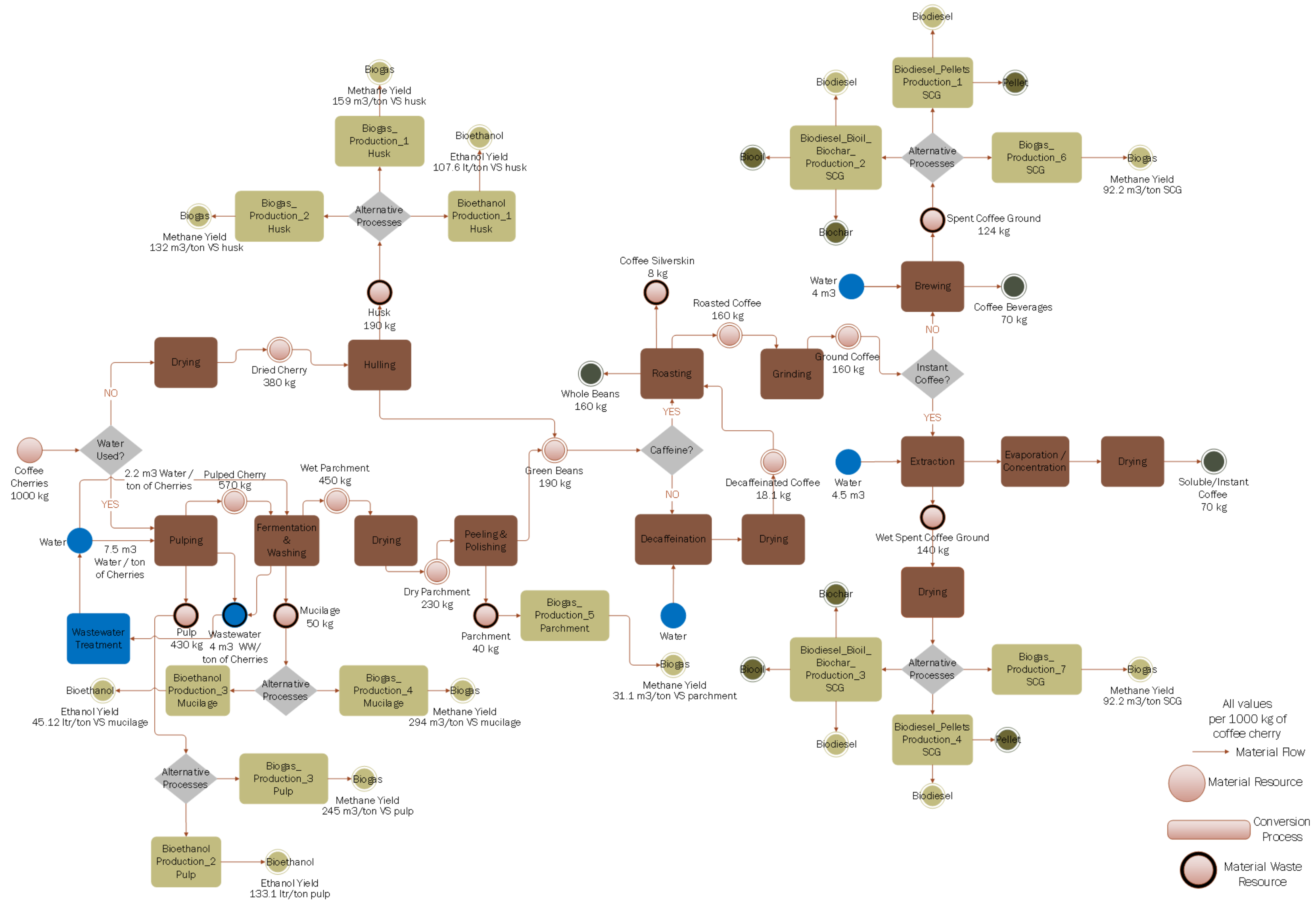

Figure 6.4: RTN of Coffee Supply Chain

6.4.4 Step 4: Mixed-Integer Linear Programming (MILP) Model

First, all available types of resources I, including material and energy resources, as well as all available types of tasks J, including the primary coffee production processes, the waste valorization and the waste treatment processes, are denoted as follows:

$$I = \{i_1, i_2, \ldots, i_{|I|}\},$$

and

$$J = \{j_1, j_2, \ldots, j_{|J|}\}$$

Also, the following subsets are denoted:

I^{WS} waste resources, $i \in \mathcal{I}^{\mathcal{WS}}$

I^{WT} water resources, $i \in \mathcal{I}^{\mathcal{WT}}$

Then, the resource and task parameters are defined. The supply and demand of the various resources form the resource parameters, while the conversion coefficients of the various processes, along with the CO_2 emissions coefficients and the energy consumption or generation coefficients form the process parameters. In particular,

sup_i resource supply parameter, $i \in \mathcal{I}$

dem_i resource demand parameter, $i \in \mathcal{I}$

$pc_{i,j}$ process conversion coefficient, $i \in \mathcal{I}$, and $j \in \mathcal{J}$

$co2_j$ CO_2 conversion coefficient, $j \in \mathcal{J}$

pw_j energy conversion coefficient, $j \in \mathcal{J}$

l_{sup_i} lower bound of supply resource i

u_{sup_i} upper bound of supply resource i

l_{dem_i} lower bound of demand resource i

u_{dem_i} upper bound of demand resource i

Moreover, the design and operational decisions are governed by the following positive variables:

p_i amount of resource i purchased or supplied, $\forall i \in \mathcal{I}$ $\{l_{sup_i} \leq p_i \leq u_{sup_i}\}$

s_i amount of resource i sold or demanded, $\forall i \in \mathcal{I}$ $\{l_{dem_i} \leq s_i \leq u_{dem_i}\}$

x_j production level of task j, $\forall j \in \mathcal{J}$ $\{0 \leq x_j \leq \infty\}$

Finally, the selection or not of a process is governed by the following binary variable:

y_j 1 if the corresponding task is selected, 0 otherwise, $\forall j \in \mathcal{J}$ $\{0 \leq y_j \leq 1\}$

The following two equations express the constraints that govern the coffee supply chain. Equation (6.1) represents the total mass balance of the coffee supply chain. For any resource i in the model, the amount of resource purchased or supplied ($\mathcal{P}_i$) plus the amount of resource produced or consumed by the tasks j, ($\sum_{j \in \mathcal{J}} pc_{i,j} \cdot x_j$) must be equal to the amount of resource sold or demanded ($\mathcal{S}_i$).

$$p_i + \sum_{j \in \mathcal{J}} pc_{i,j} \cdot x_j = s_i \; \forall \; i \in \mathcal{I} \tag{6.1}$$

Equation (6.2) represents the big-M constraint for the production level of task j. The coefficient M introduces a very large number in the equation, which actually dictates specific outcomes or limitations to the model e.g. a task is selected only if it is built, and then an upper bound M is enforced to the production level of this task.

$$x_j \leq M \cdot y_j \; \forall \; j \in \mathcal{J} \tag{6.2}$$

6.4.5 Step 5: Single or Multi-Objective Optimization and Assessment

The final step involves a multi-objective optimization strategy to obtain trade-offs among multiple CE objectives, such as maximizing the energy output while minimizing the coffee cherries consumption, under different demand scenarios for the final products i.e. coffee beverages, instant coffee and whole beans, while considering the subject constraints. A variety of single or multi-objective functions can be optimized depending on the scenario under consideration. For the design of a CE-FSC, and as is discussed in section 6.3.4 and presented in Table 6.1, the objective functions are matched with the CE goals and key characteristics.

Therefore, by looking to increase the share of the renewable resources and energy, the energy output of the supply chain (CEO) is maximized, while by looking to reduce the input, the coffee cherries consumption (CCC) is minimized. Likewise, by targeting the reduction of natural resources, the consumption of water (CWC) is minimized, while the reduction of material losses and emission levels will be achieved through minimizing the waste generation (CWG) and the CO_2 emissions (CEM) respectively.

Equation (6.3) – (6.7), contemplate the goals of CE-FSC as five different single objective functions.

$$\begin{aligned} \text{Objective 1}: \quad & \text{min CWG} = min \sum_{i \in \mathcal{I}^{\mathcal{WS}}} s_i \\ \text{s.t.} \quad & \text{Eqs. } (6.1) - (6.2) \end{aligned} \tag{6.3}$$

$$\begin{aligned} \text{Objective 2}: \quad & \text{min CCC} = min \;\; p_{cherries} \\ \text{s.t.} \quad & \text{Eqs. } (6.1) - (6.2) \end{aligned} \tag{6.4}$$

$$\begin{aligned} \text{Objective 3}: \quad & \text{min CWC} = min \sum_{i \in \mathcal{I}^{\mathcal{WT}}} p_i \\ \text{s.t.} \quad & \text{Eqs. } (6.1) - (6.2) \end{aligned} \tag{6.5}$$

$$
\begin{aligned}
\text{Objective 4 :} \quad & \text{max CEO} = max \sum_{j \in \mathcal{J}} pw_j \cdot x_j \\
\text{s.t.} \quad & \text{Eqs. } (6.1) - (6.2)
\end{aligned}
\tag{6.6}
$$

$$
\begin{aligned}
\text{Objective 5 :} \quad & \text{min CEM} = min \sum_{j \in \mathcal{J}} co2_j \cdot x_j \\
\text{s.t.} \quad & \text{Eqs. } (6.1) - (6.2)
\end{aligned}
\tag{6.7}
$$

Equation (6.8) – (6.12) contemplate the same CE goals, but this time simultaneously as a multi-objective optimization problem. For example, Equation (6.8) describes the minimization of coffee cherries consumption, while maximizing the total energy output.

$$
\begin{aligned}
\text{Multi-Objective 1 :} \quad & \text{min CCC} \quad \& \quad \text{max CEO} \\
\text{s.t.} \quad & \text{Eqs. } (6.1) - (6.2)
\end{aligned}
\tag{6.8}
$$

$$
\begin{aligned}
\text{Multi-Objective 2 :} \quad & \text{min CCC} \quad \& \quad \text{min CWG} \\
\text{s.t.} \quad & \text{Eqs. } (6.1) - (6.2)
\end{aligned}
\tag{6.9}
$$

$$
\begin{aligned}
\text{Multi-Objective 3 :} \quad & \text{min CWG} \quad \& \quad \text{max CEO} \\
\text{s.t.} \quad & \text{Eqs. } (6.1) - (6.2)
\end{aligned}
\tag{6.10}
$$

$$
\begin{aligned}
\text{Multi-Objective 4 :} \quad & \text{min CWC} \quad \& \quad \text{max CEO} \\
\text{s.t.} \quad & \text{Eqs. } (6.1) - (6.2)
\end{aligned}
\tag{6.11}
$$

$$
\begin{aligned}
\text{Multi-Objective 5 :} \quad & \text{min CEM} \quad \& \quad \text{max CEO} \\
\text{s.t.} \quad & \text{Eqs. } (6.1) - (6.2)
\end{aligned}
\tag{6.12}
$$

The multi-objective optimization problems are solved using the ϵ-constraint method [282, 283], which converts the multi-objective optimization problem to a series of single-objective optimization sub-problems. As an example, for solving multi-objective problem 1, the first step requires the solution of the problem using only one objective function f_1, in this case described by Eq. 6.4. This leads to an optimal solution, denoted as x_1^*. The minimum of the second objective function f_2 (Eq. 6.6) is obtained at this optimal point x_1^*, since any value lower than this for f_2 will not increase the value of f_1. Hence, the minimum of f_2 is denoted as $\theta^L = f_2(x_1^*)$.

The next step involves the solution of another optimization problem, this time with only the other objective function f_2, as it is described by Eq. 6.6. Similarly, another optimal solution is obtained, denoted as x_2^*, which is the maximum of f_2, so it is denoted as $\theta^U = f_2(x_2^*)$. Thus, the feasible region of f_2 is defined as [θ^L, θ^U]. This region is divided equally into N intervals, and so $\theta \in$ [θ^L, θ^U]. Hence, the original multi-objective problem can be converted into the following single objective optimization problems:

$$\begin{aligned} \min \quad & \text{CCC} \\ \text{s.t.} \quad & \text{CEO} \geq \theta \\ & \text{Eqs. } (6.1) - (6.2) \end{aligned} \tag{6.13}$$

6.5 Results and Discussion

The CE-FSC mixed-integer optimization model is implemented in Python and solved utilizing Gurobi V9.0.2 default solver [305] on an Intel 3.5GHz Quad-Core i7 Processor with 16 GB of RAM. For the multi-objective function problems (Eqs. (6.8) – (6.12)) under one scenario, the model features 138 equations, 58 continuous variables, and 18 binary variables, and the average time to solve it is 0.01 seconds.

Five different scenarios for the supply of coffee cherries and the demand of final coffee products are investigated for each of the single or multi-objective optimization problems. They are chosen so as to demonstrate the applicability and effectiveness of the framework in conducting quantitative analysis of any food supply chain under circular economy considerations while capturing even the most extreme cases. The supply and the demand values are arbitrarily selected for illustration purposes. For easy comparison, the maximum supply of coffee cherries stays the same among the scenarios at 100,000 tons. For scenarios 1 and 2, the demand for the three final products is set at 2,000 tons and 1,000 tons respectively. Scenario 3 involves only demand for coffee beverages without any demand for the other two products. Similarly, scenario 5 involves only demand for whole beans without any demand for the other two products. Finally, the demand for instant coffee in scenario 4 is set higher or equal to 6,000 ton with zero demands for the other two products. Scenario 4 requires a specific demand target to be met since the production of instant coffee introduces higher environmental and production burdens in comparison to the other two products, thus under an optimization perspective, there will be no incentives to generate any amount, unless a specific target is set. Please also refer to Appendix Table I.1.

By utilizing the CE-FSC framework that is described in the previous sections, the solution of each single objective optimization problem as well as the pareto fronts of each multi-objective optimization problem are generated. The solutions of the single objective optimization problems are shown in Figures I.3 to I.7 in Appendix I. Here, the results of multi-objective optimization problems 1 (Eq. (6.8)) and 4 (Eq. (6.11)) are presented, whereas the results of the rest of the multi-objective optimization problems are shown in Figures I.8 to I.10 in Appendix I. Figures I.11 and I.12 in Appendix I expand the results of the trade-off analysis for the multi-objective optimization problems 1 and 3 respectively, by incorporating three different values (low: 0.1034, average: 0.7281 (+604%), high: 1.3528 (+1,208%), unit: MWh/ton coffee cherries) for the parameters related to the drying process [19, 306].

Figure 6.5 reveals the results of such a trade-off analysis for the multi-objective problem 1 of minimizing the coffee cherries consumption while maximizing the total energy output (minCCC & maxCEO), subject to the constraints of the coffee supply chain which are described by Eqs. (6.1) – (6.2). The colors in Figure 6.5 represent different demand scenarios for the final products.The low values of the parameters in the drying process are used. Since this is a multi-objective optimization problem, a pareto of solutions is generated and each bubble demonstrates a different optimal solution from the pareto. An optimal solution refers to the selection of specific values for the binary and continuous variables so that the imposed constraints are satisfied and the objective functions are optimized. Practically, each bubble represents a specific operational profile of the

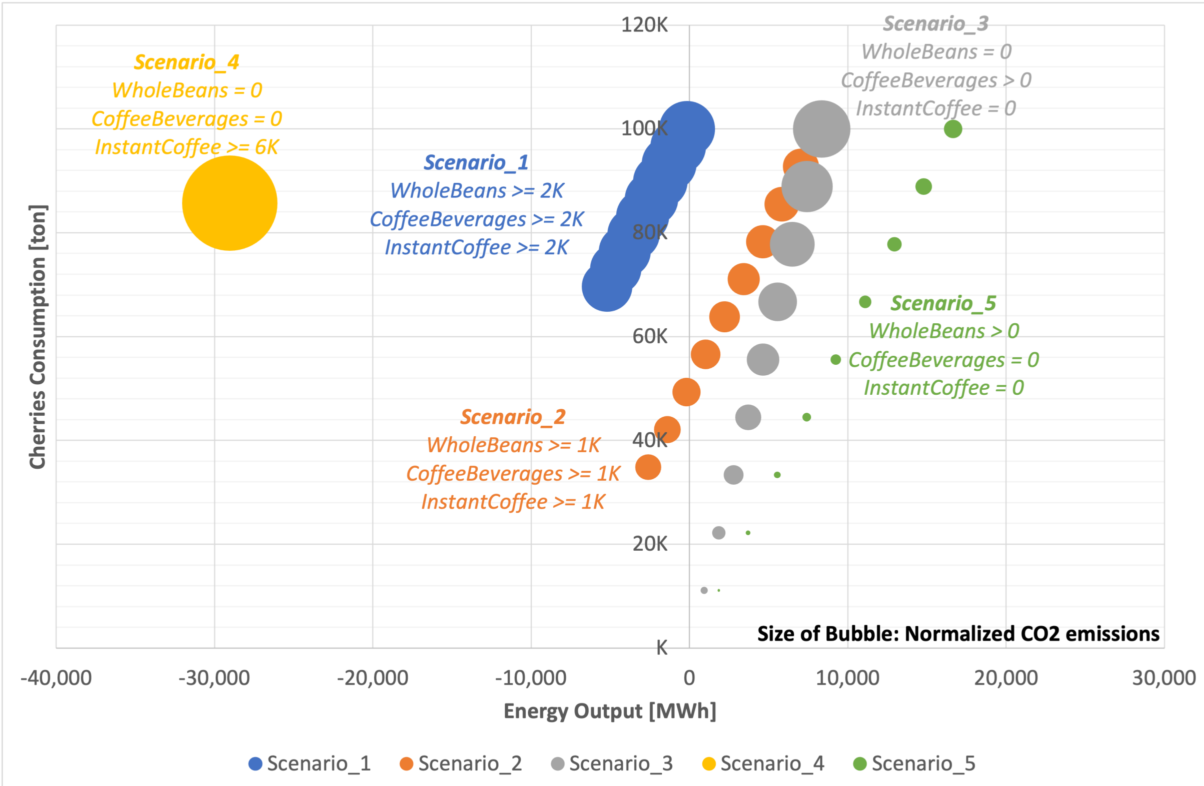

Figure 6.5: Pareto Analysis for Problem 1: Max Energy Output & Min Cherries Consumption & Normalized CO_2 Emissions

coffee supply chain, while the size of a bubble depicts the normalized CO_2 emissions (min-max normalization). As it is also discussed in section 6.3.5, the ϵ-constraint method is used for the solution of the multi-objective optimization problem. The pareto solutions for each demand scenario, meaning the bubbles with the same color, are evenly distributed over the solution space and here the number of generated efficient solutions has been specified to 10.

An upper bound of available cherries has been set at 100,000 tons for all 5 scenarios. Scenarios 1 and 2 require certain demands to be met for all 3 final products. As expected, the higher the consumption of cherries, the higher the energy produced. Once the target demands are met, the excessive amount of cherries is converted to whole beans, while the excessive amount of coffee by-product is used to produce more energy. This is because even though whole beans can be sold as a final product to the market, they require further processing, either brewing or extraction, so as to yield the end coffee drink. Thus, producing just whole beans is favorable in terms of energy and environmental footprint.

The operating profiles of scenario 1 (with higher energy demands) are more to the left on the graph than those of scenario 2, because the extra demand of coffee beverages and instant coffee requires more brewing and extraction, which are both energy intensive processes. The rest of the scenarios represent instances where the demand of only one final product is specified. In particular, scenario 5, even rather unrealistic since it refers exclusively to demand of whole beans and requires further processing to produce the coffee drinks, it demonstrates the best-case scenario in terms of both energy and environmental performance. On the contrary, scenario 4, with only instant coffee as a deliverable, is the worst-case scenario both in terms of energy and environmental efficiency. Just one operating profile is produced since the optimal solution for both objectives refers merely to the satisfaction of demand. Finally, in scenario 3 that describes the case of demand solely coming from coffee beverages, the operating profiles demonstrate a steeper slope in comparison to the ones from the other scenarios. This behavior is attributed to the different energy and environmental benefits that coffee beverages have in comparison to the other coffee products. Figures I.11 and I.12 in Appendix I highlight the effects uncertain parameters related to the drying process have on the multi-objective optimization process. As the values of drying parameters increase, the optimal solutions require more energy to meet the demand scenarios.

The second trade-off analysis is highlighted in Figure 6.6 for the multi-objective problem 4 of minimizing the water consumption while maximizing the total energy output (min CWC & max CEO), subject to the constraints of the coffee supply which are described by Eqs. (6.1) – (6.2). Similarly to the previous problem, every color in Figure 6.6 represents a different demand scenario for the final products, while the size of the bubbles represents the CO_2 emissions. Likewise, the ϵ-constraint method is utilized to solve this multi-objective problem, resulting in the generation of a pareto of solutions. The maximum supply of coffee cherries has been bounded to 100,000 ton.

In Scenarios 1 and 2, the demand of coffee beverages and instant coffee are just met and the excess is converted in whole beans because this is environmentally preferable. On the contrary,

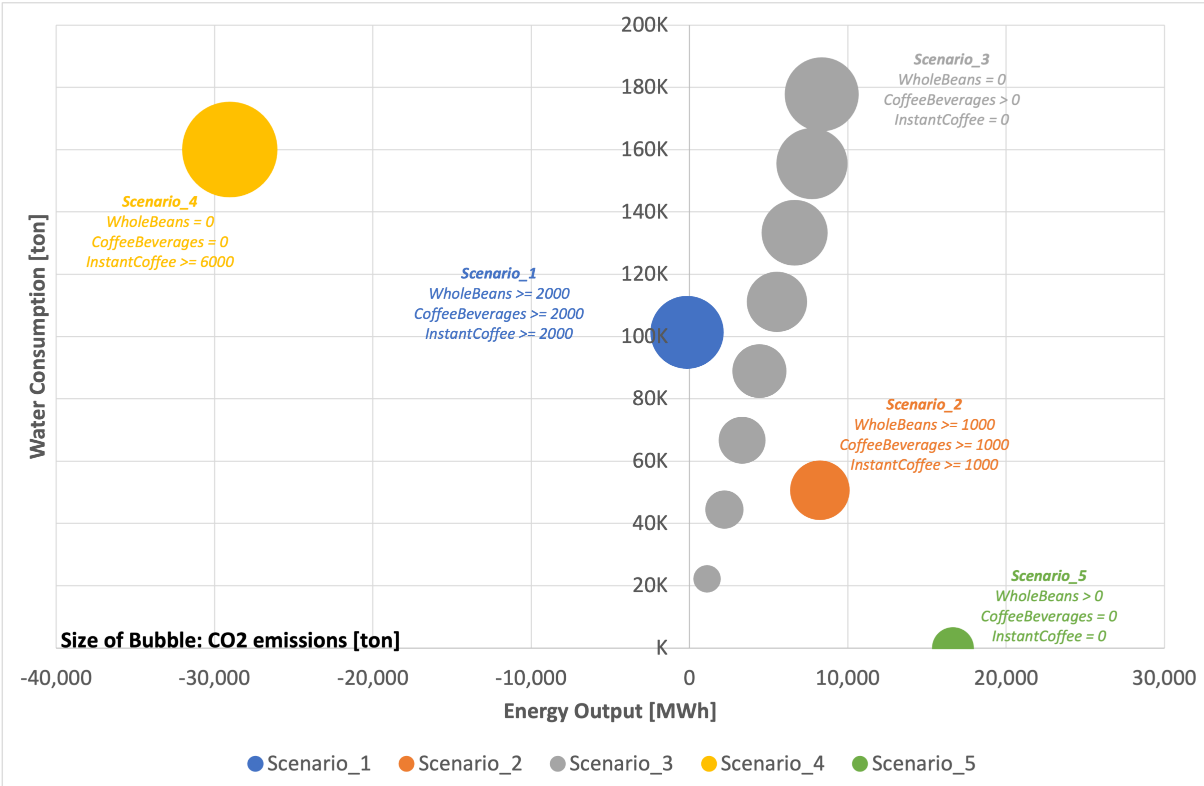

Figure 6.6: Pareto Analysis for Problem 4: Max Energy Output & Min Water Consumption & CO_2 Emissions

scenario 3 produces up to 7,000 ton of coffee beverages, because the consumption of more coffee beverages results into more spent coffee, which ultimately results in more energy generation. However, the trade-off between energy output and water consumption is clear in this scenario, since an increase in energy output of just over 7,000 MWh requires the consumption of more than 155,000 ton of water. Thus, the user is able to select its operational profile considering the environmental effects. An interesting case is revealed in scenario 4, where the optimal solution is reached once the demand is met, since it is not beneficial neither in terms of energy nor in terms of water to produce more instant coffee. This scenario also, demonstrates the higher burden with respect to CO_2 emissions. Lastly, in scenario 5, even though no water is consumed, the production reaches 17,000 tons of whole beans. The produced energy is generated from the waste of husk, as a result of the dry processing method, however and as it is mentioned before, this scenario is rather unrealistic since further processing is required for the production of the end coffee drinks. In this multi-objective optimization problem, a pareto with distinct optimal solutions is generated only for scenario 3. For the rest of the scenarios, there is only one optimal solution that satisfies the subject constraints, resulting in just one bubble for each scenario.

6.6 Conclusions

The dissemination and implementation of CE is fundamental for the fruition of the social, environmental and economic benefits of the 2030 Agenda and the Paris Agreement, along with the sustainable recovery from COVID-19. A systems engineering framework and decision-making tool for the analysis and trade-off modeling and optimization of interconnected FSCs considering the principles and goals of CE is presented. It aims to provide a holistic quantitative tool that assists towards the transition to CE-FSCs by efficiently tackling the plethora of newly introduced challenges. This is achieved through the modeling and systematic integration of recent technological, experimental, academic and industrial knowledge in the design and operation of FSCs using a RTN superstructure representation. The resulting MILP model incorporates all the unique characteristics of the FSC network, any constraints along with all the alternative production, processing and valorization pathways, and is optimized under single or multi-objective CE criteria. Since CE introduces conflicting or competing objectives, the multi-objective optimality is critical, and is implemented through the generation of the pareto optimal set over the entire feasible space.

The developed framework contributes to the literature by explicitly incorporating all CE goals and objectives into the design and operation of FSCs. It also serves a dual role, since it does not only allow the identification and selection of the optimal tasks from the list of alternatives under specific CE objectives, but also enables the identification of any potential bottlenecks. This feature promotes the research and development of certain, less efficient parts of the supply chain. The framework is also flexible since the set of resources and the corresponding available supply of inputs as well as the target demands of the final products can be constantly updated, reflecting new trends and developments. It can be also utilized from users with different backgrounds and considerations. Academics and experimentalists could focus more on the improvement of existing tasks, or the creation of completely new ones, private corporations could focus on optimizing their entire FSCs through the lens of CE holistically, and finally governmental policymakers could quantitatively identify areas that require funding and/or specific legislative actions.

The supply chain of coffee has been selected as an indicative case study for demonstrating the unique features of the proposed framework. In particular, the effectiveness and the applicability of the framework in transforming the linear supply chain to a circular one while analyzing different supply and demand scenarios, under CE objectives simultaneously is demonstrated. Since the objectives of CE and its stakeholders are usually competing, a multi-objective optimization approach is utilized. The computational results prove that the MILP problem can be optimally solved, producing different pareto fronts depending on the CE objectives. Therefore, it can be used as a decision-making tool that captures all the potential sets of resources and tasks under any design and operational criteria and/or external conditions.

7. A QUANTITATIVE AND HOLISTIC CIRCULAR ECONOMY ASSESSMENT FRAMEWORK AT THE MICRO LEVEL*

7.1 Background & Motivation

The unprecedented economic development and the social advancement that occurred over the last centuries were inextricably linked to a "take-make-waste extractive" industrial model, which inevitably placed huge stresses on the natural resources and led to enormous environmental and socioeconomic impacts [27, 233]. The concept of Circular Economy (CE) has emerged as a potential solution to this challenging issue contributing to all dimensions of sustainable development [307]. It promotes the transition to renewable energy sources [308, 309, 310], designs out waste and pollution [311, 312, 313], and focuses on improving recycling processes [314, 315, 316]. Moreover, it decouples growth from the consumption of natural resources [317], and eventually leads to the regeneration of natural systems [27, 284, 262]. To this direction, the full exploitation of synergies among pioneering business models, revolutionary products' design and new systemic conditions is necessary [27, 184, 120]. In parallel, systematic and quantitative approaches are needed to identify, exploit and assess alternative pathways for production, distribution and recycling, ensuring that the CE goals related to the optimization of resources' consumption and minimization of the environmental burden are thoroughly captured and implemented [318, 319, 320].

Despite the fact that CE has gained a lot of attention across various disciplines and it seems a rather straightforward concept, it still generates confusion among the involved parties. This is due to the vagueness of the definition, its extensive and universal nature as well as its lack of specificity in the implementation [252, 321]. Therefore, and before proceeding with any further analysis, it is important to clarify this vagueness.

*Reprinted from "A quantitative and holistic circular economy assessment framework at the micro level" by S.G. Baratsas, E.N. Pistikopoulos, S. Avraamidou, Computers & Chemical Engineering, 2021. A summary of the work is given in this chapter, with additional details provided in Appendix J.

7.1.1 Circular Economy vs. Sustainability

CE was founded on the principles of the triple bottom line (TBL) [322] as an intentionally designed restorative, regenerative and environmentally benign system that promotes the concepts of reduction, reuse, recycling and recovery. CE aims to attain sustainable development through innovation and disruption at different systemic levels i.e. micro level (product, individual enterprises, consumers), meso level (industrial symbiosis) and macro level (city, region, nation and beyond) [27, 323, 324]. Ultimately, nature must be preserved and enhanced by optimizing the recirculation of materials, resources and products, while improving the integration and efficiency of renewable resources. Any negative externalities should be eliminated [325] and the loops should be closed.

However, CE should not be muddled with sustainability but rather perceived as a roadmap or a toolbox to achieve sustainability. This can be done through the utilization of CE targeted practices and synergies towards the implementation of the majority of the sustainability goals [326]. Geissdoerfer et al. (2017) [251] concluded that academic researchers deem three relationships between CE and sustainability: 1) CE being a condition for sustainability, 2) CE and sustainability having a beneficial relationship, or 3) a trade-off relationship between CE and sustainability. This can lead to the inference that a subset relation between the two concepts is adequate, which also coincides with the general understanding of CE as a concept that entails two of the three dimensions of sustainability, while lacks social considerations [252, 327]. Recent literature reviews of CE metrics and indicators are also in agreement with this argument, claiming that the social dimension is the least covered one [328, 323, 329].

7.2 Introduction

The effective and the successful implementation of the transition towards CE on a global scale requires systematic assessment of the alternative pathways and scenarios along with the development of holistic metrics to evaluate the different aspects of CE [255, 330]. This presumes a clear and solid understanding of what needs to be measured and assessed, before considering how this will be measured, what are the metrics to be used and against what benchmarks the CE implementation should be evaluated and the CE targets must be set [331].

To this respect, in this chapter a quantitative, holistic and robust CE assessment framework for the micro level is presented. "MICRON" *(MIcro CirculaR ecOnomy iNdex)* is a GRI-based tool that takes into consideration all goals and objectives of CE holistically. Based on these goals and objectives, a set of principal categories is defined so as to establish transparency and clarity in the scope and goal setting. Four sectors are introduced to classify the economic activity and to improve granularity. Then, sector specific indicators and metrics that are matched with GRI standards are used for each of the principal categories. This structure enables the assessment of circularity at the category's level, leading to the derivation of the Category-based Circularity Index. The linear average of the category-based indices constitutes the Overall Circularity Index. As such, the framework provides i) a set of indicators and metrics with sector-specific dimensions, ii) quantitative, holistic and robust CE overall and category-based metrics, iii) media for data visualization and analysis of CE indicators, and iv) an analytical tool to assess multi-national businesses and interconnected CE supply chains.

The explicit incorporation of CE goals and objectives as assessment criteria, the classification of economic activity into distinct parent sectors, the conception of GRI matched, sector specific indicators and metrics are key contributions of the proposed framework to the literature. The metrics are normalized and standardized using sector specific relevant information, ensuring that assessments are up-to-date and dynamically adjusted. Overall, the high level of granularity covering all CE goals, the comprehensive nature of the framework and the enhanced interpretability are key features and important contributions of the framework.

7.3 Literature Review

A plethora of approaches and metrics have been proposed in the literature to measure different aspects of CE [332, 333, 183, 334, 335], without consistency in their objectives, scopes, and potential applications [323]. Nevertheless, the CE assessment still lacks standardized methods [336, 337, 328, 329], while even the used terminology has not be formalized yet, i.e. metrics vs. indicators. Such a plethora of different approaches and metrics create confusion and ambiguity to the involved parties [338, 336], and set a barrier towards the prevalence of the CE concept [339]. Undoubtedly, CE related measuring and assessment tools at the different systemic levels are necessary for the transition towards CE systems [340, 341, 342], and eventually sustainable development [343, 323, 337]. Despite that numerous CE indicators, metrics and assessment tools have been reviewed and proposed over the last years, the research and discussion is still ongoing at every level [329]. Here, some of the key outcomes from reviewing the recent literature are briefly discussed.

Elia et al. (2017) [183] highlighted a lack of CE indicators, measuring tools and standardized ways to assess circularity, especially in the micro level, which is in line with the findings of other researchers [323, 344, 337, 336]. Elia et al. (2017) [183] proposed a four level framework for CE assessment at the micro level, which did not capture all the CE characteristics, since the main focus was in the environmental evaluation. Saidani et al. (2019) [323] categorized 55 indicators from the academic and business world into 10 groups based on the main CE features and characteristics as well as their potential usage i.e. level of implementation, performance, usage, degree of transversality etc. A CE indicator selection tool based on user's requirements was also presented. Parchomenko et al. (2019) [332] analyzed 63 CE metrics based on 24 CE elements using a Multiple Correspondence Analysis (MCA). They assessed the interconnections of metrics and elements as well as the most and least frequently elements used, but their analysis did not recommend what CE characteristics need to be evaluated. Waste disposal, primary vs. secondary use of resources, resource efficiency/productivity and recycling efficiency were the most popular CE elements assessed, while preservation of value and product and system dynamic elements were poorly represented.

Moraga et al. (2019) [345] developed a classification framework based on six CE strategies and three measuring scopes in line with the Life Cycle Thinking (LCT) by considering the CE as an umbrella concept without been limited by indicators' definitions. Nevertheless, the proposed framework cannot adequately capture the causality between CE and sustainability development, while it cannot support neither the distinction of CE indicators for inputs and outputs nor for the retention of functions. Sassanelli et al. (2019) [328] presented another classification framework for CE assessment metrics using the product life-cycle stages, variables and circularity degree as criteria. Based on the results from its application in 45 papers, they proposed a framework for evaluating the circularity of companies under the TBL concept. The analysis revealed a lack of an overall CE evaluation with just half of the cases been analyzed under a mixed lifecycle stages perspective and a rather strong concentration on the environmental and material aspects. Similar findings were reported by Corona et al. (2019) [254], with none of the assessed metrics been able to fully capture the CE or the three dimensions of sustainability, while little emphasis was put towards reviewing the scarcity and multi-functionality of materials or the importance of introducing new waste valorization techniques.

After reviewing 137 articles published over the last 20 years, De Pascale et al. (2020) [329] identified 61 CE indicators using a double classification that takes into account the spatial dimensions of sustainability i.e. micro, meso, and macro, as well as the 3Rs core principles i.e. reduce, reuse, and recycle. The lack of systematic and standardized methodologies to evaluate and assess CE comprehensively at the different levels along with the known vagueness on what needs to be measured was reaffirmed. It was also shown that less than half of the indicators cover all the sustainability dimensions or all the 3Rs principles while none focus specifically on the social dimension. Also, just 13 CE indicators cover simultaneously all the sustainability dimensions and 3Rs core principles, with only one though been used at the micro level. Thus, it appears that the assessment and evaluation of CE and sustainable development at the company/product/consumer level is more challenging.

Concentrating the analysis at the micro level, Kristensen and Mosgaard (2020) [337] reviewed 30 CE indicators and also inferred that the attention was directed mainly to the economic dimension of CE while the environmental and notably the social dimensions were considered to a lesser extent. The majority of the reviewed CE indicators, from single quantitative ones to more complex indicator sets, put emphasis on the recycling, end-of-life management, and re-manufacturing, with less focus towards life-time extension, waste management, disassembly and resource-efficiency. In addition, the CE indicators at the micro level primarily evaluate single products and materials, so they provide a unique decision-making tool for the companies [346]. At the same time, they introduce a challenge since the transition to circular solutions normally affects not just single products but rather the entire supply chain. A myopic approach could lead to sub-optimal solutions and therefore undermining the holistic CE viewpoint. To this respect, Pauliuk (2018) [347] suggested the utilization of CE relevant information in conjunction with CE indicators so as to extent the CE coverage, although such a scheme would launch new challenges due to complexity issues and the inability for information disaggregation. An attractive suggestion by Kristensen and Mosgaard (2020) [337] was the development of industry specific indicators, which will boost the prevalence of CE within the various industries and promote the respective indicators.

Likewise, Vinante et al. (2020) [336] reviewed 365 CE metrics at the micro level and introduced a classification based on value chain framework, composed of 23 categories. This framework associates CE metrics with company's functions and structure, enabling the disaggregation of the CE assessment. Moreover, the generalized nature of most CE metrics, along with their applicability in evaluating CE procedures regardless of company's specific characteristics, offset any contingency factors. The extensive literature review uncovers also the fragmentation of the current CE assessment at the micro level, along with the diverging interpretations of CE's goals. The dominance of environmental metrics in comparison to the shortage of social metrics was reaffirmed, with the former demonstrating a more quantitative approach as opposed to the more qualitative approach of the latter.

7.4 Circular Economy Assessment Framework for the Micro Level

The vast majority of CE and sustainability analyses focus on the macro and meso levels, creating a shortage of CE assessment methods and tools at the micro level [183, 323, 344, 337, 348, 349]. This is attributed to some of the intrinsic characteristics of circularity assessment at micro level. In particular, Kristensen and Mosgaard (2020) [337] pointed out that reuse, repair or maintenance dimensions of CE that are considered major contributors to TBL principles require greater consideration. Also, CE indicators frequently concentrate on just a subset of CE principles, missing the bigger picture and leading to sub-optimal results. This further exacerbates the inherent issue of CE indicators at micro level which are mainly designed with a narrow focus to specific products and materials, leading again to sub-optimal solutions due to the lack of a systems perspective. The plethora of different aspects and types under CE consideration at the micro level, introduce extra obstacles for companies and organization who want to pursue CE, and thus potentially jeopardize the overall succession of CE concept. To this respect, "MICRON" *(MIcro CirculaR ecOnomy iNdex)* is developed, as a quantitative, holistic and robust CE assessment framework for the micro level. This is an attempt to address the generic challenges related to the CE assessment as well as those arise from the application specifically to the micro level.

According to the Gabrielsen and Bosch (2003) [350], a proper indicator should have the following features: i) communicate with simplicity complex and critical matters, ii) be interpretable and traceable, iii) be used as a point of reference, iv) provide a systems analysis perspective, v) reflect all causality relations and driving forces. On top of these features, CE indicators should equally reflect on material and energy aspects, with extra care for critical raw materials and resource efficiency [343]. They should also raise public awareness on local and global effects of human activities through the lens of TBL concept.

7.4.1 Structure of the framework

Figure 7.1 summarizes the key steps undertaken for the development of the proposed framework. The known issues of CE metrics and indicators are overcame by designing five principal categories of indicators which are selected and matched with the goals and key characteristics of CE [182]. Table 7.1 shows the correspondence between CE goals and key characteristics with principal categories of indicators. This is a necessary first step towards transparency in the scope and goal setting. Identifying and setting specific boundaries and targets of what must be measured and evaluated is crucial before establishing the indicators and metrics [351]. An extra principal category, named "Organization" is also used for providing general information about a company's business activity e.g. company's revenue, number of products sold etc.

Four parent sectors are introduced to represent the economic activity, namely Energy and Utilities (EnU), Services (SrV), Manufacturing (MaN), and Automotive (AuT). A series of industries is assigned to each of the parent sectors based on their primary business activity. For example, the industries Energy, Energy Utilities, Waste Management, and Waste Utilities are assigned to the Energy and Utilities sector. The list of industries is taken from the GRI sustainability Disclosure Database [352].

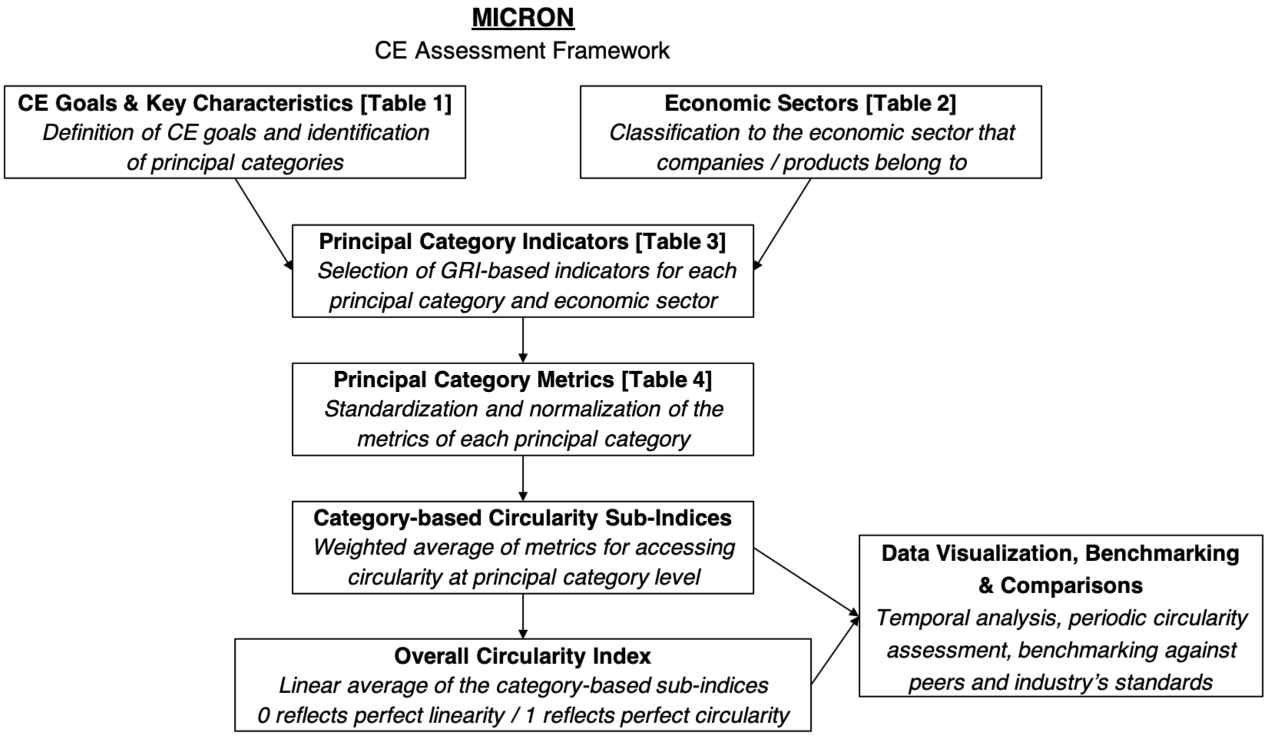

Figure 7.1: Step by step Analysis of Circularity Assessment Framework MICRON

Table 7.1: Matching of the Principal Categories with CE Goals

#	CE Goals & Key Characteristics		Principal Categories of Indicators
1	Reduction of material losses/residuals: Waste and pollutants minimization through the recovery and recycle of materials and products.	$\leftrightarrow$	Waste
2	Reduction of input and use of natural resources: The reduction of the stresses posed on natural resources through the efficient use of natural resources.	$\leftrightarrow$	Water, Procurement
3	Increase in the share of renewable resources and energy: Replacement of non-renewable resources with renewable ones, limiting the use of virgin materials.	$\leftrightarrow$	Energy
4	Reduction of emission levels: The reduction in direct and indirect emissions / pollutants.	$\leftrightarrow$	Emissions, Spillages
5	Increase the value durability of products: Extension of product lifetime through the redesign of products and high-quality recycling.	$\leftrightarrow$	Durability

The breakdown of sectors and industries is shown in Table 7.2.

Table 7.2: Classification of the Economic Activity into Parent Sectors

Energy & Utilities (EnU)	**Services (SrV)**	**Manufacturing (MaN)**	**Automotive (AuT)**
Energy	Aviation	Agriculture	Automotive
Energy Utilities	Commercial Services	Chemicals	
Waste Management	Financial Services	Computers	
Water Utilities	Healthcare Services	Conglomerates	
	Logistics	Construction	
	Media	Construction Materials	
	Non-Profit / Services	Consumer Durables	
	Public Agency	Equipment	
	Railroad	Food and Beverages Products	
	Real Estate	Forest and Paper Products	
	Retailers	Healthcare Products	
	Telecommunications	Household and Personal Products	
	Tourism / Leisure	Metals Products	
	Universities	Mining	
		Technology Hardware	
		Textiles and Apparel	
		Tobacco	
		Toys	

Each sector consists of a number of industries and has its own unique assessment indicators and quantitative metrics which cover all principal categories, so as to capture the special characteristics of each company and the industry that belongs under CE and sustainability considerations. The developed assessment framework should not be confused with Life Cycle Assessment (LCA) which is an inherent attribute towards analysis, modeling, implementation and/or assessment of the CE [255]. Since the terminology is not standardized in the literature and in order to maintain consistency throughout the document, here the relevant terms are defined as follows:

As *indicator* is defined the smallest unit of information that must be measured and evaluated under a CE goal, standard or principal category, e.g. total renewable energy consumed within the company. As *metric* is defined the composite, normalized measure of an indicator to gauge company's level of business activity and productivity, e.g. total renewable energy consumed within the company over company's revenue. This is essential to capture the progress and efficacy of a company's circularity year over year, as well as to conduct meaningful comparisons among companies [353]. The term *category* refers to the upper level grouping of indicators within the framework, e.g. Waste, Energy etc. If a category is broken down further so as to reflect a particular theme, e.g. environmental, economic etc., then the sub-categories will be called *aspects* [353]. Aspects may refer to a single indicator or a group of indicators depending on the scheme.

The indicators determine the type of information and data that must be collected and reviewed for each principle category over a specific period of time, normally one full year. Then metrics are defined to mathematically express and interpret the information and data that is stored in the indicators over the period of interest. For easy and objective comparison, metrics are normalized. The CE assessment of each principal category is based on the weighted average of its metrics, and is called *Category-based Circularity Sub-Index* of this particular principal category. For example, three different metrics are used to assess the circularity of principal category of Water on yearly basis. The annual Circularity Sub-Index of Water is calculated from the weighted average of the corresponding metrics (weights of metrics may not be equal). The varying levels of significance of the metrics are contemplated using weighted averages. The linear average of the category-based sub-indices determines the *Overall Circularity Index* for each company, product or supply chain.

7.4.2 Selection of indicators and metrics

The selection of appropriate indicators and metrics for each principal category is critical since they must incorporate all the characteristics that mentioned earlier, while successfully capture the dynamics of companies and industries at different levels. The indicators have been also matched with the Global Reporting Initiative (GRI) Standards [354], ensuring uniformity in the reported results while providing a reference guide for those who want to use the proposed index. Different indicators are used for the different sectors. This increases the flexibility and the universal nature of the framework while improves the specificity in the implementation. Having specific indicators to measure over predetermined periods of time facilitates the data collection process and the comparisons among peers. Large companies with diversified activities in multiple countries may decide to split their CE assessment to individual business segments or regions for better benchmarking and accurate planning, which can be readily accommodated within the framework. As such, these companies will be able to measure the effectiveness of circular strategies deployed at international, national and regional levels or at each business segment individually. Table 7.3 illustrates the complete set of indicators for all principal categories and sectors. The sector specific indicators individually are shown in Tables J.1 to J.4 in Appendix J.

Table 7.3: CE Indicators with Sector Allocation [EuN: Energy and Utilities, MaN: Manufacturing, Au: Automotive], SrV: Service]

Principal Categories	Indicators	GRI Standards Correspondence	Sectors Allocation			
Organization	Revenues [million $]	GRI-201-1	EuN	MaN	AuT	SrV
	Total social investment for environmental sustainability and circular economy [million $]	GRI-203-1	EuN	MaN	AuT	SrV
	Products sold [weight or volume]	GRI-301-3		MaN		
	Number of products sold [# of products]	GRI-301-3			AuT	
	Full time employees (FTE) [# of people]	GRI-401-1			AuT	SrV
	Operational building/facilities space	GRI-302-3				SrV
Waste	Waste generated - Hazardous [weight]	GRI-306-3	EuN	MaN	AuT	SrV
	Waste generated - Non Hazardous [weight]	GRI-306-3	EuN	MaN	AuT	SrV
	Diverted waste from disposal (reused, recycled, recovered) [weight]	GRI-306-4	EuN	MaN	AuT	SrV
Water	Water withdrawal [volume]	GRI-303-3	EuN	MaN	AuT	SrV
	Fresh water discharge (<= 1,000mg/L TDS) [volume]	GRI-303-4	EuN	MaN	AuT	SrV
	Other water discharge (>= 1,000mg/L TDS) [volume]	GRI-303-4	EuN	MaN	AuT	SrV
	Water recycled or reused [volume]	GRI-303-3 (2016)	EuN	MaN	AuT	SrV
Procurement: Production & Packaging	Non-renewable material used [volume or weight]	GRI-301-1			AuT	SrV
	Non-renewable packaging material used [volume or weight]	GRI-301-1		MaN		
	Renewable material used [volume or weight]	GRI-301-1			AuT	SrV
	Renewable packaging material used [volume or weight]	GRI-301-1		MaN		
	Recycled input material used [volume or weight]	GRI-301-2			AuT	SrV
	Recycled packaging material used [volume or weight]	GRI-301-2		MaN		
	Reusable, compostable or recyclable material [%]	GRI-301-3			AuT	
	Reusable, compostable or recyclable packaging material [%]	GRI-301-3		MaN		
	Paper consumption [weight]	GRI-301-1				SrV
	Single-use plastics consumption [weight]	GRI-301-1				SrV
Energy	Total energy generated [joules or multiples]	GRI-302-1	EuN			
	Total non fossil fuel energy generated [joules or multiples]	GRI-302-1	EuN			
	Total energy consumed [joules or multiples]	GRI-302-1		MaN	AuT	SrV
	Renewable energy consumed [joules or multiples]	GRI-302-1		MaN	AuT	SrV
	Certified buildings and facilities i.e LEED [%]	GRI-302-3				SrV
GHG Emissions	Direct GHG emissions (Scope 1) [tCO2e]	GRI-305-1	EuN	MaN	AuT	SrV
	Energy indirect GHG emissions (Scope 2) [tCO2e]	GRI-305-2	EuN	MaN	AuT	SrV
	Total use of products (Scope 3) [metric tons CO2 equivalent (tCO2e)]	GRI-305-3	EuN	MaN	AuT	SrV
	Average specific CO2 emissions [gCO2/km]	GRI-305-4			AuT	
	Emissions neutralized by carbon offset projects [tCO2e]	GRI-305-5	EuN	MaN	AuT	SrV
	Emissions of ozone-depleting substances (ODS) [metric tons of CFC-11 equivalent]	GRI-305-6	EuN	MaN	AuT	SrV
	Nitrogen oxides [NOx], sulfur oxides [SOx] & other significant air emissions [kg or multiples]	GRI-305-7	EuN	MaN	AuT	SrV
Spillages & Discharges	Environmental fines [$]	GRI-307-1	EuN	MaN	AuT	SrV
	Volume of flared hydrocarbon [tCO2e]	GRI-306-3	EuN			
	Volume of vented hydrocarbon [tCO2e]	GRI-306-3	EuN			
Durability	Packaging Material to be reclaimed/recovered [# of products or %]	GRI-306-2		MaN		
	Material to be reclaimed/recovered [%]	GRI-306-2			AuT	
	Average lifespan of product or Warranty provided [years]	GRI-306-2			AuT	

Similarly, one or more metrics are chosen to standardize the indicators of each principal category. Different metrics are determined for each principal category of each sector of the economy in an attempt to reflect accurately the specific features and attributes of each sector. As an example, three or four different metrics are utilized in GHG Emissions principal category depending on the sector. Table 7.4 illustrates the complete set of metrics for all principal categories and sectors. The sector specific metrics individually are shown in Tables J.5 to J.8 in Appendix J.

Table 7.4: CE Metrics with Sector Allocation [EuN: Energy and Utilities, MaN: Manufacturing, AuT: Automotive, SrV: Service]

Principal Categories	**Metric**		**Upper Bound**	**Formula Used**	**Sectors Allocation**			
Waste	1a	% of Hazardous waste over Total waste generated	100%	100%-1a	EuN	MaN	AuT	SrV
	1b	% of Diverted waste over Total waste generated	100%	1b	EuN	MaN	AuT	SrV
	1ca	Waste generated over Products sold [kg waste over tons of product]	200	1-norm[1ca]		MaN		
	1cb	Waste generated over Number of products sold [kg waste over # of products]	1500	1-norm[1cb]			AuT	
	1cc	Waste generated over Full Time Employees [kg waste over # of FTE]	1000	1-norm[1cc]				SrV
Water	2a	% of Recycled/reused water over Total water withdrawal	100%	2a	EuN	MaN	AuT	SrV
	2b	% of Other water discharge over Total water discharge	100%	100%-2b	EuN	MaN	AuT	SrV
	2c	% of Water consumed over Total water withdrawal	100%	100%-2c	EuN	MaN	AuT	SrV
	2da	Water withdrawal over Products sold [m3 water over tons of product]	10	1-norm[2da]		MaN		
	2db	Water consumption over Number of products sold [m3 water over # of products]	30	1-norm[2db]			AuT	
	2dc	Water consumption over Full Time Employees [m3 water over # of FTE]	100	1-norm[2dc]				SrV
Procurement: Production & Packaging	2paa	% of Recycled input material used	100%	2paa			AuT	SrV
	2pab	% of Recycled packaging material used	100%	2pab		MaN		
	2pba	% of Renewable material used	100%	2pba			AuT	
	2pbb	% of Renewable packaging material used	100%	2pbb		MaN		
	2pca	% of Reusable, compostable or recyclable material used	100%	2pca			AuT	
	2pcb	% of Reusable, compostable or recyclable packaging material used	100%	2pcb		MaN		
	2pd	Paper consumption over Full Time Employees [kg over # of FTE]	365	1-norm[2pd]				SrV
	2pe	Single-use plastics consumption over Full Time Employees [kg plastic over # of FTE]	50	1-norm[2pe]				SrV
Energy	3aa	% of Non fossil fuel energy generated over Total energy generated	100%	3aa	EuN			
	3ab	% of Renewable energy consumed over Total energy consumed	100%	3ab		MaN	AuT	SrV
	3ba	Total energy consumed over Products sold [joules or multiples over tons of product]	10	1-norm[3ba]		MaN		
	3bb	Total energy consumed over Number of products sold [joules or multiples over # of products]	15	1-norm[3bb]			AuT	
	3bc	Total energy consumed over Operational space [joules or multiples over surface area]	1	1-norm[3bc]				SrV
	3bd	% of Certified buildings and facilities i.e LEED	100%	3bd				SrV
GHG Emissions	4aa	Net total emissions over Total energy delivered [tCO2e over joules or multiples]	600	1-norm[4aa]	EuN			
	4ab	Net total emissions over Products sold [tCO2e over tons of product]	500	1-norm[4ab]		MaN		
	4ac	Net total emissions over Number of products sold [tCO2e over # of products]	2,000	1-norm[4ac]			AuT	
	4ad	Net total emissions over Operational space [tCO2e over surface area]	300	1-norm[4ad]				SrV
	4ba	Emissions of ODS over Total energy delivered [metric tons of CFC-11 eq. over joules or multiples]	0.1	1-norm[4ba]	EuN			
	4bb	Emissions of ODS over Products sold [metric tons of CFC-11 eq. over tons of product]	0.1	1-norm[4bb]		MaN		
	4bc	Emissions of ODS over Number of products sold [metric tons of CFC-11 eq. over # of products]	0.1	1-norm[4bc]			AuT	
	4bd	Emissions of ODS over Operational space [metric tons of CFC-11 eq. over surface area]	1	1-norm[4bd]				SrV
	4ca	NOx, SOx, and other significant air emissions over Total energy delivered [metric tons over joules or multiples]	1.0	1-norm[4ca]	EuN			
	4cb	NOx, SOx, and other significant air emissions over Products sold [metric tons over tons of product]	1	1-norm[4cb]		MaN		
	4cc	NOx, SOx, and other significant air emissions over Number of products sold [metric tons over # of products]	10	1-norm[4cc]			AuT	
	4cd	NOx, SOx, and other significant air emissions over Operational space [metric tons over surface area]	0.05	1-norm[4cd]				SrV
	4d	Average specific CO2 emissions [gCO2/km]	200	1-norm[4d]			AuT	
Spillages & Discharges	4da	Environmental fines over Total energy delivered [$ over joules or multiples]	1.0	1-norm[4da]	EuN			
	4db	Environmental fines over Products sold [$ over tons of product]	10	1-norm[4db]		MaN		
	4dc	Environmental fines over Number of products sold [$ over # of products]	10	1-norm[4dc]			AuT	
	4dd	Environmental fines over Operational space [$ over surface area]	0.5	1-norm[4dd]				SrV
Durability	5a	% of Packaging material to be reclaimed/recovered	100%	5a		MaN		
	5b	% of Material to be reclaimed/recovered	100%	5b			AuT	
	5c	Average lifespan of product or Warranty provided [years]	20	norm[5c]			AuT	

Equal weights are used for the calculation of the Category-based Circularity Sub-Index of Waste, Water, Procurement, and Durability across the sectors. One metric with 100% weight is used for the Energy principal category in Energy and Utilities sector, while for the Manufacturing and Automotive sectors, higher weight (75%) is assigned to the metric related to the evaluation of renewables utilization, and lower weight (25%) is assigned to the metric related to the energy efficiency. In the Service sector, an extra metric is used to evaluate the performance and leadership of companies towards CE for their buildings and facilities, with an assigned weight of 25% (which is subtracted from the renewables utilization metric that becomes 50% for this sector). Furthermore, three plus one metrics are used within the GHG Emissions & Spillages principal categories in the Energy and Utilities, Manufacturing and Service sectors. The highest emphasis is put towards the Net Emissions Intensity (50-55%), followed by lower weights for the rest of the metrics i.e. 5% - 20%. In the Automotive sector, the Average Specific CO_2 Emissions metric is introduced, which gets the highest weight (40%), followed by the weight in the Net Emissions Intensity metric (35%), while for the rest of the metrics the weights range from 5% to 10%.

7.4.3 Collection and analysis of data

A key advantage of the proposed framework originates from the explicit definition of the specific indicators and metrics that prevents vagueness and ambiguity on the data to be collected as well as on the type of data that are needed. The data are generally easily accessible from a variety of sources and trackable over a long period of time. Here, each company's annual "Sustainability", "Environmental-Social-Governance (ESG)" and "Financial" reports are recommended as the main sources of data. Each company's data from multiple years are collected and analyzed based on the proposed indicators and metrics so as to calculate the annual "Category-based Circularity Sub-Index" and the annual "Overall Circularity Index" for each principal category e.g. 2019 "Circularity Index for Energy", "Circularity Index for Waste", 2019 "Overall Circularity Index" etc. Therefore, a company's Overall "Circularity" as well as its "Category-based Circularity" versus every CE goal can be tracked on annual basis and/or against its peers.

The values of the "Overall Circularity Index" and its sub-indices lie between 0 and 1, with the target value of circularity being always 1 or 100%. Thereby, a value of 1 for either the Overall or any of the sub-indices reflects perfect circularity on the assessed company or principal category while a value of 0 reflects perfect linearity on the assessed company or principal category. The formulas used for each metric have been designed to reflect to the target of 1 or 100% and are shown in Table 7.4. For example, metric 1a that captures the percentage of hazardous waste over total waste generated shall be preferably 0, but since our target is 1 then the formula *100%-1a* is used. On the contrary, metric 1b that tracks the percentage of diverted waste over total waste generated shall preferably approaches 1, and thus the formula used is *1b*.

In case data for a metric are not available for a specific period of time, then the corresponding metric gets a value of 0 for this particular period. The metrics that are not expressed as percentages and have different units are normalized using an upper bound value, and then the formula is selected based on the target value. As such, only metric 5c that reflects the average lifespan of product or warranty provided and shall preferably approaches 1 is calculated based on the formula *norm[metric]*. The rest of the normalized metrics shall approach 0, and hence the formula *1-norm[metric]* is used. The upper bound value of each metric is estimated as 1.5 times higher than the average of the already collected data so as to reflect a reasonable and realistic upper bound for each principle category. Clearly, this is a parameter of the framework that is updated once more data become available and companies use the framework. For example, the upper bound of metric 4d that captures the average specific CO_2 emissions (gCO_2/km) of vehicles is set at 200 gCO_2/km based on analysis of data from various automotive manufactures. A hypothetical measurement of 100 gCO_2/km results to a 4d metric of 0.5. In case the value of a metric is higher than its upper bound and in order to avoid negative (when formula *1-norm[metric]* is used) or larger than 1 (when *norm[metric]* is used) index numbers, the final normalized metric is set to 0 or 1 respectively.

7.4.4 A holistic and robust CE assessment framework

The developed quantitative framework combines data and information from the academic and industrial literature along with a novel structure to effectively assess the circularity at the micro level in any sector of the economy. It provides media for data visualization and analysis at different levels of granularity and is an analytical tool to assess the multi-scale, multi-faceted and interconnected CE supply chains and business activities. This structure provides a holistic approach in capturing both the CE and sustainability attributes across the different sectors while it improves the interpretability and traceability of the integrated CE within the various aspects of a business. It also enhances the robustness of the framework allowing the successful treatment of outliers which is crucial for comparison among peers or among different industries and sectors as well as for tracking year over year performance. Specific CE targets and benchmarks can be set by taking advantage of the high level of granularity, having a positive impact on the decision-making at different operational levels and investment time horizons (short or long term).

Figure 7.2 demonstrates the schematic of the proposed CE assessment framework - MICRON. For demonstration purposes, arbitrary values are assigned to the Category-based Circularity Sub-Indices while the Overall Circularity Index is calculated as their linear average.

Illustrative Example

Let's assume that a company wants to assess its overall circularity performance, compare its performance against its competitors, track its progress over the years, and identify areas of potential improvement. First, the company is classified into one of the four economic sectors according to its business activities. For this example, let's assume that the company belongs to the Manufacturing sector. Next, the company provides annual data for a variety of indicators in 7 plus 1 principal categories. As such, the annual data of "Total energy consumed, in GJ" and "Renewable energy consumed, in GJ" must be provided for the Energy principal category, the "Waste generated - Hazardous, in metric tons", "Waste generated - Non Hazardous, in metric tons" and "Diverted waste from disposal, in metric tons" must be provided for the Waste principal category, and so on (Table 7.3). The data provided are then used for the calculation of the various standardized and normalized metrics of each principal category. The metrics are dimensionless, with values close to zero reflecting linear behavior while values close to one (or 100%) reflecting circular behavior. For the case of the Energy principal category, two metrics are calculated: "% of Renewable energy consumed over Total energy consumed", and "Total energy consumed over Products sold, in GJ per ton product". The first metric is a percentage so no further processing is required, but the second metric needs to be normalized, thus an upper bound value is used. Since this metric captures the energy consumption per unit sold, this implies that a value close to zero is preferable in circularity terms. Therefore, the normalized value is subtracted from 1. As indicative values for this example for the years 2018 and 2019, let's assume that the first metric has values of 0.20 and 0.25, and the second metric has values of 0.80 and 0.85 with an upper bound of 10 GJ per ton product. The same process is followed for the rest of the metrics in the remaining principal categories (Table 7.4). Having estimated the normalized metrics for all principal categories, then the Category-based Circularity Sub-Indices using weighted averages are calculated. In particular, for the Energy principal category, the first metric gets a 75% weight, while the second metric gets a 25%. Given the previous mentioned values, the 2018 "Circularity Index for Energy" is 0.35, which increased to 0.40 in 2019. Conducting the analogous process for the rest of the principal categories, the annual Circularity Sub-Index for each principal category is calculated. The linear average of all annual Circularity-based Sub-Indices leads to the Overall Circularity Index, in this case being 0.46 and 0.49 for 2018 and 2019 respectively. Finally, data visualization, benchmarking and various comparisons can be conducted and indicative analysis is shown in the next Section 7.5 Case Studies.

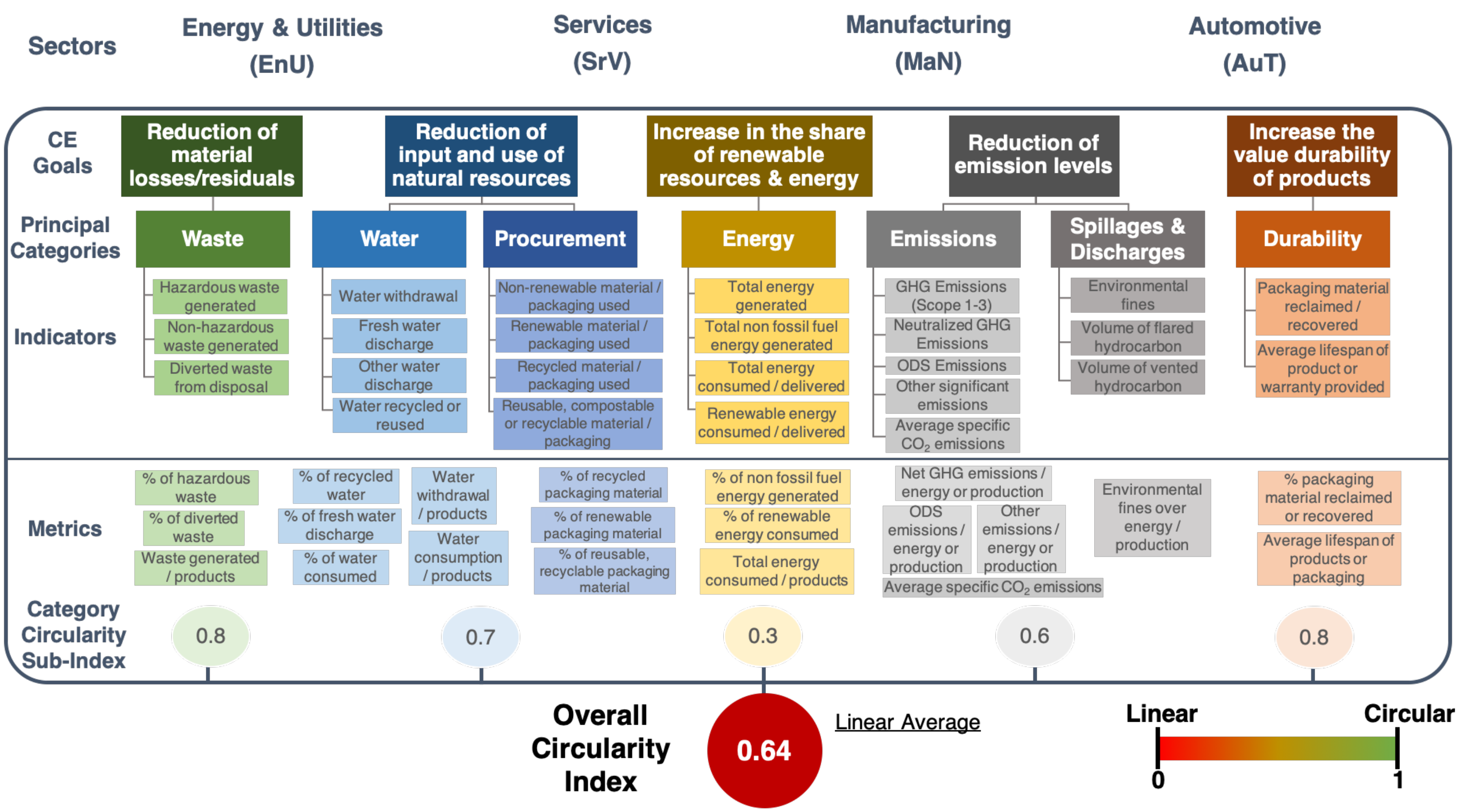

Figure 7.2: Schematic of MICRON CE Assessment Framework, with arbitrary values on Category-based Circularity Sub-Indices

7.5 Case Studies

Leading companies from the Energy and Utilities, Manufacturing, and Automotive sectors are used as working examples to illustrate the extent, use and applicability of the proposed framework.

7.5.1 MICRON applied in Energy and Utilities (EnU) sector

First, the developed CE assessment framework is applied to Energy Utilities companies which operate in Energy and Utilities sector so as to estimate their Overall Circularity Index as well as their Category-based Circularity Sub-Indices. In particular, the circularity of the following companies over the a number of years are evaluated: **PG&E** (2014-2019), **NextEra** (2016-2019) and **Uniper** (2016-2019). The data used for the subject calculations and analysis are taken from the following sources: PG&E: "Corporate Responsibility and Sustainability" reports (2015-2020), NextEra: "Environmental, Social and Governance" report (2020) and "Sustainability: By the Numbers" report (2014-2018), Uniper: "Sustainability" reports (2017-2019) and "2019 Annual Report - Financial Results" [355, 356, 357, 358, 359]. First, the annual metrics of each indicator are calculated using the methodology described in sections 7.4.2 and 7.4.3, and are summarized in Table 7.5.

Table 7.5: CE Metrics of Energy Utilities Companies (2014-2019) - Energy and Utilities Sector

Principal Categories / Year	**Waste**		**Water**			**Energy**	**GHG Emissions**			**Spillages and Discharges**
	1a	**1b**	**2a**	**2b**	**2c**	**3aa**	**4aa**	**4ba**	**4ca**	**4da**
Weights	***50%***	***50%***	***33.33%***	***33.33%***	***33.33%***	***100%***	***50%***	***20%***	***20%***	***10%***
Company	**PG&E**									
2014	0.4104	0.4630	0.0000	0.0000	0.9999	0.7893	0.6952	0.0000	0.9883	0.9893
2015	0.2072	0.2712	0.0000	0.0000	0.9997	0.7621	0.6799	0.0000	0.9872	0.3866
2016	0.2466	0.2741	0.0000	0.0000	0.9997	0.8294	0.7539	0.0000	0.9894	0.5954
2017	0.4166	0.4343	0.0000	0.0000	0.9997	0.8361	0.7777	0.0000	0.9890	0.9187
2018	0.3225	0.4452	0.0000	0.0000	0.9997	0.8068	0.7674	0.0000	0.9900	0.7160
2019	0.3519	0.3328	0.0000	0.0000	0.9996	0.8133	0.7745	0.0000	0.9901	0.8611
Company	**NextEra**									
2016	0.0000	0.0000	0.0032	0.0000	0.9855	0.4838	0.6028	0.0000	0.9167	0.0000
2017	0.9972	0.9797	0.0022	0.0000	0.9851	0.5103	0.6211	0.0000	0.9219	0.0000
2018	0.9985	0.9879	0.0027	0.0000	0.9850	0.5066	0.6366	0.0000	0.9392	0.0000
2019	0.9990	0.9934	0.0035	0.0000	0.9819	0.4871	0.5985	0.0000	0.9300	0.0000
Company	**Uniper**									
2016	0.9516	0.1252	0.0000	0.0000	0.9983	0.1788	0.1113	0.0000	0.3410	0.0000
2017	0.9072	0.2597	0.0000	0.0000	0.9940	0.1912	0.1210	0.0000	0.3121	0.0000
2018	0.9716	0.1600	0.0000	0.0000	0.9917	0.1896	0.1048	0.0000	0.3207	0.0000
2019	0.9330	0.3164	0.0000	0.0000	0.9934	0.2288	0.2216	0.0000	0.4151	0.0000

PG&E scores almost the maximum (100%) with regards to the water preservation metric (2c - percentage of water consumed over water withdrawal), but data for the other two Water metrics are not available. One of the environmental GHG emissions intensity metrics (4ca - NOx, SOx, and other significant air emissions over Total energy delivered) demonstrates almost perfect score (100%) over this period, while no data are available for the third environmental GHG emissions intensity metric (4ba - Emissions of ODS over Total energy delivered). The spillages intensity metric (4da - Environmental fines over Total energy delivered) fluctuates dramatically over this period.

The majority of the required data are not available for NextEra in 2016. NextEra is the only one of the three companies which reports recycled water values, although the reported values are close to 0. It does not report any values for the spillages and discharges (4da), percentage of other water discharges (2b), and ODS emissions (4ba). NextEra scores almost 100% in the Waste principal category, the water preservation metric (2c), and one of the environmental GHG emissions intensity metrics (4ca). Finally, despite the increase in Energy and Net emissions intensity (4aa) metrics in 2017, both metrics did not improve over the years.

Data availability for Uniper is similar to PG&E, with the only difference that spillages and discharges are also not available. The company performs poorly in multiple metrics, including diverted waste (1b), Energy (3aa) and GHG emissions (4aa, 4ca).

7.5.2 MICRON applied in Manufacturing (MaN) sector

The second application of MICRON framework is at the Food and Beverages industry which is classified under the Manufacturing sector. Here, the category-based and overall circularity of the following companies from 2010-2019 are assessed: **Nestle** (2010-2019), **General Mills** (2010-2019), **Tyson** (2015-2019) and **Ferrero** (2016-2019).

The following sources are used for collecting data for the analysis: Nestle: "Progress Report" (2018-2019) and "Consolidated Nestle Environmental Performance Indicators" (2019), General Mills: "Global Responsibility" report (2016-2020) and "Annual Report to Shareholders" (2020), Tyson: "Sustainability" reports (2012-2019), and Ferrero: "Sustainability" reports (2017-2019)

[360, 361, 362, 363, 364, 365]. The annual metrics of each indicator are calculated using the methodology described in sections 7.4.2 and 7.4.3, and are summarized in Table 7.6.

Table 7.6: CE Metrics of Food and Beverages Companies (2010-2019) - Manufacturing Sector

Principal Categories /	Waste			Water				Procurement: Production and Packaging			Energy		GHG Emissions			Spillages and Discharges	Durability
Year	1a	1b	1ca	2a	2b	2c	2da	2pab	2pbb	2pcb	3ab	3ba	4ab	4bb	4cb	4db	5a
Weights	33.33%	33.33%	33.33%	25%	25%	25%	25%	33.33%	33.33%	33.33%	75%	25%	50%	20%	20%	10%	100%
Company	Nestle																
2010	0.9951	0.7140	0.8454	0.0339	0.6178	0.6555	0.6685	0.0000	0.0000	0.0000	0.1190	0.7959	0.6746	0.2112	0.6036	0.0000	0.0000
2011	0.9967	0.7631	0.8414	0.0335	0.6172	0.6530	0.6818	0.2710	0.2801	0.0000	0.1200	0.8001	0.6778	0.6887	0.6331	0.9929	0.0000
2012	0.9972	0.7757	0.8500	0.0341	0.5759	0.6106	0.7105	0.2710	0.2801	0.0000	0.1250	0.8108	0.6973	0.7223	0.6705	0.9986	0.0000
2013	0.9979	0.8273	0.8551	0.0337	0.6133	0.5958	0.7084	0.2710	0.2801	0.0000	0.1340	0.8099	0.6966	0.8052	0.6446	0.9781	0.0000
2014	0.9984	0.8511	0.8549	0.0374	0.5899	0.6019	0.7244	0.2680	0.2837	0.0000	0.1450	0.8186	0.7148	0.8197	0.6837	0.9853	0.0000
2015	0.9986	0.8954	0.8534	0.0390	0.5817	0.5835	0.7426	0.2810	0.2769	0.0000	0.1530	0.8275	0.7280	0.6491	0.7091	0.9853	0.0000
2016	0.9996	0.9352	0.8504	0.0370	0.5657	0.5759	0.7520	0.2740	0.2587	0.0000	0.1690	0.8328	0.7546	0.8813	0.7157	0.9757	0.0000
2017	0.9998	0.9620	0.8503	0.0476	0.5624	0.5907	0.7633	0.2870	0.2821	0.0000	0.1930	0.8357	0.7764	0.8714	0.7303	0.9911	0.0000
2018	0.9998	0.9790	0.8472	0.0463	0.5618	0.5939	0.7668	0.2360	0.2504	0.0000	0.2190	0.8372	0.7826	0.8883	0.7505	0.9844	0.0000
2019	0.9998	0.9913	0.8424	0.0397	0.4765	0.5585	0.7718	0.2600	0.2701	0.8700	0.2020	0.8341	0.7886	0.8935	0.7631	0.9951	0.0000
Company	General Mills																
2010	1.0000	0.0000	0.8163	0.0000	0.0000	0.0000	0.7832	0.0000	0.0000	0.0000	0.0008	0.8080	0.5917	0.0000	0.0000	0.0000	0.0000
2011	1.0000	0.0000	0.8176	0.0000	0.0000	0.0000	0.7889	0.0000	0.0000	0.0000	0.0031	0.8080	0.5872	0.0000	0.0000	0.0000	0.0000
2012	1.0000	0.0000	0.8298	0.0000	0.0000	0.0000	0.7859	0.0000	0.0000	0.0000	0.0076	0.8100	0.5872	0.0000	0.0000	0.0000	0.0000
2013	1.0000	0.0000	0.8296	0.0000	0.0000	0.0000	0.7094	0.0000	0.0000	0.0000	0.0501	0.8110	0.6208	0.0000	0.0000	0.0000	0.0000
2014	1.0000	0.0000	0.8339	0.0000	0.0000	0.0000	0.7178	0.0000	0.0000	0.0000	0.0488	0.8120	0.6381	0.0000	0.0000	0.0000	0.0000
2015	1.0000	0.8800	0.8258	0.0000	0.0000	0.0000	0.7148	0.4900	0.0000	0.8400	0.0494	0.8130	0.6415	0.0000	0.0000	0.0000	0.0000
2016	1.0000	0.8500	0.7860	0.0000	0.0000	0.0000	0.6803	0.4200	0.0000	0.8800	0.0418	0.8140	0.6616	0.0000	0.0000	0.0000	0.0000
2017	1.0000	0.8700	0.7775	0.0000	0.0000	0.0000	0.7053	0.4300	0.0000	0.8800	0.0468	0.8090	0.6593	0.0000	0.0000	0.0000	0.0000
2018	1.0000	0.9000	0.7601	0.0000	0.0000	0.0000	0.7154	0.4500	0.0000	0.8900	0.0445	0.8120	0.6664	0.0000	0.0000	0.0000	0.0000
2019	1.0000	0.9200	0.7029	0.0000	0.0000	0.0000	0.7365	0.4700	0.0000	0.8800	0.0376	0.8110	0.6805	0.0000	0.0000	0.0000	0.0000
Company	Tyson																
2015	0.0000	0.9055	0.5594	0.0000	0.0000	0.0000	0.3031	0.0000	0.0000	0.0000	0.0166	0.7581	0.3320	0.0000	0.0000	0.7547	0.0000
2016	0.0000	0.8976	0.5604	0.0638	0.0000	0.0000	0.2555	0.3000	0.0000	0.0000	0.0215	0.7453	0.2760	0.0000	0.0000	0.9405	0.0000
2017	0.0000	0.8879	0.5077	0.0627	0.0000	0.0000	0.2022	0.3000	0.0000	0.0000	0.0135	0.6585	0.2400	0.0000	0.0000	0.8625	0.0000
2018	0.0000	0.8111	0.2993	0.0634	0.0000	0.0000	0.2240	0.2990	0.0000	0.0000	0.0075	0.6542	0.2400	0.0000	0.0000	0.0000	0.0000
2019	0.0000	0.8675	0.0505	0.0637	0.0000	0.0000	0.2537	0.3550	0.0000	0.0000	0.0077	0.6135	0.2800	0.0000	0.0000	0.9772	0.0000
Company	Ferrero																
2016	0.0000	0.9500	0.5535	0.7406	0.0620	0.7406	0.6279	0.3900	0.3700	0.0000	0.0994	0.1000	0.0326	0.2580	0.0000	0.0000	0.0000
2017	0.0000	0.9500	0.5727	0.7319	0.0590	0.7319	0.6319	0.3600	0.3700	0.0000	0.1202	0.1000	0.0851	0.4076	0.0000	0.0000	0.0000
2018	0.9877	0.9465	0.5503	0.6385	0.0510	0.6385	0.5697	0.3390	0.3690	0.8170	0.1371	0.1600	0.0000	0.8661	0.0000	0.0000	0.0000
2019	0.9854	0.9677	0.5892	0.6318	0.0530	0.6318	0.5620	0.3420	0.3690	0.8170	0.1900	0.1600	0.0000	0.9178	0.0000	0.0000	0.0000

Nestle demonstrates a continuous improvement with regards to circularity in almost all principal categories. Waste is the best performing category, with close to perfect scores. As an example, the company reports on average 30 kg of total waste per ton of product produced (1ca) over the decade. The metrics for GHG Emissions & Spillages also reveal an upward trend, with about 35% decrease in the net emissions per ton of product sold metric (4ab), and even higher reductions in the ODS and other significant emissions per ton of product sold (4bb, 4cb) during the same period. The environmental fines are constantly minimal in comparison to the level of production. On the contrary, and despite the advancements over the years, there are significant opportunities for improving circularity in the Energy principal category, since just 20% of the energy consumed comes from renewable resources.

Similar findings are observed from the circularity assessment of General Mills. The introduction of recycling and reusing initiatives for the waste handling (1b) in 2015 resulted in a substantial improvement in the corresponding category. There are enormous enhancement possibilities for the rest of the principal categories, since for example less than 5% of energy consumed comes from renewable resources (3ab), or the water withdrawal per product sold has raised by 22% without any provision for recycling or reusing initiatives (2da).

Tyson is the least circular from the assessed companies in the Food and Beverages industry. As an example, the total waste generated per ton of product sold (1ca) more than doubled within five years while the GHG emissions per product sold (4ab) grew by more than 7% over this period. The portion of renewable energy in company's portfolio is less than 1% (3ab), and the energy efficiency (3ba) has deteriorated by almost 60% since 2015.

Ferrero illustrated a slightly better circular performance in comparison to Tyson. Despite the significant increase of 91% in the share of renewables sources (3ab), renewables still provide less than 20% of the total energy requirements, while GHG emissions intensity (4ab) grew by more than 30% over the last four years. The water consumed as a percentage of water withdrawal (2c) and the water withdrawal per product sold (2da) increased by almost 40% and 20% respectively.

Finally, it is worth highlighting that none of the reviewed companies in this sector reported data related to the Durability. This will be another contribution of the proposed framework towards enhancing the awareness of companies with regards to specific overlooked or under-reviewed categories, that are inextricably linked with the CE concept.

7.5.3 MICRON applied in Automotive (AuT) sector

The Automotive industry has some unique characteristics that differentiate it from the rest of the industries and require its classification into a separate sector, the Automotive sector. These characteristics refer to the output of the industry which is counted in vehicles with distinct features and as such affects all the intensity metrics, the environmental aspects of the produced vehicles, and the lifespan or the warranty that is provided by the automotive companies for their vehicles. Here, the category-based circularity sub-indices and the overall circularity index of the following companies from 2012-2019 are evaluated: **Daimler** (2012-2019), **Ferrari** (2016-2019), **Audi** (2014-2019) and **BMW** (2015-2019).

The sources of data and information for our analysis are as follows: Daimler: "sustainability" reports (2012-2019) and "GRI" (2017-2019), Ferrari: "Sustainability" reports (2017-2019) and "Annual" reports (2017-2019), Audi: "Sustainability" reports (2014-2019), and BMW: "Sustainability Value" reports (2015-2019) and "GRI" (2017-2019) [366, 367, 368, 369, 370, 371, 372]. The annual metrics of each indicator are calculated using the methodology described in sections 7.4.2 and 7.4.3, and are summarized in Table 7.7.

Table 7.7: CE Metrics of Automotive Companies (2012-2019) - Automotive Sector

Principal Categories /	Waste			Water				Procurement: Production and Packaging			Energy		GHG Emissions				Spillages and Discharges	Durability	
Year	1a	1b	1cb	2a	2b	2c	2db	2paa	2pba	2pca	3ab	3bb	4ac	4bc	4cc	4d	4dc	5a	5b
Weights	33.33%	33.33%	33.33%	25%	25%	25%	25%	33.33%	33.33%	33.33%	75%	25%	35%	10%	10%	40%	5%	50%	50%
Company	Daimler																		
2012	0.9257	0.9266	0.6406	0.0000	0.0000	0.0000	0.7674	0.0000	0.0000	0.8500	0.0000	0.6734	0.2411	0.0000	0.6989	0.2415	0.0000	0.9500	0.3500
2013	0.9104	0.9055	0.6525	0.0000	0.0000	0.0000	0.7847	0.0000	0.0000	0.8500	0.0000	0.6868	0.2871	0.0000	0.7065	0.2770	0.0000	0.9500	0.3500
2014	0.8623	0.8542	0.6426	0.0000	0.0000	0.0000	0.8062	0.0000	0.0000	0.8500	0.0000	0.7159	0.3576	0.0000	0.7429	0.3039	0.0000	0.9500	0.3500
2015	0.9111	0.9088	0.6456	0.0000	0.0000	0.3816	0.8001	0.0000	0.0000	0.8500	0.0000	0.7078	0.3527	0.0000	0.5382	0.3328	0.0000	0.9500	0.3500
2016	0.9251	0.9129	0.6780	0.0000	0.0000	0.3608	0.8022	0.0000	0.0000	0.8500	0.0000	0.7146	0.4227	0.0000	0.5171	0.3305	0.0000	0.9500	0.3500
2017	0.9291	0.9236	0.6825	0.0000	0.0000	0.3921	0.8247	0.0000	0.0000	0.8500	0.0000	0.7163	0.4456	0.0000	0.5749	0.3175	1.0000	0.9500	0.3500
2018	0.9307	0.9623	0.6652	0.0000	0.0000	0.4111	0.8186	0.0000	0.0000	0.8500	0.0000	0.7072	0.4448	0.0000	0.5558	0.2927	0.0000	0.9500	0.3500
2019	0.9288	0.9696	0.6636	0.0000	0.0000	0.4079	0.8185	0.0000	0.0000	0.8500	0.0000	0.6962	0.4923	0.0000	0.5428	0.2742	1.0000	0.9500	0.3500
Company	Ferrari																		
2016	0.6765	0.4148	0.0828	0.0000	0.0000	0.5382	0.0000	0.0000	0.0430	0.8500	0.0468	0.0000	0.0000	1.0000	0.0000	0.0000	1.0000	0.9500	0.7500
2017	0.7204	0.4325	0.0260	0.0000	0.0000	0.5041	0.0000	0.0000	0.0430	0.8500	0.0517	0.0000	0.0000	1.0000	0.0000	0.0000	1.0000	0.9500	0.7500
2018	0.7497	0.4583	0.1912	0.0000	0.0000	0.5742	0.0000	0.0000	0.0430	0.8500	0.0541	0.0000	0.0000	1.0000	0.0000	0.0000	1.0000	0.9500	0.7500
2019	0.7605	0.4429	0.2646	0.0000	0.0000	0.5899	0.1550	0.0000	0.0380	0.8500	0.0655	0.0000	0.0000	1.0000	0.1056	0.0000	1.0000	0.9500	0.7500
Company	Audi																		
2014	0.8979	0.9674	0.8424	0.0000	0.0000	0.4058	0.9295	0.0000	0.0000	0.0000	0.2747	0.8715	0.8233	0.0000	0.8794	0.3450	1.0000	0.0000	0.5000
2015	0.9023	0.9683	0.8390	0.0000	0.0000	0.4012	0.9272	0.0000	0.0000	0.0000	0.2646	0.8644	0.8237	0.0000	0.8887	0.3700	1.0000	0.0000	0.5000
2016	0.9040	0.9766	0.8309	0.0000	0.0000	0.3731	0.9269	0.0000	0.0000	0.8500	0.2493	0.8592	0.8143	0.0000	0.8948	0.3700	1.0000	0.9500	0.5000
2017	0.9031	0.9773	0.8327	0.0000	0.0000	0.3510	0.9267	0.0000	0.0000	0.8500	0.2456	0.8558	0.8078	0.0000	0.9098	0.3650	1.0000	0.9500	0.5000
2018	0.9033	0.9838	0.8393	0.0000	0.0000	0.3656	0.9271	0.0000	0.0000	0.8500	0.2993	0.8643	0.8357	0.0000	0.9286	0.3550	1.0000	0.9500	0.5000
2019	0.8973	0.9913	0.8423	0.0000	0.0000	0.3541	0.9378	0.0000	0.0000	0.8500	0.3553	0.8636	0.8422	0.0000	0.9366	0.3450	1.0000	0.9500	0.5000
Company	BMW																		
2015	0.9515	0.9884	0.7772	0.0000	0.0000	0.6450	0.9747	0.0000	0.0200	0.8500	0.0449	0.8508	0.6780	0.0000	0.8780	0.3650	1.0000	0.9500	0.3500
2016	0.9540	0.9896	0.7839	0.0000	0.0000	0.6602	0.9758	0.0000	0.0200	0.8500	0.0447	0.8490	0.6971	0.0000	0.8860	0.3800	1.0000	0.9500	0.3500
2017	0.9473	0.9885	0.7880	0.0000	0.0000	0.7162	0.9806	0.0000	0.0200	0.8500	0.0830	0.8552	0.7713	0.0000	0.8970	0.3600	1.0000	0.9500	0.3500
2018	0.9469	0.9875	0.7880	0.0000	0.0000	0.6328	0.9733	0.0000	0.0200	0.8500	0.0400	0.8612	0.7757	0.0000	0.9070	0.3600	1.0000	0.9500	0.3500
2019	0.9367	0.9875	0.7949	0.0000	0.0000	0.6606	0.9759	0.0000	0.0200	0.8500	0.0319	0.8627	0.8151	0.0000	0.9150	0.3650	1.0000	0.9500	0.3500

Waste and Durability are the top performing circularity principal categories for Daimler over a period from 2012 to 2019, followed by Emissions & Spillages and Water & Procurement, with Energy being the worst performing category. The amount of waste that is diverted from disposal (1b) continued to increase over the years, while the hazardous waste remained minimal as a percentage of the total waste (1a). Both metrics of Durability remain constant over the years, which is also the case for the rest of the automotive companies considered, with the exception of Audi, which started reporting information for the percentage of the material that is reclaimed and/or recovered (5a) in 2015. Emissions demonstrate a mix picture since the net total GHG emissions per vehicle sold (4ac) are reduced by 33% while on the other hand, the NOx, SOx and other significant air emissions per vehicle sold (4cc) have increased by 52% over the same period. The water consumption per vehicle sold (2db) declined by 22%. The company did not report any total renewable energy consumption.

With the exception of Durability metrics, the rest of Ferrari's circularity principal categories reveal room for substantial improvement. Energy is by far the worst performing circular category, with the energy consumption per vehicle sold (3bb) being 11x to 25x times higher than the other three companies. Similar results are reported for Emissions, with Ferrari's GHG emissions per vehicle sold (4ac) being between 10x to 33x times higher than the other three companies. Water & Procurement and Waste categories have slowly progressed over the years, but further improvements towards circularity are required.

Audi scores close to the maximum with regards to the Waste metrics, followed by Durability and Emission & Spillages. A significant improvement in Durability category occurs after 2016, once the company reported that 95% of the materials used are reclaimed and/or recovered (5b). The share of renewable energy in the total mix of consumed energy (3ab) has grown to almost 36%, while the energy efficiency in vehicle production (3bb) remains the highest in the sector. Water & Procurement is the worst performing circularity category despite the improvement caused by the reported high percentages of reusable and/or recyclable materials (2pca) after 2016.

BMW reveals a very similar circular behavior with Daimler, scoring almost excellent in Waste metrics. GHG Emissions per vehicle sold (4ac) decreased by more than 42%, while 30% was the reduction in the NOx, SOx and other air emissions per vessel sold (4cc) over the same period.

On the contrary, Water & Procurement metrics remain rather unchanged since 2015. Renewable energy remains a minor percent of the total energy consumed (3ab), while the energy efficiency in vehicles' production (3bb) has increased by 8%.

7.6 Results and Discussion

Having considered the individual metrics of each principal category in the previous section, here the Category-based Circularity Sub-Index and the Overall Circularity Index for each company in the three sectors are computed and assessed. Initially, the analysis is performed per sector, estimating the Category-based Circularity Sub-Index for the companies within the sector and conducting a comparison between peers. Then, the Overall Circularity Index of each company within the same sector is calculated, and a comparison between peers at this higher level is presented, enabling the identification of areas that require improvement. As it was discussed earlier, this is an advantage of the proposed framework that allows the CE assessment at different operational and structural levels and monitoring the progress towards CE goals in due time. Also, benchmarking against peers from the same industry and/or sector, or even from different sectors can be conducted.

7.6.1 Category-based and Overall Circularity Indices for Energy and Utilities (EnU) Sector

The following figures illustrate the annual Category-based Circularity Sub-Indices (Figure 7.3) and annual Overall Circularity Index (Figure 7.4) for three companies that operate in the Energy & Utilities sector from 2016 to 2019, using the weights described in previous sections. According to Figure 7.3, PG&E scores higher than the other two companies in circularity in the Energy and Emissions principal categories over the years, in comparison to Waste category in which NextEra is by far the best performing company. All three companies reveal the same steady performance in Water category. PG&E scores on average 62% and 30% higher than NextEra, and 309% and 362% higher than Uniper in the Energy and Emissions categories respectively. Conversely, NextEra outperforms on average Uniper and PG&E by 68% and 159% respectively in the Waste category between 2017-2019, while no data are available for NextEra in 2016. Figures J.1 to J.3 present Category-based Circularity Sub-indices for the three Energy Utilities companies for multiple years, while Figure J.4 in Appendix J highlights the Category-based Circularity Sub-indices for the Energy & Utilities sector for 2019.

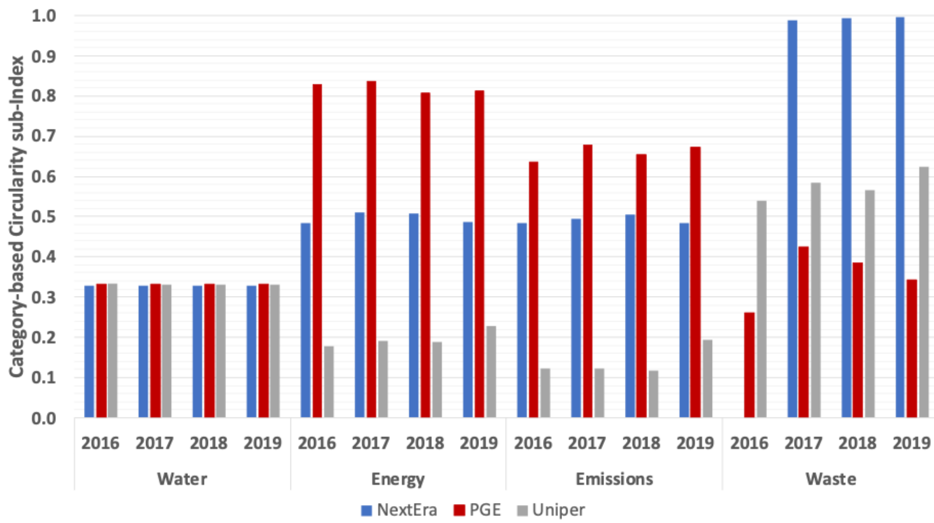

Figure 7.3: Category-based Circularity Sub-Indices in the Energy & Utilities sector (2016-2019)

The annual Overall Circularity Index for each company represents an aggregate of the annual category-based circularity metrics. As it is shown in Figure 7.4, NextEra's improvement in 2017 places the company in the top of the comparison among industry peers, with an Overall Circularity Index just below 60% of the target. The significantly lower price of NextEra's overall index in 2016 is attributed to the non availability of data for the Waste principal category that resulted in zeroing of the corresponding category. On the contrary, Uniper is the least circular company from the three under consideration. With the exception of NextEra in the Waste category, there are opportunities for enhancement in all aspects of CE for these companies.

7.6.2 Category-based and Overall Circularity Indices for Manufacturing (MaN) Sector

Figure 7.5 and Figure 7.6 highlight the category-based circularity sub-indices and the overall circularity indices of four companies from the Food and Beverages industry, which is classified within the Manufacturing sector. Figure 7.5 displays only the period from 2016-2019, due to the

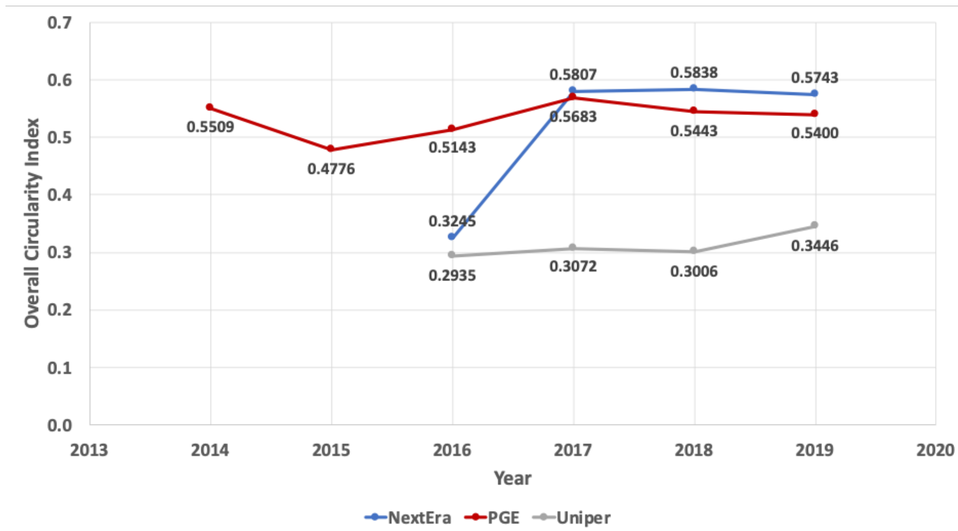

Figure 7.4: Overall Circularity Indices in the Energy & Utilities sector (2016-2019)

non-availability of data for two of the assessed companies for the previous period. An interesting finding is that none of the companies report any information or data that can be used to assess Durability. Thus, the Durability metrics for these companies are zero. Similar to the Energy & Utilities sector, companies score very well in the Waste category, with Nestle and General Mills been very close to each other and around 0.9. Ferrero achieved a major improvement the last two years with a 62% jump in this category. This is mainly attributed to the reporting of excellent handling of hazardous wastes over this period. On the contrary, Tyson's performance with regards to Waste shows a declining pattern with a 37% decrease in just four years, as a result of the deterioration of the waste generated per ton of product sold (1ca), which has more than double in such a short period of time.

Emissions & Spillages and Energy categories reveal similar trends. More specifically, Nestle is the leading company in both categories, achieving more than 0.8 in the Emissions & Spillages category, and being 143% higher than the second company of the list. Tyson performs slightly better than Ferrero in these two categories. In the Energy category, the gap between the first two companies is much smaller around 51%. Tyson and Ferrero demonstrate opposite paths in circularity in this category, with the former declining and the later increasing in values, and eventually managing to cover the initial 100% difference in just four years. In the Water & Procurement category, Ferrero has the lead, followed by Nestle, General Mills, and then Tyson. Ferrero's improvement in the last two years is attributed to the high percentage of recyclable, reusable and compostable packaging materials that was reported. A similar finding is observed also for Nestle in 2019. Figures J.5 to J.8 display the Category-based Circularity Sub-indices for the four Food and Beverages companies for multiple years, while Figure J.9 in in Appendix J shows the Category-based Circularity Sub-indices for the Manufacturing sector for 2019.

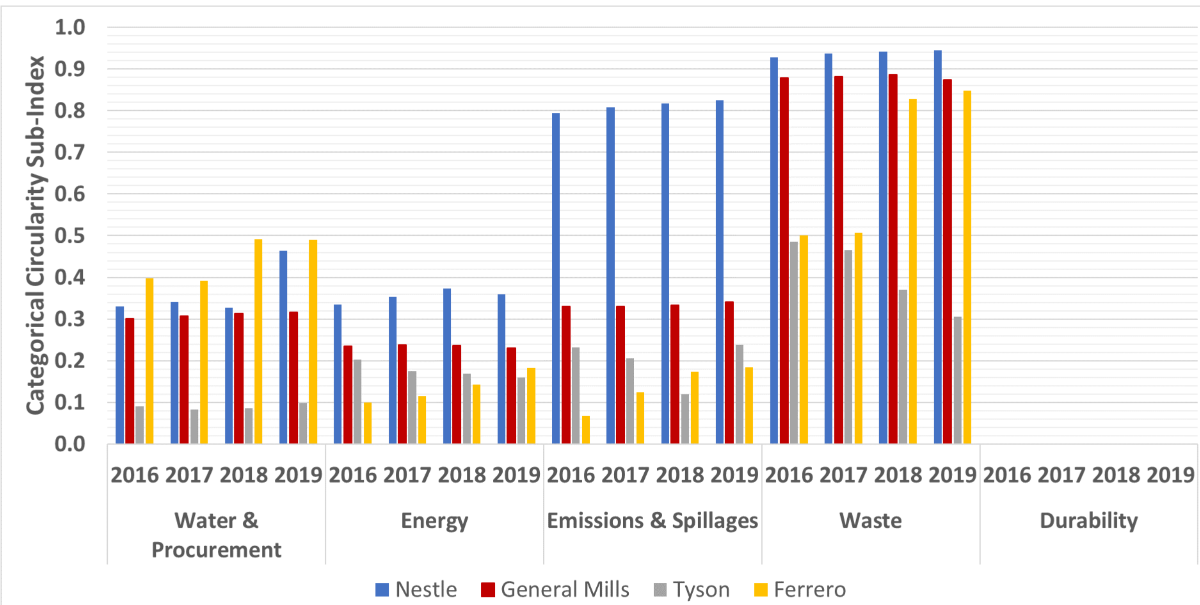

Figure 7.5: Category-based Circularity Sub-Indices in the Manufacturing sector (2016-2019)

Figure 7.6 summarizes the overall circularity assessment of the four companies since 2010. Three out of four companies demonstrate an improving upward trend in their overall circularity, with Tyson being the only one whose performance has deteriorated. More specifically, Nestle and General Mills achieved a 47% and 37% increase in their overall circularity respectively over the decade. Ferrero improved even more (up to 60%) almost reaching General Mills, while Tyson dropped by 17%. Despite the difference between the top two performing companies which is 47%

in 2019, and the rising trend of CE performance over the years, there is still big room for CE improvement for all companies, as it was also observed for the Energy & Utilities sector.

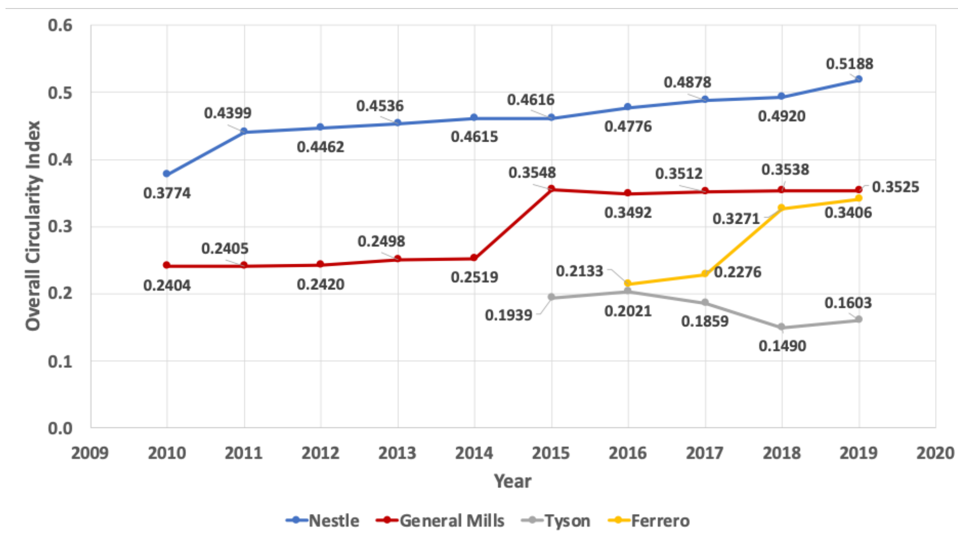

Figure 7.6: Overall Circularity Indices in the Manufacturing sector (2010-2019)

7.6.3 Category-based and Overall Circularity Indices for Automotive (AuT) Sector

Waste is the best performing circularity sub-index for three of the assessed companies, having reached and maintained values close to 0.9, as it can be seen in Figure 7.7. Audi and BMW lead the category, followed by Daimler, while Ferrari despite the improvement over the last two years, still scores almost 75% less than Daimler. However, Ferrari scores 0.85 in Durability sub-index, 17% more than Audi which comes second, and 31% higher than Daimler and BMW. This is attributed to the fact that Ferrari's vehicles have longer lifespan and they are considered collectibles. Audi and BMW are also the top performers in the GHG Emissions & Spillages category, scoring almost 50% higher than Daimler. Audi scores 71% and 72.5% higher than Daimler in net total GHG emissions per vehicle sold (4ac) and NOx, SOx, and other significant air emissions per vehicle sold (4cc) respectively. The average specific CO_2 emissions of Audi vehicles are also about 10% lower than those of Daimler. Even though Audi scores less than 0.5 in Energy sub-index, nevertheless its difference with the second in line is around 0.24.

Daimler's lack to report total renewable energy sources resulted in poor performance in this category, while Ferrari scores on average less than 0.05 due to its minimal exposure to renewable energy sources (3ab), as well as its energy intensive production (3bb). Thus, even a minor increase in both companies renewable energy footprint will boost their circularity. Water & Procurement sub-indices demonstrate a rather stable profile for all companies, with the difference gap among them being minimal. Figures J.10 to J.13 present the Category-based Circularity Sub-indices for the four automotive companies for multiple years, while Figure J.14 in Appendix J features the Category-based Circularity Sub-indices for the Automotive sector for 2019.

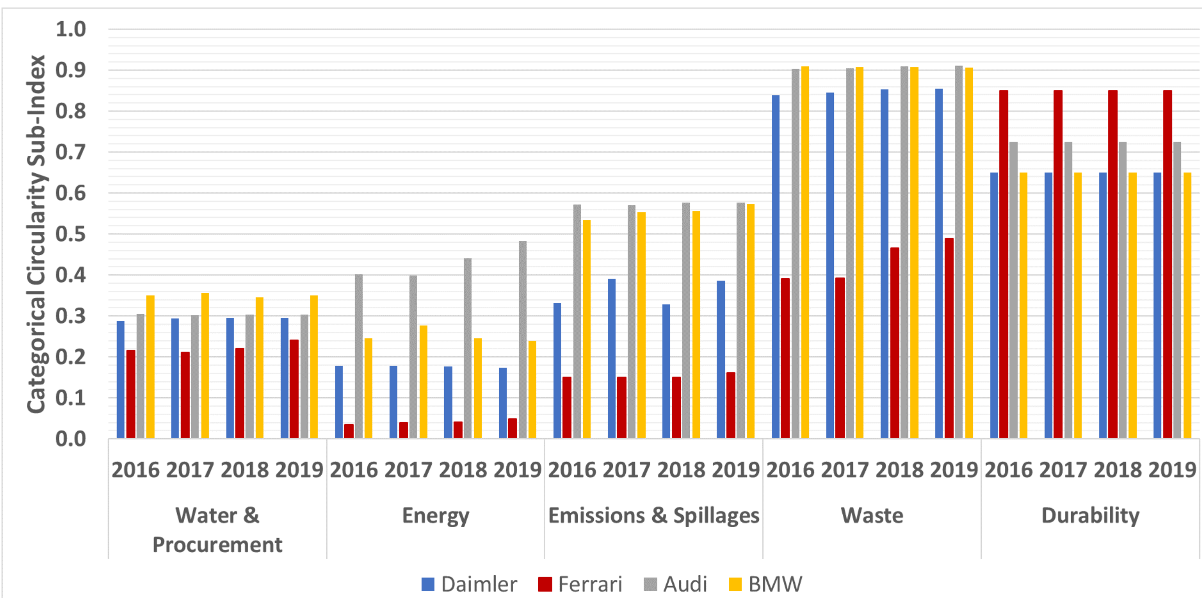

Figure 7.7: Category-based Circularity Sub-Indices in the Automotive sector (2016-2019)

The Overall Circularity Indices in the Automotive sector are displayed in Figure 7.8, revealing an upward pattern over the years. As expected from the previous analysis, Audi demonstrates the highest Overall Circularity Index the last four years, following a 26% rise in 2016 which is attributed to the improvement in Durability and Procurement principal categories. BMW and

Daimler rank second and third with an increase of just 2% and 10% respectively. Ferrari is the least circular automotive company from the ones evaluated over this period.

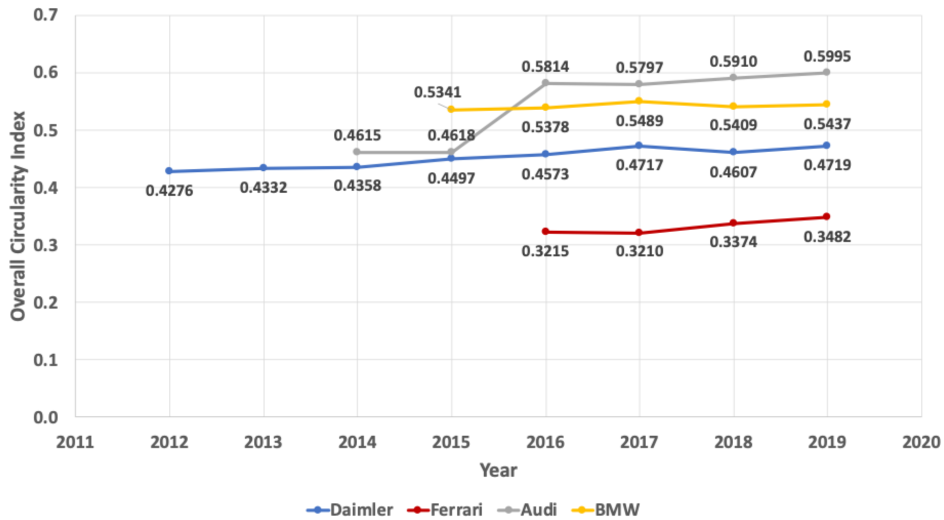

Figure 7.8: Overall Circularity Indices in the Automotive sector (2012-2019)

7.7 Conclusions

MICRON has been developed as a quantitative CE framework for assessing circularity at the micro level, in an effort to accurately measure the various aspects of CE and identify potential areas of improvement towards the transition to a CE economic model. First, principal categories are designed based on the goals and key characteristics of CE. Then, clearly specified indicators and readily measurable metrics are selected for each of these principal categories so as to provide accurate CE assessment at different operational and structural levels, along the different CE goals. This is achieved through weighted average Category-based Circularity Indices that are calculated to evaluate the CE performance of companies at each of the principal categories. The linear average of these indices constitutes the Overall Circularity Index of each company that is a numeric value between 0 and 1, with 0 representing perfect linearity and 1 representing perfect circularity. It is a holistic approach that utilizes various sector specific indicators and metrics so as to effectively capture all CE aspects across different business segments. Its structure enables better interpretability and traceability of the integrated CE characteristics, while identifying key areas that require improvement. Moreover, it is a robust framework that allows the effective capture and fair evaluation of extreme cases e.g. Ferrari, easy comparison among peers, benchmarking within business segments/industries/sectors, and tracking of CE performance on year-over-year basis. As such, it can be utilized as a decision-making tool at different operational levels and investment time horizons.

The capabilities and applicability of the subject framework are demonstrated through case studies in three sectors, namely Energy & Utilities, Manufacturing and Automotive. An upward trend is observed in most of the assessed companies, reaffirming the progress of CE across different industries and sectors of the economy. It is also evident that the aggregate prevalence of the CE concept is still far away, but important steps have already been made, and accurate assessment tools are critical to this direction. The proposed framework can act as an organization's internal CE and sustainability assessment tool, providing information about company's Category-based and Overall Circularity Indices, along with visualization mechanisms for tracking periodic progress, benchmarking against peers, and identification of areas for improvement.

The classification of industries into certain sectors, and the introduction of sector specific indicators and metrics that are matched with GRI standards are key features and contributions to the literature from the proposed framework. Furthermore, the normalization and standardization of metrics utilizing upper bounds which are derived from the statistical analysis of the given data, underline essential contributions and differentiating factors of the methodology, providing also a dynamic perspective. Ultimately, the metrics will evolve once more data become available and more CE initiatives and strategies are realized. Additionally, high level of granularity covering all CE goals, the wide range of parameters assessed, the simplicity of metrics with values ranging from 0 to 1, and the conception of the Category-based and the Overall Circularity Indices are also important contributions of the framework.

However, the non-availability or non-reporting of data complicates the evaluation process, potentially routing to misleading results. Also, social aspects are not directly captured in the current form of the framework, but can be incorporated in the future. Conglomerates or companies with diverse operations may not accurately assessed due to the extensive nature of their businesses. In such case, it might be more appropriate to assess individual segments of the company matching their activities with the proposed classification.

8. CONCLUSION AND FUTURE WORK

8.1 Conclusion

In this dissertation, various imminent challenges towards the energy transition and the successful implementation of circular economy concept are discussed. Even though there are many outstanding issues and as a society we still have a long way to go before claiming these issues as resolved, the goal here is to present a few ideas and demonstrate systematic and quantitative ways to address some of the challenges. Towards the energy transition, an extensive analysis and study of the US energy landscape was conducted and a quantitative forecasting framework that allows the accurate estimation of the price of energy for the end-use consumers are presented. By incorporating the demand and prices of all energy feedstocks and products of the energy landscape within the framework and by introducing a state-of-the-art forecasting methodology that includes optimization and machine learning techniques, a dual objective is achieved: a) the energy market dynamics are closely monitored and analyzed, and b) various policies of significant public and governmental interest can be designed, assessed and optimized.

Towards the circular economy implementation, two unique, quantitative frameworks are presented. The first one illustrates a system engineering approach and a decision-making tool for the analysis and trade-off modeling and optimization of interconnected food supply chains considering the principles and goals of circular economy. The second one introduces a holistic and robust methodology for assessing circularity at the micro level, and a decision-making tool at different operational levels and investment time horizons. Various applications of both frameworks are discussed, highlighting their applicability and capabilities.

The following are the key questions that are addressed in this dissertation:

What is the price of energy to the end-users in the United States? The response is the Energy Price Index or EPIC, the benchmark to calculate the average price of energy to the end-use consumers in the United States in units of $/MMBtu.

*What is the daily market price of energy to the end-users in the United States?*The response is the Energy Spot Price Index or ESPIC, the benchmark to calculate the daily average market price of energy to the end-use consumers in the United States in units of \$/MMBtu. ESPIC can be used as a financial tradable security for investors who look to hedge their investments against the overall energy market.

How can we monitor and analyze the energy market dynamics? By utilizing EPIC that is comprised of the demands and prices of all energy feedstocks and products within an energy network. The excellent forecasting methodologies for both the demands and the prices of these energy products facilitate such analysis to be extended into the future.

Can we estimate the impact of different policies in energy to the end-users? Yes, by using EPIC, a comprehensive, reliable and easily interpretable instrument for policymakers to determine the quantitative effects of various policies. With its accurate forecasting capabilities, EPIC can be utilized not only for retrospective analyses, but most importantly for prospective ones, up to 10 years in the future. The change of the price of energy, the tax burden in a household, the generated revenue and the environmental impacts are some of the features that can be estimated under different scenarios.

How can we redesign supply chains using circular economy principles? By utilizing frameworks like the one presented here for the food supply chains. Process Systems Engineering tools and optimization techniques are used for the modeling and systematic integration of recent technological, experimental, academic and industrial knowledge in the design and operation of food supply chains while explicitly considering circular economy goals and objectives.

Can we evaluate circularity at the company's or products level? Yes, by using MICRON, a robust, holistic and quantitative framework that accurately measures the various aspects of circular economy across different business segments through sector specific indicators and metrics while identifies potential areas of improvement towards the transition to a circular economy model. It also allows the effective capture and fair evaluation of extreme cases, easy comparison among peers, benchmarking within business segments/industries/sectors, and tracking of circular economy performance on year-over-year basis.

8.2 Key Contributions

The key contributions of the dissertation are summarized as follows:

1. EPIC represents the average price of energy over the entire energy landscape covering all the different energy sources and feedstocks (non-renewables and renewables) as well as the end-use sectors. It is region agnostic, and can be applied from a state level to international level. As such, it is not just a representative price of a sub-section of the energy landscape such as the price of electricity in the residential sector or the price of oil products in the industrial sector which is common in the existing literature. Secondly, the proposed formulation collectively captures the two key attributes of energy, the supply and demand mechanisms along with the prices of the energy feedstocks and products across the entire energy landscape. This is another unique feature since the methodologies in the literature generally focus on specific energy sectors. Thirdly, the excellent forecasting ability of the proposed mathematical framework allows the estimation of the current value of EPIC, thus the current price of energy, overcoming the issue of the non-availability of actual data. In contrast, the forecasting frameworks in the literature focus on specific energy sectors with generally much shorter forecasting horizon. Finally, an extended forecasting framework that incorporates state-of-the-art statistical and machine learning techniques and requires minimum user interference has been presented so as to accurately forecast future prices for all energy feedstocks and products.

2. The EPIC/ESPIC framework demonstrates novel features not only for the academic literature but also for the financial world. The various energy indices are primarily capitalization weighted indices, capped market capitalization indices, price weighted indices and world production weighted indices, covering mainly oil and gas sectors. On the contrary, EPIC/ESPIC capture the prices of all energy feedstocks while the weights are calculated from the actual demands of these energy feedstocks, thus reflecting and capturing the dynamics of the entire energy landscape. ESPIC has the potential to become a novel tradable

financial security.

3. EPIC is a quantitative approach to evaluate, design and optimize different policy questions of significant public interest. Four key policy case studies have been illustrated. The scenarios have been investigated parametrically for the past and the future where apart from the change of the price of energy and the tax burden in a household, the generated revenue or budget required and the environmental impacts are estimated.

4. Research challenges and PSE research opportunities to assist in the understanding, analysis and optimization of CE supply chains have been identified. A motivating example on the supply chain of coffee is introduced to illustrate the challenges of the transition towards a CE and to propose PSE research opportunities.

5. The explicit incorporation of CE goals and objectives into the design and operation of FSCs is a key contribution of the proposed CE-FSC framework. Apart from systematically capturing the extensive, up-to-date set of production, processing and valorization pathways, the proposed CE-FSC framework also contributes to the literature in a dual manner. First, it enables the identification and selection of the optimal tasks from the list of all alternative processes based on certain CE objectives. It also allows the identification of the least efficient processes or even sections of the network, which introduce potential bottlenecks within the supply chain. This is a key feature that refocuses the interest and promotes the research and development on the less developed sections of the supply chain. Additionally, different users can benefit from the framework e.g. academics and experimentalists by focusing on the improvement of existing processes or introduction of new ones, policymakers by determining areas of improvement etc.

6. The explicit incorporation of CE goals and objectives as assessment criteria, the classification of economic activity into distinct parent sectors, the conception of GRI matched, sector specific indicators and metrics are key contributions of MICRON. The metrics are normalized and standardized using sector specific relevant information, ensuring that assessments

are up-to-date and dynamically adjusted. Overall, the high level of granularity covering all CE goals, the comprehensive nature of the framework and the enhanced interpretability are key features and important contributions of the framework.

8.3 Future Work

There are plenty of challenges that need to be addressed towards energy transition and the implementation of CE. By no means, these challenges can be addressed through a single dissertation. A non-exhaustive list of future research directions is highlighted below.

8.3.1 EPIC Forecasting Framework

EPIC framework has been applied so far to the US energy landscape. Therefore, it can be applied to other energy landscapes of different size, from state and/or regional level to national and/or international level. This would provide new insights into the dynamics of the energy markets as well as the factors that affect the pricing of energy feedstocks.

It would also be interesting to investigate the effects of key economic and monetary indicators such as GDP growth, inflation, currency exchange rates etc. on the price of energy. Having better understanding on these relationships would allow more accurate forecasts and policy studies. Future work can expand further the forecasting capabilities of the framework by incorporating multivariate time series forecasting techniques along with different statistical and machine learning methods. Moreover, it would be of great interest to integrate the findings from the analysis of the key economic and monetary indicators and how they affect the price of energy into the forecasting tools. Since machine learning techniques proved to be the most accurate ones, research work towards increasing their interpretability as well as into incorporating uncertainty shall be contacted. Currently, the uncertainty of the forecasts is not properly addressed. Additionally, the lack of understanding on how these methods work and how the corresponding forecasts are generated, create a barrier for their acceptance within the research community. As such, improving the transparency and comprehension of machine learning methods will have a positive impact in a variety of ways i.e. assisting towards understanding better the strengths and weaknesses of models, providing new insights on the data, allowing the integration of domain expertise within the models, and finally increasing their adoption from the community [373, 374].

Future work can also address different policy questions, such as how EPIC would respond to financial or monetary shocks, natural disasters and other disruptions, as well as to technological advancements. To address such questions, a simultaneous evaluation of multiple energy sources within the same framework across different production targets and subsidies would be required, taking into consideration potential limitations on the availability and production of each energy source. The vulnerability of the energy systems to dynamically changing conditions and the resilience of the energy infrastructure to potential disruptions can be incorporated and studied within the EPIC framework, allowing the identification of potential bottlenecks in the existing networks and the investigation of their cascading effects on the demand and price of energy. Moreover, modelling of the up-to-date technological solutions for accurate representation of the prices and levelized costs would be beneficial. The goal remains EPIC to be used for the design and optimisation of a federal energy policy for mitigating climate change, while ensuring that the price of energy remains affordable so as to not have a negative impact on short-term economic activity. To this respect, EPIC can be integrated with a multi-scale energy systems methodology [275] and a circular economy systems engineering methodology [262, 375], introducing a novel modeling, optimization and scenario analysis framework. Such a framework, as it is shown in Figure 8.1, would include i) detailed data and models for the description of the energy landscape and the various supply chains along with their corresponding main and alternative processes, ii) identification and assessment of alternative pathways for the production of the products and the valorization of the wastes under circular economy objectives, iii) a detailed time-varying scheduling model [376], iv) a library of surrogate modelling techniques, for both the nonlinear process models, as well as scheduling decisions, and v) an effective multi-period, multi-location mixed-integer optimization solution strategy, coupled with environmental, risk and uncertainty analysis.

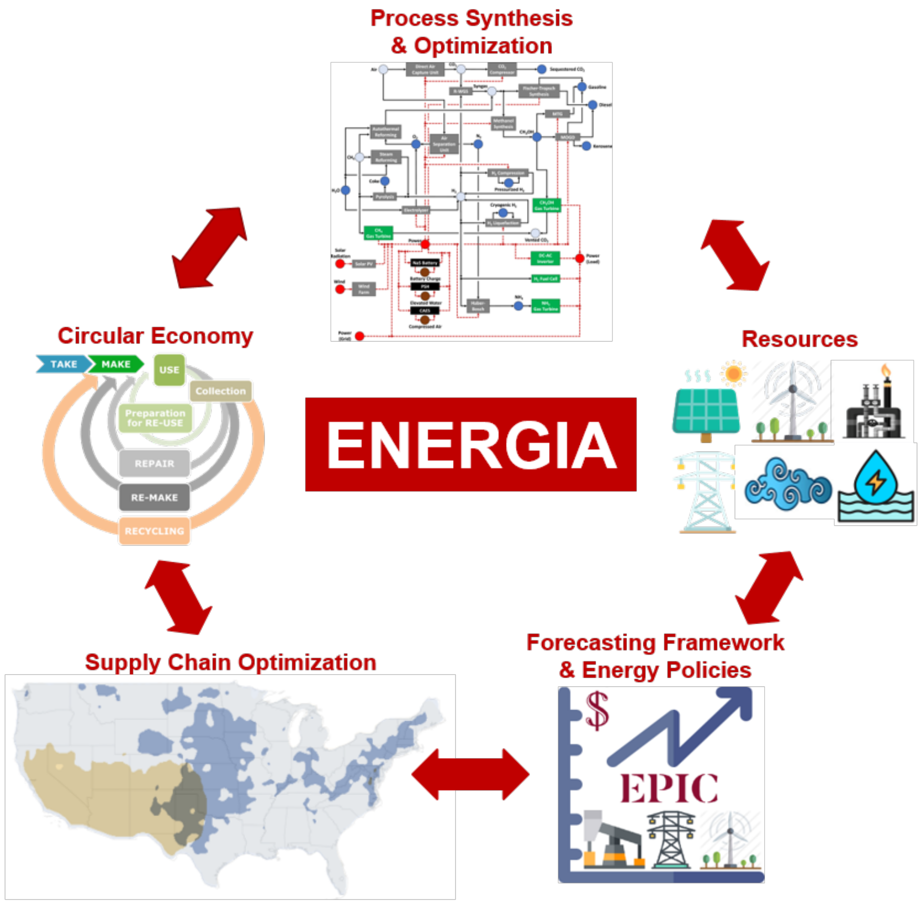

Figure 8.1: Energia Systems Engineering Framework

8.3.2 Systems Engineering Framework for Circular Economy Food Supply Chains

The proposed framework can be utilized in other food supply chains, ensuring their effective transition towards circularity. Moreover, extra constraints in the modeling can be introduced to capture inherent characteristics of FSCs systematically, such as perishability and quality decay of dairy, meat-poultry, vegetable products. The identification of valorization techniques to eliminate wastes and produce new valuable products along with the ability to simulate different demand and supply scenarios provide a powerful tool towards circularity.

Future work may expand into other classes of problems, including phenomena, objective functions and/or constraints with non-linear terms, thus resulting into mixed-integer nonlinear programming (MINLP) problems. In addition, uncertainty issues related to system's externalities or inherent characteristics such as weather conditions, consumer preferences, demand and supply fluctuations and so on [377, 378], can be also taken into consideration in future work by incorporating sensitivity analysis, parametric optimization, stochastic and robust optimization into the framework [379, 380, 381]. Finally, the current framework considers a central planner deciding for the entire supply chain. Future work would involve the decomposition of the supply chain into its different stakeholders, resulting into multi-agent optimization formulations, and requiring other optimization approaches for its solution [382, 383].

Future developments on the illustrative case study of the coffee supply chain could include valorization pathways for the utilization of wastes and by-products for the production of high added value products. Scaling issues from the laboratory and proof of concept levels to the full scale and product release levels must be always taken into consideration. Hence, analytical process design and synthesis along with feedback from experimentalists are crucial. The model approximations could be also revisited, and high-fidelity models can be developed for proper testing. Validation strategies through energy systems engineering optimization approaches will be also required for the efficient design and operation of the most promising processes.

8.3.3 MICRON: Circular Economy Assessment Framework at Micro level

Advanced data analytics can be incorporated into the framework, enabling the faster and more accurate execution of the evaluation process. Ideally, the framework will be embedded into a website as a web-based index calculator where the users will be able to i) measure a firm's "circularity", ii) track firm's periodic progress, iii) benchmark against firm's peers, and iv) visualize the analysis online. The collection of more data from companies in different industries and sectors, and their evaluation within the framework would provide more insights about the effectiveness of the current indicators and metrics. The non-availability or non-reporting of data complicates the evaluation process, potentially routing to misleading results. Therefore, it would be interesting to explore ways to handle such cases. Also, social aspects are not directly captured in the current form of the framework, and must be incorporated in the future.

Conglomerates or companies with diverse operations may not accurately assessed due to the extensive nature of their businesses. In such case, it might be more appropriate to assess individual segments of the company matching their activities with the proposed classification. Future work could introduce a new sector that would reflect and capture the special characteristics of this type of companies. In addition, future research should focus on conducting similar analysis at the meso and macro levels, especially in relation to the alignment between CE indicators and the three dimensions of sustainability. This can be done by investigating the interconnections of these dimensions with indicators and metrics at the meso and macro level.

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APPENDIX A

ENERGY CONVERSION CALCULATIONS

Table A.1: Conversion Factors

Fuel	Units	Approximate Heat Content
Asphalt and Road Oil	MMBtu per bbl	6.636
Aviation Gasoline	MMBtu per bbl	5.048
Biodiesel	MMBtu per bbl	5.359
Diesel	MMBtu per bbl	5.770
Distillate Fuel Oil	MMBtu per bbl	5.817
Ethanol	MMBtu per bbl	3.563
Gasoline	MMBtu per bbl	5.222
HGL	MMBtu per bbl	3.841
Kerosene	MMBtu per bbl	5.670
Lubricants	MMBtu per bbl	6.065
Petroleum Coke	MMBtu per bbl	6.124
Residual Fuel Oil	MMBtu per bbl	6.287
Electricity	BTU per kWh	3,412
Coal	MMBtu per short ton	38.2425

APPENDIX B

LOOKBACK PERIOD AND PARAMETER ESTIMATION SCHEMES

Energy demand is highly seasonal [77] (see Figure 2.2), so each month needs to be trained separately. Thus, all the schemes involve the parameter estimation for each month individually, so as to capture the seasonality effects which are crucial for accurate forecasting. Four different approaches for minimizing the sum of the squared error were tested over four different lookback periods (24months, 36months, 48months, 60 months), with each month being trained separately. Approaches 1 and 2 are "weight-based", while approaches 3 and 4 are "demand-based". The mathematical formulations are shown below for the lookback period of 36 months. Table B.1 summarises the results for the four approaches and four lookback periods.

Approach 1 - (weight-based)

$$min \sum_{m} Err_m$$

$$Err_m = \sum_{m'} (EPIC_{m'} - \widehat{EPIC}_{m'})^2$$

$$\widehat{EPIC}_{m'} = \sum_{p} (C_{m',p} * \widehat{w}_{m,p})$$

$$EPIC_m = \sum_{p} (C_{m,p} * w_{m,p})$$

$$\sum_{p} \widehat{w}_{m,p} = 1$$

$$\widehat{w}_{m,p} \geq 0$$

$$\forall m' \mid (m' - m) = (-36) \quad or \quad (-24) \quad or \quad (-12)$$

Approach 2 - (weight-based)

$$min \sum_m Err_m$$

$$Err_m = \sum_{m',p} (w_{m',p} - \widehat{w}_{m,p})^2$$

$$\sum_p \widehat{w}_{m,p} = 1$$

$$\widehat{w}_{m,p} \geq 0$$

$$\forall m' \mid (m' - m) = (-36) \quad or \quad (-24) \quad or \quad (-12)$$

where $\widehat{w}_{m,p}$ represents the predicted weight of product *p* in month *m*.

Approach 3 - (demand-based)

$$min \sum_m Err_m$$

$$Err_m = \sum_{m',p} (D_{m',p} - a_{m,p} * m' + b_{m,p})^2$$

$$a_{m,p} * m + b_{m,p} \geq 0$$

$$\widehat{w}_{m,p} = \frac{a_{m,p} * m + b_{m,p}}{\sum_{p'} a_{m,p'} * m + b_{m,p'}}$$

$$\forall m' \mid (m' - m) = (-36) \quad or \quad (-24) \quad or \quad (-12)$$

Approach 4 - (demand-based)

$$min \sum_{m} Err_m$$

$$Err_m = \sum_{p} (D_{m-12,p} - (a_{m,p} * D_{m-24,p} + b_{m,p} * D_{m-36,p}))^2$$

$$a_{m,p} * D_{m-12,p} + b_{m,p} * D_{m-24,p} \geq 0$$

$$\widehat{w}_{m,p} = \frac{a_{m,p} * D_{m-12,p} + b_{m,p} * D_{m-24,p}}{\sum_{p'} a_{m,p'} * D_{m-12,p'} + b_{m,p'} * D_{m-24,p'}}$$

where $D_{m,p}$ represents the demand of product *p* in month *m*, $a_{m,p}$ and $b_{m,p}$ represent the fitted parameter 1 and 2 of product *p* in month *m* respectively.

Table B.1: Results on Prediction of Weights (Different Lookback Periods)

	lookback_24				**lookback_36**			
	App1	App2	App3	App4	App1	App2	App3	App4
Min Error	0.052%	0.049%	0.064%	0.067%	0.058%	0.053%	0.051%	0.127%
Max Error	0.263%	0.221%	0.410%	0.351%	0.292%	0.228%	0.290%	0.624%
Average Error	0.106%	0.099%	0.147%	0.154%	0.121%	0.104%	0.127%	0.336%
	lookback_48				**lookback_60**			
	App1	App2	App3	App4	App1	App2	App3	App4
Min Error	0.064%	0.057%	0.052%	0.233%	0.064%	0.065%	0.054%	0.394%
Max Error	0.265%	0.209%	0.289%	0.776%	0.261%	0.196%	0.255%	0.839%
Average Error	0.137%	0.107%	0.120%	0.454%	0.158%	0.113%	0.115%	0.536%

As it can be seen, approaches 1 and 2 outperform approaches 3 and 4, regardless of the look-back period. Between the weight-based approaches, approach 2 is the one with the lowest errors regardless of the lookback period, so it is the one selected. With regards to the lookback periods, the cases for 24 and 36 months produce the lowest errors in comparison to the 48 and 60 months. Since, the results for the 24 and 36 months are comparable, the longer lookback period is selected, which will capture better the increasing volatility of the energy demand in the future. Therefore, the methodology selected is Approach 2 with 36 months lookback period.

APPENDIX C

FORECASTING RESULTS FOR THE DEMANDS AND PRICES OF ENERGY PRODUCTS

Table C.1: Sum of Squared Errors for the Forecasting of the Weights

Year of Forecasting	1st year	2nd year	3rd year	4th year
2006 January	0.00169025	0.00000000	0.00000000	0.00000000
2006 February	0.00058085	0.00000000	0.00000000	0.00000000
2006 March	0.00021295	0.00000000	0.00000000	0.00000000
2006 April	0.00023641	0.00000000	0.00000000	0.00000000
2006 May	0.00023087	0.00000000	0.00000000	0.00000000
2006 June	0.00016016	0.00000000	0.00000000	0.00000000
2006 July	0.00027143	0.00000000	0.00000000	0.00000000
2006 August	0.00025395	0.00000000	0.00000000	0.00000000
2006 September	0.00017492	0.00000000	0.00000000	0.00000000
2006 October	0.00017026	0.00000000	0.00000000	0.00000000
2006 November	0.00018149	0.00000000	0.00000000	0.00000000
2006 December	0.00064226	0.00000000	0.00000000	0.00000000
2007 January	0.00015041	0.00060949	0.00000000	0.00000000
2007 February	0.00043464	0.00026794	0.00000000	0.00000000
2007 March	0.00008725	0.00017743	0.00000000	0.00000000
2007 April	0.00015412	0.00020004	0.00000000	0.00000000
2007 May	0.00013978	0.00024963	0.00000000	0.00000000
2007 June	0.00021104	0.00030346	0.00000000	0.00000000
2007 July	0.00012475	0.00024875	0.00000000	0.00000000
2007 August	0.00017119	0.00029990	0.00000000	0.00000000
2007 September	0.00014788	0.00018094	0.00000000	0.00000000
2007 October	0.00017521	0.00020705	0.00000000	0.00000000
2007 November	0.00010496	0.00011980	0.00000000	0.00000000
2007 December	0.00009077	0.00010847	0.00000000	0.00000000

Table C.1 continued from previous page

Year of Forecasting	1st year	2nd year	3rd year	4th year
2008 January	0.00032132	0.00024880	0.00018570	0.00000000
2008 February	0.00016441	0.00027061	0.00014792	0.00000000
2008 March	0.00017691	0.00018144	0.00020354	0.00000000
2008 April	0.00017740	0.00021688	0.00020193	0.00000000
2008 May	0.00024392	0.00026156	0.00028559	0.00000000
2008 June	0.00023788	0.00031761	0.00039532	0.00000000
2008 July	0.00030059	0.00030920	0.00039746	0.00000000
2008 August	0.00031008	0.00038352	0.00040577	0.00000000
2008 September	0.00023943	0.00029728	0.00028647	0.00000000
2008 October	0.00023759	0.00023697	0.00032100	0.00000000
2008 November	0.00030642	0.00036109	0.00041720	0.00000000
2008 December	0.00059325	0.00069510	0.00048058	0.00000000
2009 January	0.00108481	0.00140707	0.00119094	0.00055285
2009 February	0.00029712	0.00037806	0.00053460	0.00055477
2009 March	0.00027061	0.00037076	0.00045481	0.00060045
2009 April	0.00055190	0.00063837	0.00069210	0.00076995
2009 May	0.00069059	0.00080875	0.00087938	0.00101184
2009 June	0.00044950	0.00054766	0.00073642	0.00089440
2009 July	0.00039833	0.00041351	0.00045663	0.00067383
2009 August	0.00040358	0.00056169	0.00066491	0.00071660
2009 September	0.00030008	0.00038579	0.00047867	0.00052521
2009 October	0.00047339	0.00059461	0.00058672	0.00067339
2009 November	0.00046843	0.00057918	0.00066024	0.00073549
2009 December	0.00044028	0.00076489	0.00089168	0.00054722
2010 January	0.00050146	0.00095165	0.00138620	0.00111124
2010 February	0.00020387	0.00025136	0.00038191	0.00067702
2010 March	0.00019686	0.00020734	0.00029272	0.00034912
2010 April	0.00035647	0.00038397	0.00043434	0.00041693
2010 May	0.00017466	0.00027801	0.00044686	0.00048967

Table C.1 continued from previous page

Year of Forecasting	1st year	2nd year	3rd year	4th year
2010 June	0.00016701	0.00021507	0.00039571	0.00052869
2010 July	0.00022884	0.00028372	0.00049476	0.00052390
2010 August	0.00019238	0.00018884	0.00031042	0.00049674
2010 September	0.00012943	0.00016054	0.00028821	0.00043820
2010 October	0.00012734	0.00027152	0.00039537	0.00046585
2010 November	0.00025037	0.00029519	0.00054799	0.00068644
2010 December	0.00042858	0.00070206	0.00115439	0.00134016
2011 January	0.00021389	0.00038182	0.00093742	0.00155177
2011 February	0.00013790	0.00024556	0.00026940	0.00040602
2011 March	0.00017760	0.00028759	0.00024051	0.00035482
2011 April	0.00022301	0.00033708	0.00030631	0.00044203
2011 May	0.00031429	0.00041710	0.00043910	0.00075276
2011 June	0.00021235	0.00029840	0.00029525	0.00058370
2011 July	0.00020819	0.00032540	0.00037061	0.00061394
2011 August	0.00037387	0.00053666	0.00039633	0.00057551
2011 September	0.00021589	0.00029985	0.00027488	0.00047573
2011 October	0.00024626	0.00028698	0.00038359	0.00061847
2011 November	0.00032169	0.00047778	0.00042772	0.00072872
2011 December	0.00038633	0.00038742	0.00045440	0.00059754
2012 January	0.00057636	0.00054090	0.00047292	0.00043356
2012 February	0.00067800	0.00073623	0.00077378	0.00075570
2012 March	0.00123748	0.00135595	0.00165884	0.00163334
2012 April	0.00041933	0.00058776	0.00091836	0.00086678
2012 May	0.00027936	0.00044817	0.00063041	0.00074209
2012 June	0.00023195	0.00035312	0.00052385	0.00047865
2012 July	0.00034525	0.00047865	0.00072545	0.00064491
2012 August	0.00014917	0.00023680	0.00037191	0.00040482
2012 September	0.00027757	0.00041687	0.00057491	0.00062005
2012 October	0.00025045	0.00039858	0.00044428	0.00065313

Table C.1 continued from previous page

Year of Forecasting	1st year	2nd year	3rd year	4th year
2012 November	0.00037108	0.00057765	0.00088953	0.00082820
2012 December	0.00036841	0.00058808	0.00058131	0.00064413
2013 January	0.00010127	0.00027885	0.00029095	0.00035500
2013 February	0.00010706	0.00015261	0.00021184	0.00037195
2013 March	0.00082384	0.00045289	0.00047756	0.00058032
2013 April	0.00028868	0.00031848	0.00049716	0.00056462
2013 May	0.00009598	0.00015510	0.00031695	0.00053958
2013 June	0.00008989	0.00015755	0.00027637	0.00045884
2013 July	0.00012326	0.00017354	0.00027117	0.00042244
2013 August	0.00014871	0.00022407	0.00026159	0.00037983
2013 September	0.00007371	0.00009969	0.00020611	0.00035424
2013 October	0.00011646	0.00022361	0.00038529	0.00046822
2013 November	0.00017070	0.00034287	0.00055814	0.00099078
2013 December	0.00039171	0.00040291	0.00043969	0.00094699
2014 January	0.00057984	0.00057454	0.00043747	0.00075951
2014 February	0.00047937	0.00057258	0.00030567	0.00040910
2014 March	0.00079868	0.00136995	0.00070764	0.00083020
2014 April	0.00010063	0.00018766	0.00028241	0.00059331
2014 May	0.00008448	0.00013227	0.00019535	0.00047191
2014 June	0.00008456	0.00013527	0.00026661	0.00051652
2014 July	0.00023581	0.00031970	0.00038393	0.00048197
2014 August	0.00018367	0.00027932	0.00036830	0.00039371
2014 September	0.00005026	0.00007510	0.00015449	0.00037376
2014 October	0.00008603	0.00010004	0.00012764	0.00027284
2014 November	0.00018230	0.00028655	0.00053636	0.00085352
2014 December	0.00014036	0.00012652	0.00021581	0.00056836
2015 January	0.00005743	0.00018343	0.00019034	0.00029665
2015 February	0.00061479	0.00099938	0.00117982	0.00065863
2015 March	0.00012664	0.00032864	0.00082904	0.00030563

Table C.1 continued from previous page

Year of Forecasting	1st year	2nd year	3rd year	4th year
2015 April	0.00012457	0.00015214	0.00019489	0.00041076
2015 May	0.00009819	0.00011612	0.00017901	0.00029074
2015 June	0.00009817	0.00011147	0.00015043	0.00029612
2015 July	0.00008353	0.00013741	0.00022390	0.00033523
2015 August	0.00008172	0.00009634	0.00014406	0.00023443
2015 September	0.00019669	0.00019709	0.00017889	0.00025847
2015 October	0.00034115	0.00040917	0.00036567	0.00032838
2015 November	0.00071305	0.00064959	0.00053344	0.00038099
2015 December	0.00096012	0.00110267	0.00069011	0.00109389
2016 January	0.00020630	0.00021139	0.00014699	0.00019528
2016 February	0.00116565	0.00074876	0.00040817	0.00038036
2016 March	0.00184829	0.00171524	0.00096200	0.00037059
2016 April	0.00015478	0.00018638	0.00018682	0.00019884
2016 May	0.00013943	0.00017763	0.00019108	0.00022649
2016 June	0.00013494	0.00016383	0.00017843	0.00021491
2016 July	0.00018386	0.00019399	0.00020255	0.00023609
2016 August	0.00015108	0.00020368	0.00017272	0.00020652
2016 September	0.00012569	0.00021716	0.00022069	0.00024754
2016 October	0.00013478	0.00021873	0.00026180	0.00027459
2016 November	0.00056906	0.00097518	0.00078647	0.00059570
2016 December	0.00016671	0.00014584	0.00017481	0.00023973
2017 January	0.00045718	0.00064802	0.00061956	0.00029457
2017 February	0.00159470	0.00257694	0.00171943	0.00097086
2017 March	0.00014028	0.00052119	0.00045170	0.00026143
2017 April	0.00025569	0.00035292	0.00043381	0.00039786
2017 May	0.00007100	0.00010955	0.00016608	0.00019561
2017 June	0.00009699	0.00016182	0.00019772	0.00021556
2017 July	0.00006016	0.00011393	0.00013784	0.00019388
2017 August	0.00007710	0.00010518	0.00015797	0.00024488

Table C.1 continued from previous page

Year of Forecasting	1st year	2nd year	3rd year	4th year
2017 September	0.00007262	0.00011236	0.00019369	0.00021705
2017 October	0.00015230	0.00022606	0.00031845	0.00038520
2017 November	0.00017257	0.00020567	0.00033253	0.00025249
2017 December	0.00041363	0.00058545	0.00029348	0.00026426
2018 January	0.00017560	0.00011151	0.00013114	0.00017954
2018 February	0.00017124	0.00042569	0.00107039	0.00051946
2018 March	0.00031268	0.00032542	0.00022566	0.00025018
2018 April	0.00089452	0.00069845	0.00067844	0.00061453
2018 May	0.00017771	0.00021000	0.00024117	0.00032392
2018 June	0.00009946	0.00013556	0.00021927	0.00027993
2018 July	0.00010703	0.00011836	0.00019312	0.00025247
2018 August	0.00009161	0.00011507	0.00019802	0.00032078
2018 September	0.00023493	0.00026516	0.00029111	0.00036375
2018 October	0.00032381	0.00034609	0.00039674	0.00036155
2018 November	0.00101193	0.00117265	0.00068887	0.00034122
2018 December	0.00010260	0.00024116	0.00040453	0.00029445
2019 January	0.00011171	0.00018582	0.00014774	0.00026694
2019 February	0.00079592	0.00080607	0.00032463	0.00037609
2019 March	0.00061980	0.00090504	0.00082239	0.00021272
2019 April	0.00013723	0.00015497	0.00016199	0.00024742
2019 May	0.00012416	0.00018282	0.00023362	0.00026705
2019 June	0.00009340	0.00012781	0.00014591	0.00022097
2019 July	0.00007390	0.00012145	0.00013615	0.00024600
2019 August	0.00007350	0.00009100	0.00014265	0.00023201
2019 September	0.00008590	0.00016635	0.00018172	0.00024659
2019 October	0.00006140	0.00014909	0.00021073	0.00031819
2019 November	0.00042966	0.00096256	0.00116242	0.00059594
2019 December	0.00010884	0.00013570	0.00024827	0.00044538
2020 January	0.00033701	0.00034522	0.00029330	0.00060895

Table C.1 continued from previous page

Year of Forecasting	1st year	2nd year	3rd year	4th year
2020 February	0.00009060	0.00021529	0.00024230	0.00036097
2020 March	0.00060887	0.00070588	0.00089502	0.00092804
2020 April	0.00516623	0.00507030	0.00652467	0.00588608
2020 May	0.00259839	0.00276708	0.00293191	0.00285565
2020 June	0.00134370	0.00133813	0.00142056	0.00137575
2020 July	0.00105790	0.00108082	0.00121768	0.00123202
2020 August	0.00094581	0.00095579	0.00102573	0.00094769
2020 September	0.00069657	0.00073136	0.00088994	0.00090819
2020 October	0.00077923	0.00086822	0.00117532	0.00121506
2020 November	0.00060094	0.00057358	0.00076594	0.00105741
2020 December	0.00087452	0.00090562	0.00109122	0.00164638
2021 January	0.00045517	0.00041579	0.00051259	0.00072194
2021 February	0.00164641	0.00168494	0.00274646	0.00275953
2021 March	0.00025026	0.00036102	0.00033686	0.00046802
2021 April	0.00044854	0.00025617	0.00031994	0.00053150

Table C.2: Average Absolute Error of Prices up to 3 months

Product No.	Average Abs. Error Ahead ($/MMBtu)			Forecasting Required	Forecasting Function (Rolling Horizon)
	1 month	2 months	3 months	(months)	
2	1.868	2.472	2.929	3	Trigonometric & Commodity based linear (9 months)
4	0.757	0.977	1.107	3	Trigonometric & Commodity based linear (9 months)
5	1.868	2.472	2.929	3	Trigonometric & Commodity based linear (9 months)
6	1.025	1.404	1.712	3	Trigonometric & Commodity based linear (9 months)

Table C.2 continued from previous page

Product No.	Average Abs. Error Ahead ($/MMBtu)			Forecasting Required (months)	Forecasting Function (Rolling Horizon)
	1 month	2 months	3 months		
7	0.773	0.954	1.024	3	Trigonometric & Commodity based linear (9 months)
8	0.233	0.328	0.389	3	Trigonometric & Commodity based linear (9 months)
9	0.605	0.783	0.902	3	Trigonometric & Commodity based linear (9 months)
10	1.386	1.945	2.413	1	Trigonometric & Commodity based linear (9 months)
11	0.757	0.977	1.107	3	Trigonometric & Commodity based linear (9 months)
12	1.868	2.472	2.929	3	Trigonometric & Commodity based linear (9 months)
13	1.025	1.404	1.712	3	Trigonometric & Commodity based linear (9 months)
14	1.457	2.158	2.836	1	Trigonometric & Commodity based linear (9 months)
15	0.773	0.954	1.024	3	Trigonometric & Commodity based linear (9 months)
16	0.233	0.328	0.389	2	Trigonometric & Commodity based linear (9 months)
17	0.605	0.783	0.902	3	Trigonometric & Commodity based linear (9 months)
18	1.27	1.697	1.861	1	Trigonometric & Commodity based linear (9 months)
19	1.053	1.315	1.397	3	Trigonometric & Commodity based linear (9 months)

Table C.2 continued from previous page

Product No.	Average Abs. Error Ahead ($/MMBtu)			Forecasting Required	Forecasting Function (Rolling Horizon)
	1 month	2 months	3 months	(months)	
20	0.42	0.577	0.664	3	Trigonometric & Commodity based linear (9 months)
21	0.371	0.481	0.558	3	Trigonometric & Commodity based linear (9 months)
22	1.025	1.404	1.712	3	Trigonometric & Commodity based linear (9 months)
23	1.457	2.158	2.836	1	Trigonometric & Commodity based linear (9 months)
24	0.919	1.151	1.208	1	Trigonometric & Commodity based linear (9 months)
25	0.605	0.783	0.902	3	Trigonometric & Commodity based linear (9 months)
35	0.994	1.233	1.399	3	Trigonometric & Commodity based linear (9 months)
42	0.994	1.233	1.399	3	Trigonometric & Commodity based linear (9 months)
44	0.994	1.233	1.399	3	Trigonometric & Commodity based linear (9 months)
45	1.189	1.452	1.572	3	Trigonometric & Commodity based linear (9 months)
46	0.855	0.984	1.075	3	Pure Trigonometric (12 months)
47	0.414	0.579	0.729	3	Trigonometric & Commodity based Linear(12 months)
48	0.514	0.648	0.781	3	Trigonometric & Commodity based linear (9 months)
50	0.656	0.906	1.105	2	Trigonometric & Commodity based Linear(12 months)

Table C.2 continued from previous page

Product No.	Average Abs. Error Ahead ($/MMBtu)			Forecasting Required	Forecasting Function (Rolling Horizon)
	1 month	2 months	3 months	(months)	
51	0.573	0.699	0.788	2	Pure Trigonometric (12 months)
52	0.548	0.645	0.715	2	Pure Trigonometric (12 months)
53	1.144	1.512	1.803	2	Trigonometric & Commodity based linear (9 months)
55	0.102	0.147	0.188	1	Trigonometric & Commodity based linear (9 months)
56	0.069	0.098	0.125	1	Trigonometric & Commodity based linear (9 months)

APPENDIX D

ACCURACY OF EPIC FORECASTS

Table D.1: Actual versus Forecasts values of EPIC

Month	**Actual EPIC**	**Initial EPIC Release**	**Initial Release Abs Percent Error**	**1st EPIC Adj.**	**1st Adj. Abs Percent Error**	**2nd EPIC Adj.**	**2nd Adj. Abs Percent Error**
	$/MMBtu	**$/MMBtu**	**%**	**$/MMBtu**	**%**	**$/MMBtu**	**%**
2006 January	17.165	13.661	20.42	15.039	12.39	16.217	5.52
2006 February	16.928	14.631	13.57	15.53	8.26	16.182	4.41
2006 March	16.895	15.883	5.99	16.368	3.12	16.655	1.42
2006 April	18.296	17.499	4.36	17.892	2.21	18.09	1.13
2006 May	19.296	17.79	7.80	18.862	2.25	18.754	2.81
2006 June	19.754	18.787	4.89	19.105	3.28	19.512	1.22
2006 July	20.494	19.259	6.03	19.645	4.14	20.146	1.69
2006 August	20.537	19.05	7.24	19.938	2.92	20.13	1.98
2006 September	18.784	17.87	4.87	18.679	0.56	18.88	0.51
2006 October	17.023	16.822	1.18	17.495	2.77	17.221	1.16
2006 November	16.665	17.148	2.89	16.792	0.76	16.579	0.52
2006 December	16.837	17.324	2.90	16.744	0.55	16.657	1.07
2007 January	16.462	16.006	2.77	16.244	1.33	16.334	0.78
2007 February	16.493	16.435	0.36	16.524	0.18	16.505	0.07
2007 March	17.646	17.085	3.18	17.246	2.27	17.324	1.82
2007 April	18.765	18.32	2.37	18.476	1.54	18.664	0.54
2007 May	19.945	19.093	4.27	19.755	0.95	19.684	1.31
2007 June	20.387	19.739	3.18	20.197	0.93	20.328	0.29
2007 July	20.653	20.826	0.84	20.662	0.04	20.363	1.40
2007 August	20.134	19.65	2.40	19.678	2.27	19.892	1.20
2007 September	19.929	20.111	0.91	19.635	1.48	19.805	0.62
2007 October	19.864	19.643	1.11	19.502	1.82	19.526	1.70
2007 November	20.246	19.799	2.21	19.832	2.04	19.743	2.49
2007 December	19.629	19.405	1.14	19.164	2.37	19.475	0.78
2008 January	19.499	19.115	1.97	19.411	0.46	19.492	0.04
2008 February	19.708	19.04	3.39	19.507	1.02	19.571	0.70
2008 March	21.194	20.92	1.29	21.072	0.58	21.254	0.28
2008 April	22.773	22.26	2.25	22.686	0.38	22.706	0.29
2008 May	24.861	24.574	1.15	24.793	0.27	24.866	0.02
2008 June	26.843	25.664	4.39	26.495	1.29	26.74	0.38
2008 July	27.556	25.992	5.67	27.029	1.91	27.356	0.72
2008 August	25.989	23.987	7.70	25.318	2.58	25.763	0.87

Table D.1 continued from previous page

Month	Actual EPIC	Initial EPIC Release	Initial Release Abs Percent Error	1st EPIC Adj.	1st Adj. Abs Percent Error	2nd EPIC Adj.	2nd Adj. Abs Percent Error
	$/MMBtu	$/MMBtu	%	$/MMBtu	%	$/MMBtu	%
2008 September	25.072	22.655	9.64	24.468	2.41	24.555	2.06
2008 October	22.082	18.972	14.08	20.852	5.57	21.319	3.46
2008 November	18.009	15.434	14.30	16.874	6.30	17.857	0.85
2008 December	16.076	15.147	5.78	15.686	2.43	15.758	1.98
2009 January	16.183	15.596	3.63	15.697	3.00	15.993	1.18
2009 February	16.186	16.29	0.65	15.996	1.17	16.22	0.21
2009 March	16.008	16.816	5.05	16.617	3.81	16.195	1.17
2009 April	16.377	17.757	8.43	16.903	3.21	16.571	1.19
2009 May	17.569	19.279	9.73	17.848	1.59	17.581	0.07
2009 June	19.459	20.331	4.48	19.65	0.98	19.439	0.10
2009 July	19.683	20.018	1.71	19.581	0.51	19.38	1.54
2009 August	20.041	21.034	4.95	20.006	0.18	19.69	1.75
2009 September	19.399	19.506	0.55	19.121	1.43	19.034	1.88
2009 October	18.772	19.633	4.58	18.986	1.14	18.801	0.16
2009 November	18.609	18.877	1.44	18.579	0.16	18.223	2.07
2009 December	17.907	18.465	3.11	17.983	0.42	17.842	0.36
2010 January	18.175	18.657	2.65	17.929	1.36	17.87	1.68
2010 February	18.163	17.65	2.82	17.772	2.15	17.877	1.58
2010 March	18.926	18.352	3.03	18.634	1.54	18.595	1.75
2010 April	19.795	19.204	2.99	19.478	1.60	19.569	1.14
2010 May	20.242	19.51	3.61	20.006	1.16	19.988	1.25
2010 June	20.512	20.01	2.45	20.091	2.05	20.204	1.50
2010 July	20.923	20.451	2.26	20.534	1.86	20.569	1.69
2010 August	20.922	20.553	1.76	20.571	1.68	20.731	0.91
2010 September	20.302	20.614	1.54	20.344	0.21	20.473	0.84
2010 October	20.106	20.402	1.47	20.198	0.46	20.084	0.11
2010 November	19.344	19.709	1.89	19.523	0.93	19.598	1.31
2010 December	19.109	19.303	1.02	19.312	1.06	19.142	0.17
2011 January	19.239	18.952	1.49	19.095	0.74	19.258	0.10
2011 February	19.927	19.544	1.92	19.708	1.10	19.788	0.70
2011 March	21.737	20.923	3.75	21.523	0.98	21.816	0.36
2011 April	23.43	23.021	1.75	23.698	1.14	23.485	0.24
2011 May	24.328	23.476	3.50	24.538	0.86	24.408	0.33
2011 June	24.576	23.9	2.75	24.528	0.19	24.56	0.06
2011 July	24.916	25.104	0.75	24.969	0.21	24.959	0.17
2011 August	24.745	24.452	1.18	24.57	0.71	24.607	0.56
2011 September	24.26	23.875	1.59	24.164	0.40	24.16	0.41
2011 October	22.888	22.901	0.06	23.054	0.72	23.096	0.91
2011 November	21.901	21.704	0.90	22.003	0.47	21.956	0.25

Table D.1 continued from previous page

Month	Actual EPIC	Initial EPIC Release	Initial Release Abs Percent Error	1st EPIC Adj.	1st Adj. Abs Percent Error	2nd EPIC Adj.	2nd Adj. Abs Percent Error
	$/MMBtu	$/MMBtu	%	$/MMBtu	%	$/MMBtu	%
2011 December	20.613	20.676	0.31	20.63	0.08	20.657	0.21
2012 January	20.465	20.626	0.78	20.376	0.44	20.428	0.18
2012 February	21.265	21.124	0.67	20.984	1.33	21.005	1.22
2012 March	23.049	21.305	7.56	22.586	2.01	22.502	2.37
2012 April	23.469	22.439	4.39	23.57	0.43	23.53	0.26
2012 May	23.644	23.352	1.24	23.942	1.26	23.702	0.24
2012 June	23.11	23.298	0.82	23.526	1.80	23.261	0.65
2012 July	23.358	24.234	3.75	23.76	1.72	23.69	1.42
2012 August	24.27	24.904	2.61	24.54	1.11	24.456	0.77
2012 September	24.293	23.851	1.82	24.471	0.73	24.494	0.83
2012 October	23.321	22.622	3.00	23.404	0.36	23.391	0.30
2012 November	21.361	21.917	2.60	21.617	1.20	21.751	1.83
2012 December	20.41	20.647	1.16	20.458	0.23	20.487	0.37
2013 January	20.084	20.318	1.17	20.126	0.21	20.115	0.15
2013 February	21.149	21.281	0.62	21.093	0.27	21.183	0.16
2013 March	21.5	21.771	1.26	21.989	2.28	22.077	2.68
2013 April	22.24	22.251	0.05	22.419	0.81	22.374	0.60
2013 May	23.295	23.009	1.23	23.157	0.59	23.26	0.15
2013 June	24.007	23.637	1.54	23.843	0.68	24.049	0.18
2013 July	24.325	24.56	0.96	24.357	0.13	24.572	1.02
2013 August	24.177	24.083	0.39	24.335	0.65	24.405	0.94
2013 September	23.841	23.561	1.18	23.75	0.38	23.835	0.03
2013 October	22.511	22.482	0.13	22.526	0.07	22.559	0.21
2013 November	20.756	21.35	2.86	21.129	1.80	21.198	2.13
2013 December	20.206	20.73	2.59	20.463	1.27	20.467	1.29
2014 January	20.104	19.823	1.40	20.03	0.37	20.284	0.90
2014 February	20.979	20.494	2.31	20.674	1.45	21.044	0.31
2014 March	21.962	21.379	2.66	21.662	1.37	21.867	0.43
2014 April	22.943	22.934	0.04	22.884	0.26	22.913	0.13
2014 May	23.91	23.237	2.81	23.755	0.65	23.828	0.34
2014 June	24.566	24.255	1.27	24.497	0.28	24.677	0.45
2014 July	24.658	24.117	2.19	24.657	0.00	24.8	0.58
2014 August	24.231	23.738	2.03	24.126	0.43	24.251	0.09
2014 September	23.603	23.367	1.00	23.461	0.60	23.612	0.04
2014 October	22.051	21.351	3.17	21.783	1.22	21.683	1.67
2014 November	19.629	20.315	3.50	19.621	0.04	19.838	1.07
2014 December	18.224	18.256	0.18	17.945	1.53	17.999	1.24
2015 January	16.333	16.034	1.83	16.404	0.44	16.408	0.46
2015 February	16.666	17.591	5.55	17.124	2.75	17.17	3.03

Table D.1 continued from previous page

Month	Actual EPIC	Initial EPIC Release	Initial Release Abs Percent Error	1st EPIC Adj.	1st Adj. Abs Percent Error	2nd EPIC Adj.	2nd Adj. Abs Percent Error
	$/MMBtu	$/MMBtu	%	$/MMBtu	%	$/MMBtu	%
2015 March	17.6	17.815	1.22	17.896	1.68	17.722	0.69
2015 April	18.036	18.578	3.01	18.335	1.66	18.17	0.74
2015 May	19.523	20.129	3.11	19.792	1.38	19.607	0.43
2015 June	20.199	20.396	0.97	20.35	0.75	20.161	0.19
2015 July	20.465	20.1	1.79	20.354	0.54	20.309	0.76
2015 August	19.727	19.047	3.45	19.537	0.96	19.637	0.46
2015 September	18.913	18.328	3.09	18.71	1.07	18.803	0.58
2015 October	17.746	17.247	2.81	17.711	0.19	17.601	0.81
2015 November	16.379	16.64	1.59	16.43	0.31	16.333	0.28
2015 December	15.565	16.043	3.08	15.536	0.18	15.298	1.71
2016 January	14.511	15.262	5.18	14.703	1.33	14.589	0.54
2016 February	14.353	15.061	4.93	14.293	0.42	14.24	0.79
2016 March	15.239	15.762	3.43	15.16	0.51	15.152	0.57
2016 April	15.804	16.727	5.84	16.199	2.50	16.131	2.07
2016 May	17.049	18.097	6.14	17.387	1.98	17.168	0.70
2016 June	18.349	18.674	1.77	18.332	0.09	18.245	0.57
2016 July	18.305	18.424	0.65	18.156	0.82	18.028	1.51
2016 August	18.165	18.254	0.49	17.906	1.42	17.936	1.26
2016 September	18.118	18.042	0.42	17.803	1.74	17.833	1.58
2016 October	17.452	17.651	1.14	17.417	0.20	17.383	0.40
2016 November	16.441	16.305	0.82	16.262	1.08	16.294	0.90
2016 December	16.096	16.531	2.70	16.392	1.84	16.325	1.42
2017 January	16.298	16.107	1.17	15.917	2.34	15.916	2.34
2017 February	16.842	16.026	4.84	15.93	5.42	16.208	3.76
2017 March	16.835	16.421	2.46	16.516	1.90	16.727	0.64
2017 April	17.626	17.092	3.03	17.322	1.73	17.36	1.51
2017 May	17.959	17.543	2.32	17.819	0.78	17.901	0.32
2017 June	18.534	18.069	2.51	18.213	1.73	18.414	0.65
2017 July	18.786	18.553	1.24	18.603	0.98	18.745	0.22
2017 August	19.042	19.028	0.08	18.88	0.85	19.109	0.35
2017 September	19.602	19.049	2.82	19.478	0.63	19.681	0.41
2017 October	18.581	18.072	2.74	18.452	0.70	18.555	0.14
2017 November	17.687	17.754	0.38	17.907	1.24	17.955	1.52
2017 December	16.878	17.318	2.61	17.378	2.96	17.238	2.13
2018 January	17.307	17.334	0.16	17.202	0.60	17.182	0.72
2018 February	17.828	17.268	3.14	17.343	2.72	17.444	2.16
2018 March	17.822	17.872	0.28	17.899	0.43	18.094	1.53
2018 April	18.578	18.831	1.36	19.249	3.61	19.158	3.12
2018 May	20.399	20.129	1.32	20.509	0.54	20.362	0.18

Table D.1 continued from previous page

Month	Actual EPIC	Initial EPIC Release	Initial Release Abs Percent Error	1st EPIC Adj.	1st Adj. Abs Percent Error	2nd EPIC Adj.	2nd Adj. Abs Percent Error
	$/MMBtu	$/MMBtu	%	$/MMBtu	%	$/MMBtu	%
2018 June	21.074	20.82	1.21	21.013	0.29	20.986	0.42
2018 July	21.375	21.262	0.53	21.286	0.41	21.335	0.19
2018 August	21.377	21.166	0.99	21.276	0.47	21.311	0.31
2018 September	20.965	21.133	0.80	21.182	1.04	21.149	0.88
2018 October	20.311	20.209	0.50	20.602	1.43	20.557	1.21
2018 November	18.329	17.685	3.51	18.674	1.88	18.809	2.62
2018 December	17.238	16.963	1.60	17.285	0.27	17.165	0.42
2019 January	16.587	17.051	2.80	16.588	0.01	16.627	0.24
2019 February	17.084	17.578	2.89	17.171	0.51	17.218	0.79
2019 March	17.674	18.255	3.29	17.978	1.72	17.995	1.81
2019 April	19.378	19.315	0.32	19.244	0.69	19.14	1.23
2019 May	19.944	19.54	2.03	20.03	0.43	20.024	0.40
2019 June	20.037	19.487	2.74	20.178	0.70	20.276	1.19
2019 July	20.668	19.928	3.58	20.71	0.20	20.701	0.16
2019 August	20.179	19.914	1.31	20.138	0.20	20.18	0.01
2019 September	19.763	19.913	0.76	19.785	0.11	19.829	0.34
2019 October	19.01	19.081	0.38	19.219	1.10	19.15	0.74
2019 November	17.681	18.023	1.93	18.1	2.37	18.126	2.52
2019 December	17.052	17.243	1.12	17.27	1.28	17.153	0.59
2020 January	17.063	16.835	1.33	16.724	1.99	16.746	1.86
2020 February	16.63	16.845	1.29	16.705	0.45	16.786	0.94
2020 March	16.194	15.47	4.47	16.165	0.18	15.986	1.29
2020 April	15.215	15.261	0.30	15.324	0.72	15.012	1.33
2020 May	15.767	16.203	2.76	15.362	2.57	16.005	1.51
2020 June	17.659	17.511	0.83	17.63	0.16	17.207	2.56
2020 July	18.481	18.467	0.08	18.056	2.30	17.898	3.16
2020 August	18.302	18.121	0.99	17.927	2.05	17.908	2.15
2020 September	17.917	17.251	3.72	17.456	2.57	17.664	1.41
2020 October	16.881	16.73	0.89	16.75	0.77	16.768	0.67
2020 November	16.258	16.171	0.53	15.889	2.27	15.933	2.00
2020 December	16.108	16.234	0.78	15.978	0.81	15.984	0.77
2021 January	16.44	16.287	0.94	16.187	1.54	16.394	0.28
2021 February	18.381	17.467	4.98	17.269	6.05	18.345	0.20
2021 March	19.231	17.576	8.60	18.333	4.67	18.792	2.28
2021 April	19.625	18.121	7.67	19.25	1.91	19.438	0.95
2021 May	NA	20.122	NA	20.71	NA	20.583	NA
2021 June	NA	21.488	NA	22.255	NA	NA	NA
2021 July	NA	22.568	NA	NA	NA	NA	NA

APPENDIX E

RESULTS OF FUTURE FORECASTS

Table E.1: Selected Forecasting Models, Best Configurations and their Accuracy Measures

Energy Product	Selected Forecasting Method	Best Configuration	Average RMSE	Average sMAPE	Average MAE
			$/MMBtu	%	$/MMBtu
p1	**fc7**	# of indices tested = 74, # of MLP inputs = 12, # of nodes = 32, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 16, differences taken = 1, data scaled = False, future horizon = 12	1.4363	4.7603	1.0025
p2_5_12	**fc9**	# of indices tested = 85, # of LSTM inputs = 28, # of nodes = 64, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 16, differences taken = 1, data scaled = True, future horizon = 14	3.4035	8.9818	1.9617
p3	**fc8**	# of indices tested = 70, # of RNN inputs = 12, # of nodes = 32, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 8, differences taken = 12, data scaled = True, future horizon = 12	1.4301	5.0035	1.1110

Table E.1 continued from previous page

Energy Product	Selected Forecasting Method	Best Configuration	Average RMSE	Average sMAPE	Average MAE
			$/MMBtu	%	$/MMBtu
p4_11	**fc7**	# of indices tested = 85, # of MLP inputs = 14, # of nodes = 32, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 8, differences taken = 1, data scaled = True, future horizon = 14	1.0247	4.2619	0.7747
p6_13_22	**fc7**	# of indices tested = 85, # of MLP inputs = 14, # of nodes = 32, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 16, differences taken = 1, data scaled = True, future horizon = 14	1.0137	4.2411	0.7674
p7_15	**fc8**	# of indices tested = 85, # of RNN inputs = 14, # of nodes = 32, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 8, differences taken = 1, data scaled = True, future horizon = 14	1.0497	4.1301	0.8243
p8_16	**fc9**	# of indices tested = 32, # of LSTM inputs = 14, # of nodes = 32, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 8, differences taken = 1, data scaled = True, future horizon = 14	0.2323	9.7916	0.1941

Table E.1 continued from previous page

Energy Product	Selected Forecasting Method	Best Configuration	Average RMSE	Average sMAPE	Average MAE
			$/MMBtu	%	$/MMBtu
p9_17_25	**fc8**	# of indices tested = 51, # of RNN inputs = 28, # of nodes = 64, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 16, differences taken = 1, data scaled = True, future horizon = 14	0.7083	5.8563	0.5456
p10	**fc9**	# of indices tested = 45, # of LSTM inputs = 13, # of nodes = 64, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 8, differences taken = 1, data scaled = False, future horizon = 13	1.0687	7.4925	0.8343
p14_23	**fc9**	# of indices tested = 45, # of LSTM inputs = 13, # of nodes = 64, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 8, differences taken = 1, data scaled = True, future horizon = 13	1.0437	7.4431	0.8291
p18	**fc7**	# of indices tested = 42, # of MLP inputs = 26, # of nodes = 64, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 16, differences taken = 1, data scaled = False, future horizon = 13	1.0852	6.6006	0.8166

Table E.1 continued from previous page

Energy Product	Selected Forecasting Method	Best Configuration	Average RMSE	Average sMAPE	Average MAE
			$/MMBtu	%	$/MMBtu
p19	**fc9**	# of indices tested = 51, # of LSTM inputs = 28, # of nodes = 32, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 16, differences taken = 1, data scaled = False, future horizon = 14	1.6683	4.9817	1.2286
p20	**fc8**	# of indices tested = 51, # of RNN inputs = 28, # of nodes = 64, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 16, differences taken = 1, data scaled = True, future horizon = 14	0.8356	3.8567	0.6634
p21	**fc9**	# of indices tested = 51, # of LSTM inputs = 14, # of nodes = 32, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 8, differences taken = 1, data scaled = False, future horizon = 14	1.0712	5.7650	0.7710
p24	**fc9**	# of indices tested = 51, # of LSTM inputs = 26, # of nodes = 32, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 16, differences taken = 1, data scaled = False, future horizon = 13	1.0196	3.9501	0.8130

Table E.1 continued from previous page

Energy Product	Selected Forecasting Method	Best Configuration	Average RMSE	Average sMAPE	Average MAE
			$/MMBtu	%	$/MMBtu
p26_30_37	**fc9**	# of indices tested = 26, # of LSTM inputs = 24, # of nodes = 64, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 8, differences taken = 1, data scaled = False, future horizon = 12	0.5268	0.5100	0.1254
p27	**fc9**	# of indices tested = 26, # of LSTM inputs = 12, # of nodes = 32, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 16, differences taken = 1, data scaled = False, future horizon = 12	0.4836	0.2802	0.1570
p28_33_34_40_41_43	**fc9**	# of indices tested = 26, # of LSTM inputs = 12, # of nodes = 32, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 16, differences taken = 1, data scaled = True, future horizon = 12	0.1756	0.2995	0.0825
p29_36	**fc7**	# of indices tested = 26, # of MLP inputs = 12, # of nodes = 32, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 16, differences taken = 1, data scaled = False, future horizon = 12	0.4676	1.6008	0.2058

Table E.1 continued from previous page

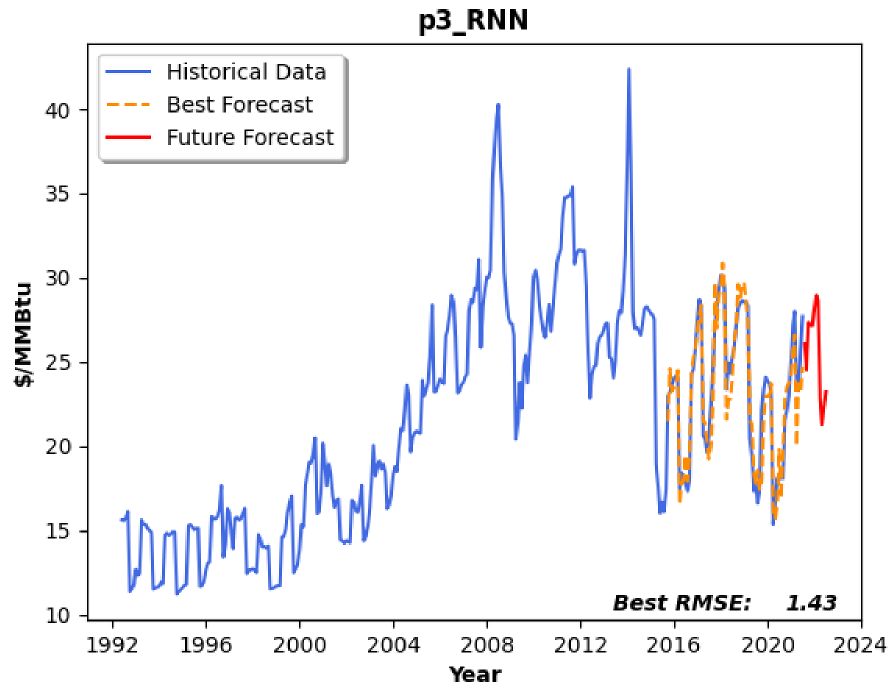
Energy Product	Selected Forecasting Method	Best Configuration	Average RMSE	Average sMAPE	Average MAE
			$/MMBtu	%	$/MMBtu
p31_38	**fc7**	# of indices tested = 26, # of MLP inputs = 12, # of nodes = 64, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 16, differences taken = 1, data scaled = False, future horizon = 12	1.0348	0.9974	0.3488
p32_39	**fc8**	# of indices tested = 26, # of RNN inputs = 24, # of nodes = 64, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 16, differences taken = 1, data scaled = False, future horizon = 12	0.0887	0.3646	0.0433
p35_42_44	**fc9**	# of indices tested = 49, # of LSTM inputs = 14, # of nodes = 32, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 16, differences taken = 1, data scaled = False, future horizon = 14	1.0941	3.7128	0.8561
p45	**fc9**	# of indices tested = 37, # of LSTM inputs = 28, # of nodes = 64, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 16, differences taken = 1, data scaled = True, future horizon = 14	1.4440	5.0645	1.1654

Table E.1 continued from previous page

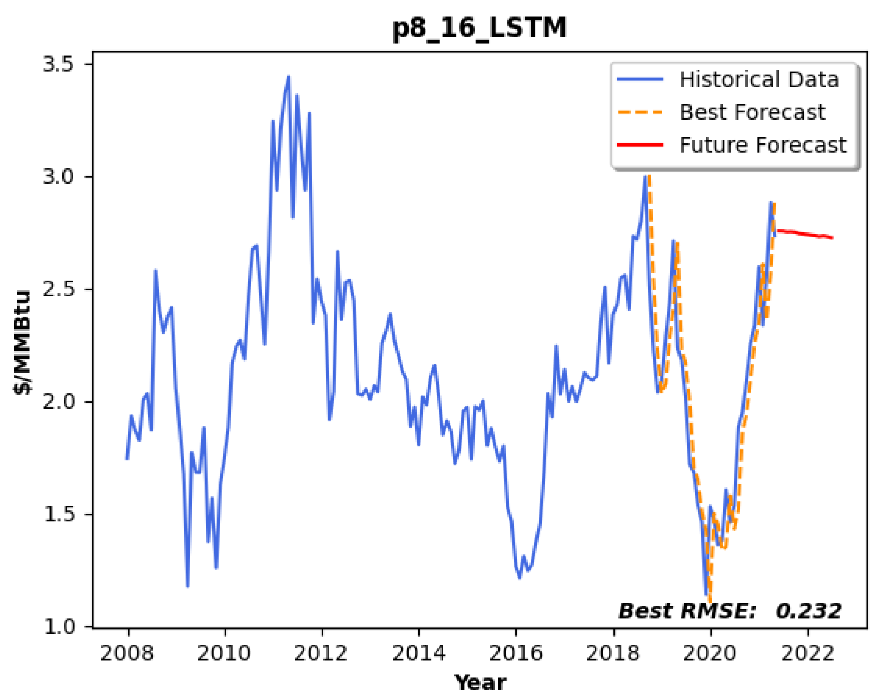
Energy Product	Selected Forecasting Method	Best Configuration	Average RMSE	Average sMAPE	Average MAE
			$/MMBtu	%	$/MMBtu
p46	**fc8**	# of indices tested = 85, # of RNN inputs = 28, # of nodes = 32, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 16, differences taken = 1, data scaled = False, future horizon = 14	0.5969	4.1835	0.4676
p47	**fc8**	# of indices tested = 85, # of RNN inputs = 28, # of nodes = 64, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 16, differences taken = 0, data scaled = True, future horizon = 14	0.2628	2.6852	0.2044
p48	**fc8**	# of indices tested = 49, # of RNN inputs = 28, # of nodes = 32, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 8, differences taken = 0, data scaled = False, future horizon = 14	0.8913	8.8456	0.3935
p49	**fc9**	# of indices tested = 59, # of LSTM inputs = 12, # of nodes = 32, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 16, differences taken = 0, data scaled = True, future horizon = 12	0.6111	4.2230	0.4015

Table E.1 continued from previous page

Energy Product	Selected Forecasting Method	Best Configuration	Average RMSE $/MMBtu	Average sMAPE %	Average MAE $/MMBtu
p50	**fc10**	# of indices tested = 49, # of nodes = 64, learn_rate = 1e-06, # of epochs = 1000, # of batches = 64, # of sequences = 3, # of steps = 12, # of filters = 256, # of kernels = 3, future horizon = 14	0.5506	1.1251	0.4301
p51	**fc4a**	Arima(2, 1, 0)(2, 1, 0) 12	0.6510	1.1150	0.3540
p52	**fc8**	# of indices tested = 49, # of RNN inputs = 28, # of nodes = 64, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 8, differences taken = 0, data scaled = True, future horizon = 14	0.8101	1.9149	0.3896
p53	**fc2d**	stlf(method = "rwdrift"")	0.6640	1.8550	0.5320
p55	**fc9**	# of indices tested = 51, # of LSTM inputs = 13, # of nodes = 32, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 8, differences taken = 1, data scaled = False, future horizon = 13	0.0592	0.9531	0.0418
p56	**fc9**	# of indices tested = 51, # of LSTM inputs = 13, # of nodes = 64, dropout = 0.1, learn_rate = 0.0001, # of epochs = 250, # of batches = 8, differences taken = 1, data scaled = False, future horizon = 13	0.0372	0.7046	0.0269

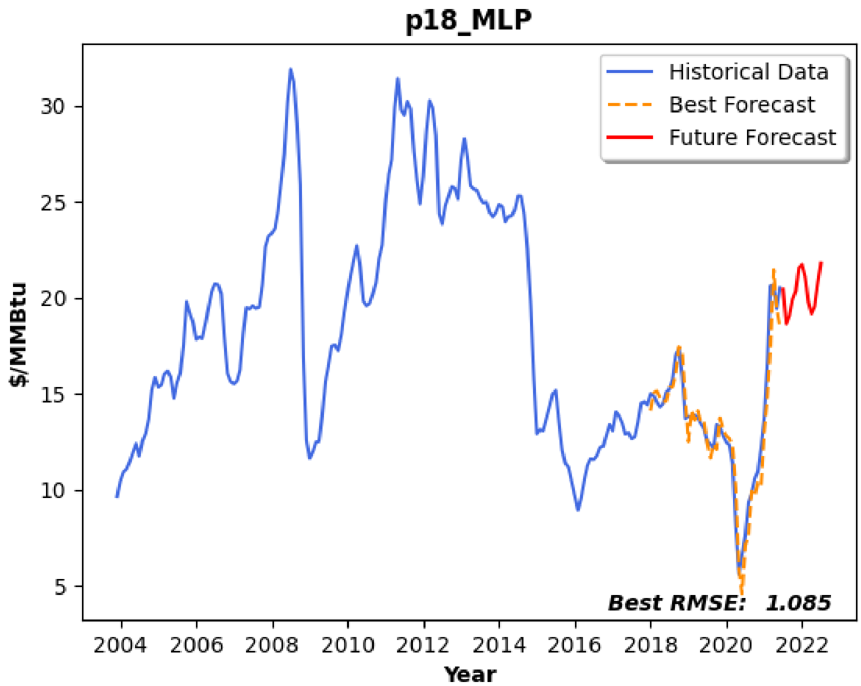


(a) HGL (Propane) in Residential Sector

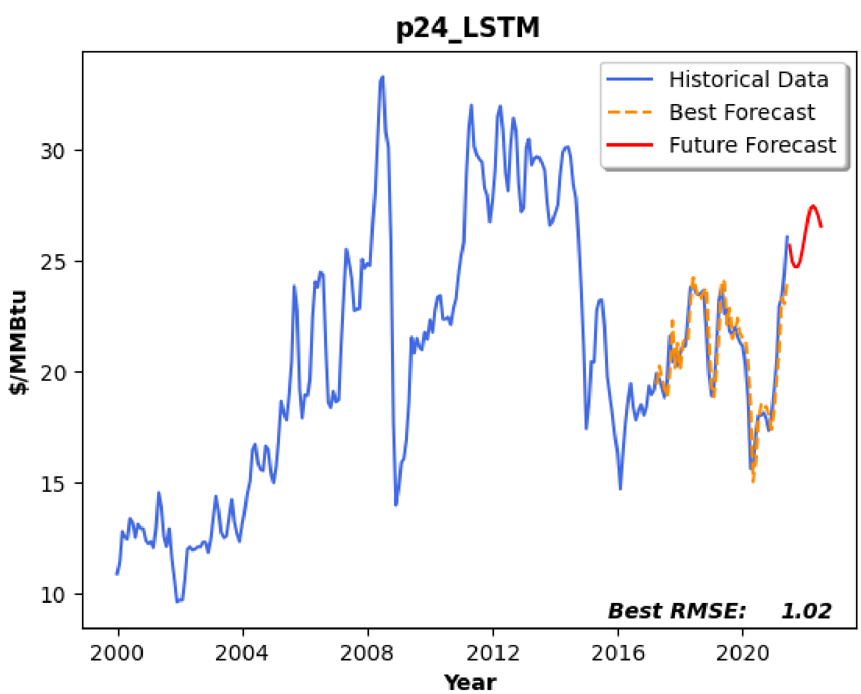


(b) Petroleum Coke in Commercial Sector

Figure E.1: Historical Data, Best Models, and Future Forecasts for Product 3 and Products 8 & 16

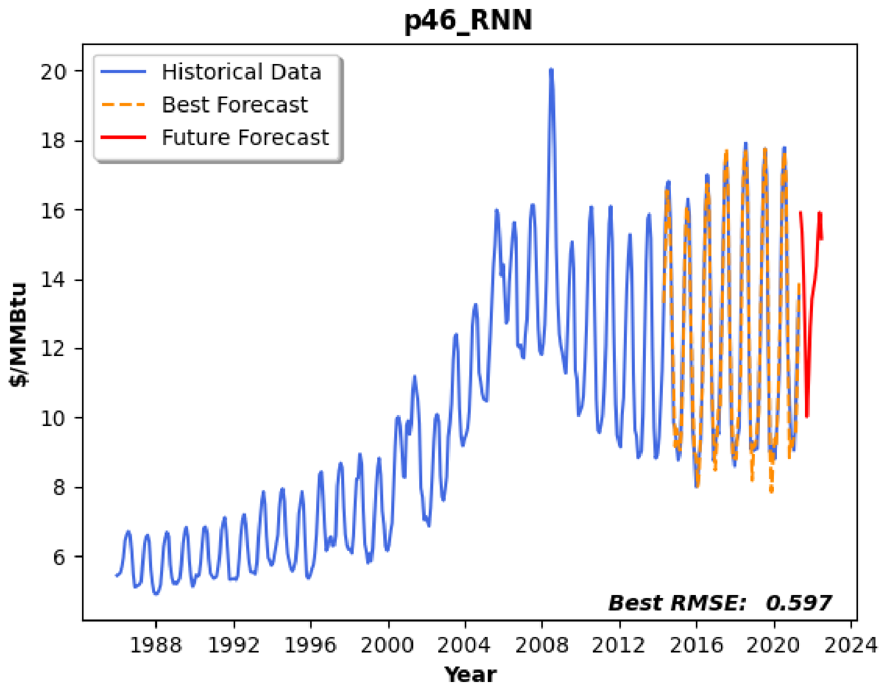


(a) Other Petroleum Products in Industrial Sector

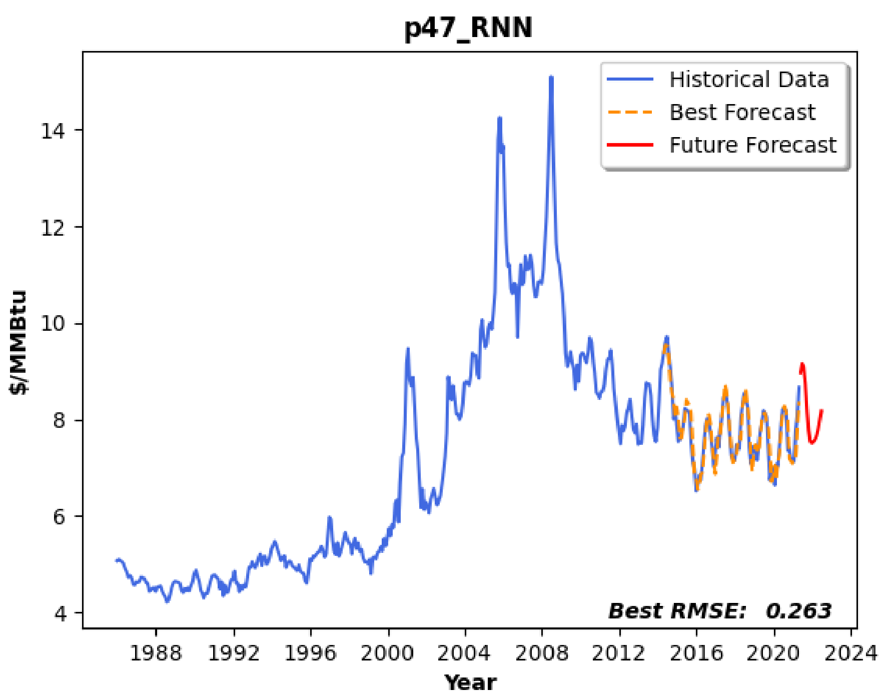


(b) Motor Gasoline in Transportation Sector

Figure E.2: Historical Data, Best Models, and Future Forecasts for Products 18 & 24

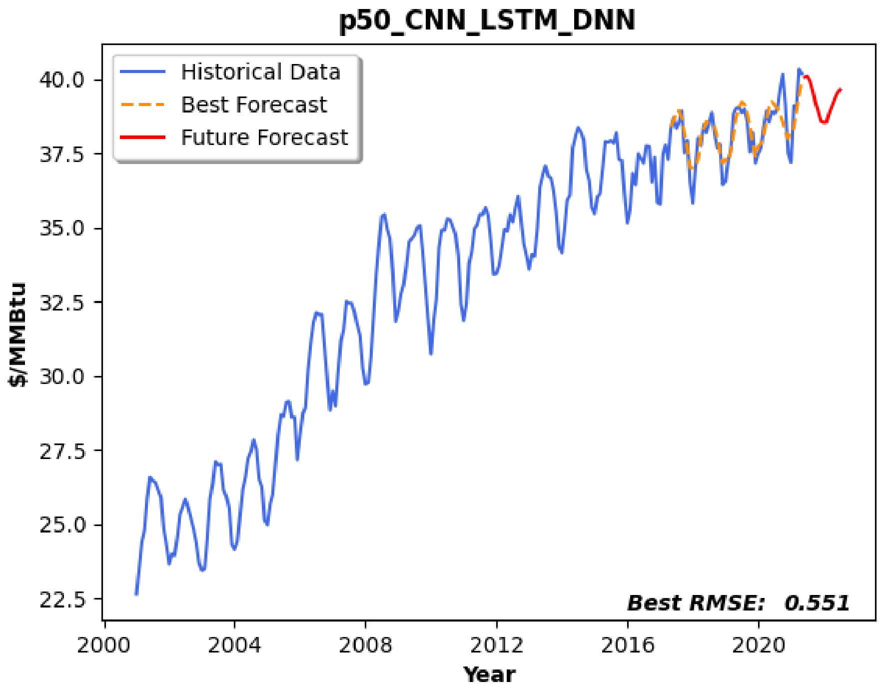


(a) Natural Gas in Residential Sector

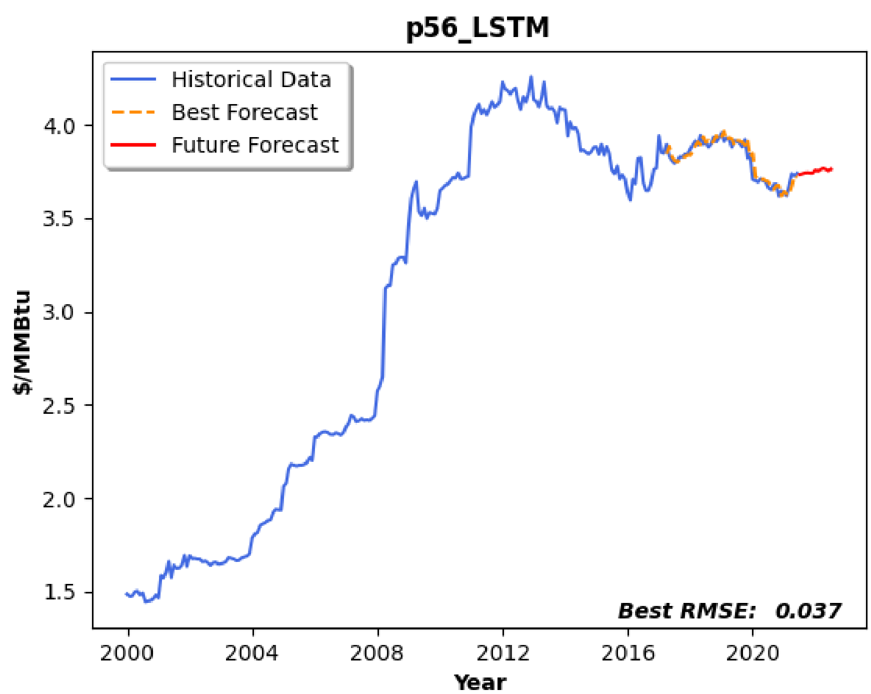


(b) Natural Gas in Commercial Sector

Figure E.3: Historical Data, Best Models, and Future Forecasts for Products 46 & 47



(a) Electricity in Residential Sector



(b) Coal in Industrial Sector

Figure E.4: Historical Data, Best Models, and Future Forecasts for Products 50 & 56

APPENDIX F

COMMODITIES WITH SPOT PRICES

Table F.1: Commodities with Spot Prices from Bloomberg

Commodity	Commodity with Available Spot Price	Bloomberg Ticker
Motor Gasoline	US NYH Gasoline 83.5 Octane CBOB Prompt-Month Spot	MOINCB87 Comdty
	US XBQ9 Commodity Spot	XB1 Comdty
	US NYH Gasoline 87 Conventional Prompt-Month Spot	MOINY87P Comdty
	US Gulf Coast Gasoline 87 Octane Conventional Prompt Spot	MOIGC87P Comdty
	Danaher Oil Mid-Continent 85 Octane CBOB Gasoline Prompt Month Spot/Chicago Area	CHOR87PC Index
	US Los Angeles Gasoline 88.5 Sub-Octane Premium Prompt-Month Spot	MOILPR92 Index
	US San Francisco Gasoline 88.5 Sub-Oct Premium Prompt-Month Spot	MOISPR92 Index
	US Portland Gasoline 90 Sub-Oct Conventional Prompt-Month Spot	MOGHS92P Comdty
	US Portland Gasoline 84 Sub-Oct Conventional Prompt-Month Spot	MOGHS87P Comdty
Ethanol	US New York Harbor Ethanol Prompt Spot	ETHNNYPR Index
	US Chicago Argo Ethanol FOB Spot	ETHNCHIC Comdty
	Bloomberg Ethanol Prompt Month fob Spot Price/U.S. Gulf Coast	ETHNUSGC Index
	Bloomberg Ethanol Prompt Month fob Spot Price/U.S. West Coast	ETHNWCPR Comdty
Bio-Diesel	Biodiesel B100 Soy Methyl Esters Midwest Spot Price	BIDISMMW Comdty
	Biodiesel B100 Soy Methyl Esters Gulf Coast Spot Price	BIDISMGC Index
	Biodiesel B100 Fatty Acid Methyl Esters West Coast Spot Price	BIDIFAWC Index
Electricity	PJM ISO Western Hub 5 Minute Wtd Avg LMP ON PEAK AVG	PJE35MON Index
	PJM ISO Eastern Hub Day Ahead LMP ON PEAK AVG	PJB6DAON Index
Distillate Fuel Oil	US New York Harbor No. 2 Heating Oil Prompt Spot	NO2INYPR Index

Continued on next page

Table F.1 – continued from previous page

Commodity	Commodity with Available Spot Price	Bloomberg Ticker
	US Boston Heating Oil 2000 ppm Sulfur FOB Prompt-Month Spot	NO2IBSTN Index
	US Gulf Coast No. 2 Heating Oil Prompt Spot	NO2IGCPR Index
Kerosene	Danaher Oil Mid-Continent Jet Fuel Prompt Month Outright Chicago	CHORJETP Index
	US New York Harbor Jet Fuel 54 Prompt Spot	JETINYPR Index
	US Los Angeles Jet Fuel Any-Month Spot	JETFLAPL Index
	US Gulf Coast Jet Fuel 54 Prompt Spot	JETIGCPR Index
	US Mid-Continent Jet Fuel Prompt-Month Spot	G3ORJETP Index
	US NYH Jet Kerosene 55 Prompt-Month Spot	JETINYP5 Index
Diesel	US Los Angeles CARB Ultra Low Sulfur Diesel Prompt Spot	DIEILCAM Index
	US San Francisco EPA Ultra Low Sulfur Diesel Prompt Month Spot	DIEISFAM Index
	US Portland EPA Ultra Low Sulfur Diesel Prompt Month Spot	DIEISTPR Index
HGL (Propane, Butane, Isobutane)	North American Spot LPG Propane Price/Hattiesburg	LPGTHAPP Index
	North American Spot LPG Propane Price/Mont Belvieu LST	LPGSMBPP Index
	North American Spot LPG Propane Price/Conway Kansas	LPGSCWPP Index
	North American Spot LPG Normal Butane Price/Mont Belvieu LST	LPGSMBNB Index
	North American Spot LPG Normal Butane Price/Conway Kansas	LPGSCWNB Index
	North American Spot LPG Iso-Butane Price/Mont Belvieu Texas LST	LPGSMBIL Index
	North American Spot LPG Isobutane Price/Conway Kansas	LPGSCWIB Index
Natural Gas	Henry Hub Natural Gas Spot Price	NGUSHHUB Index
	Mid-Continent Natural Gas Spot Price/Chicago City Gate	NAGANGPL Index
	Leidy Hub Natural Gas Spot Price	NGNELEID Index
	Cheyenne Hub Natural Gas Spot Price	NGRMCHEY Index

Continued on next page

Table F.1 – continued from previous page

Commodity	Commodity with Available Spot Price	Bloomberg Ticker
	Rocky Mountain Natural Gas Spot Price/Kern River Opal Wyoming	NGRMKERN Index
Residual Fuel Oil	US New York Harbor No. 6 1.0% Sulfur Residual Fuel Oil Cargo Spot	N6NY1LC Index
	US Gulf Coast No 6 Fuel Oil 1.0% Sulfur FOB Barge Spot	N6GF1.0L Index
Coal	Bloomberg 1% Sulfur Coal Spot Price Fob/Utah Colorado	COALCO1S Index
	Bloomberg Powder River Basin 8800 Btu Coal Spot Price Fob/Gillette Wyoming	COALPWDR Index
	Bloomberg Low Sulfur Compliance Coal Spot Price/Big Sandy Barge Fob	COALBGSD Index

APPENDIX G

POLICY CASE STUDIES

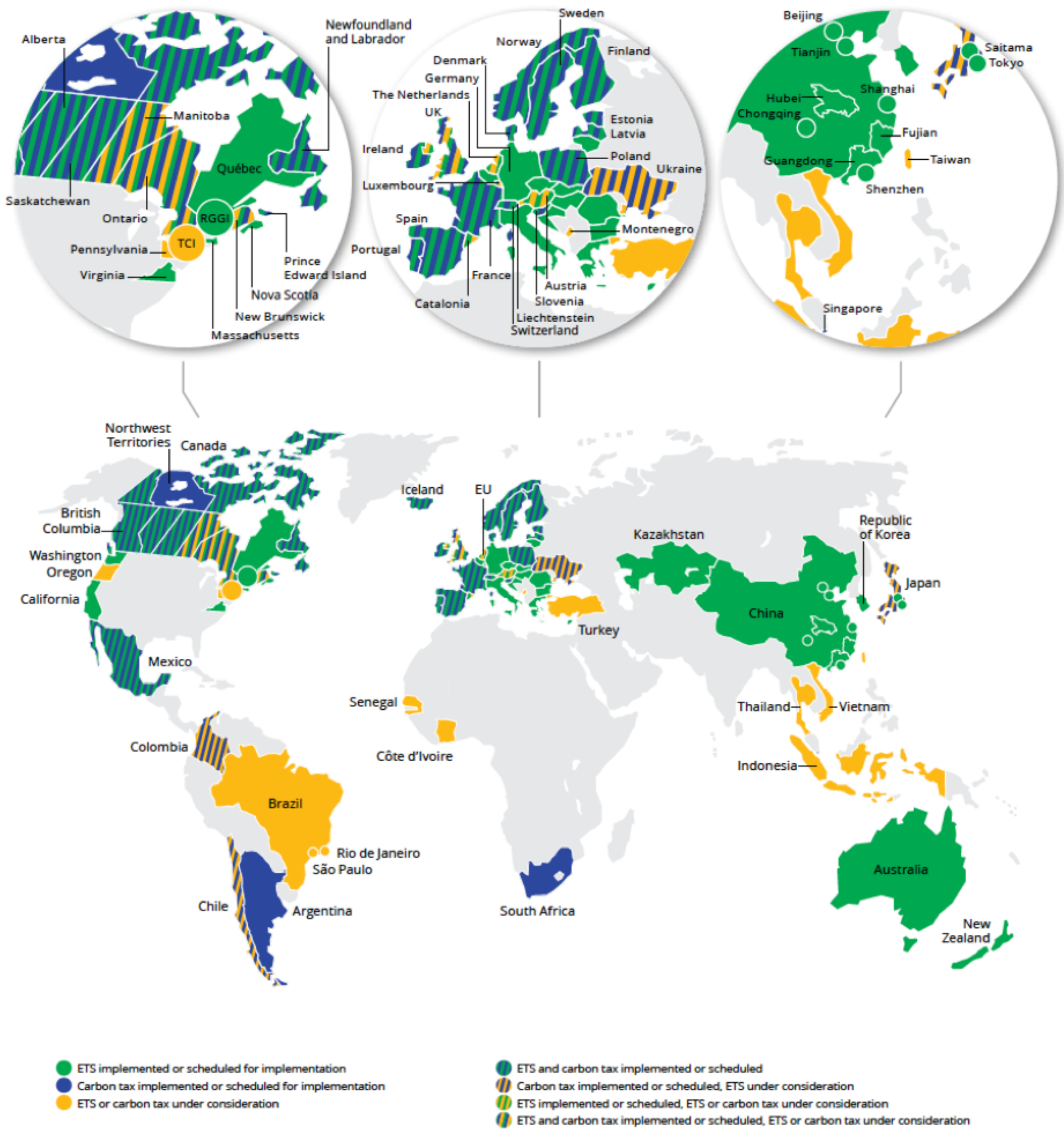


Figure G.1: Summary Map of Regional, National and Sub-national Carbon Pricing Initiatives Implemented, Scheduled for Implementation and under Consideration (ETS and Carbon Tax) [2]

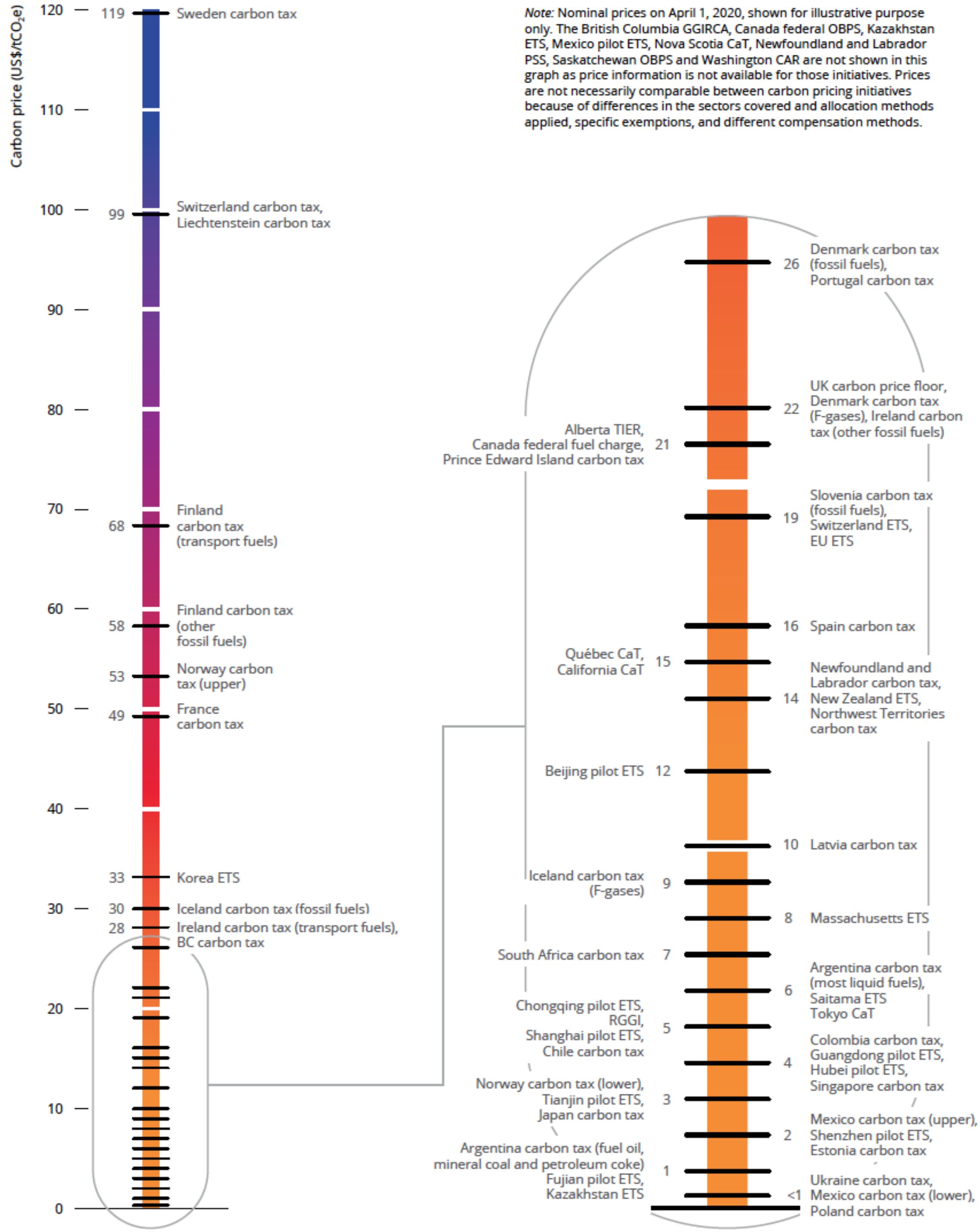


Figure G.2: Prices in Implemented Carbon Pricing Initiatives [2]

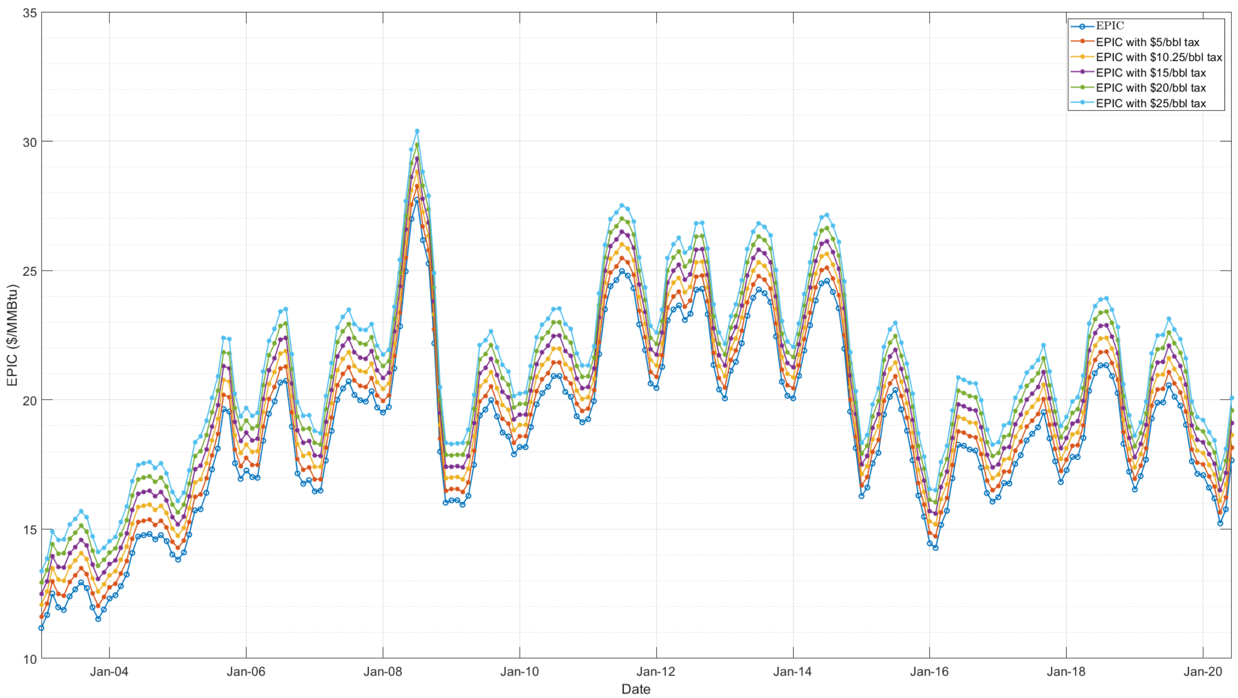


Figure G.3: Impact on EPIC from an increase in the Federal Tax on Crude Oil (January 2003 to June 2020)

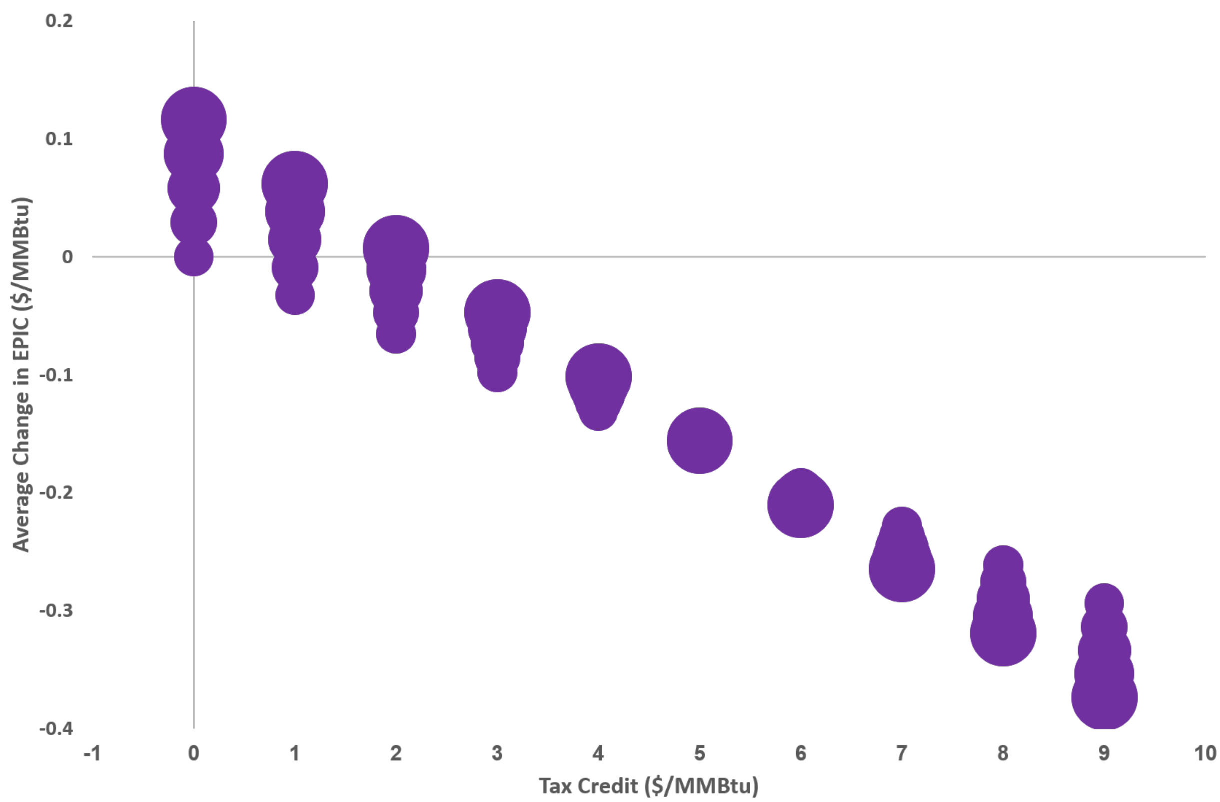


Figure G.4: Nuclear Power at different Target Weights & Tax Credits, 2020-2024

The grid of results for nuclear energy at different target weights and tax credits from 2020 to 2024 is shown in this figure. Due to the relatively higher levelized cost of nuclear energy, EPIC tends to increase at low tax credit levels, whereas EPIC decreases substantially (about $0.4/MMBtu) at the highest target weight (30%) and tax credit. At maximum weight (30%) and without tax credit, EPIC increases by 0.657% with no budget required, whereas at maximum weight (30%) and maximum tax credit ($9/MMBtu), EPIC decreases by 2.107% requiring around $38.0 billion annually from the government's budget.

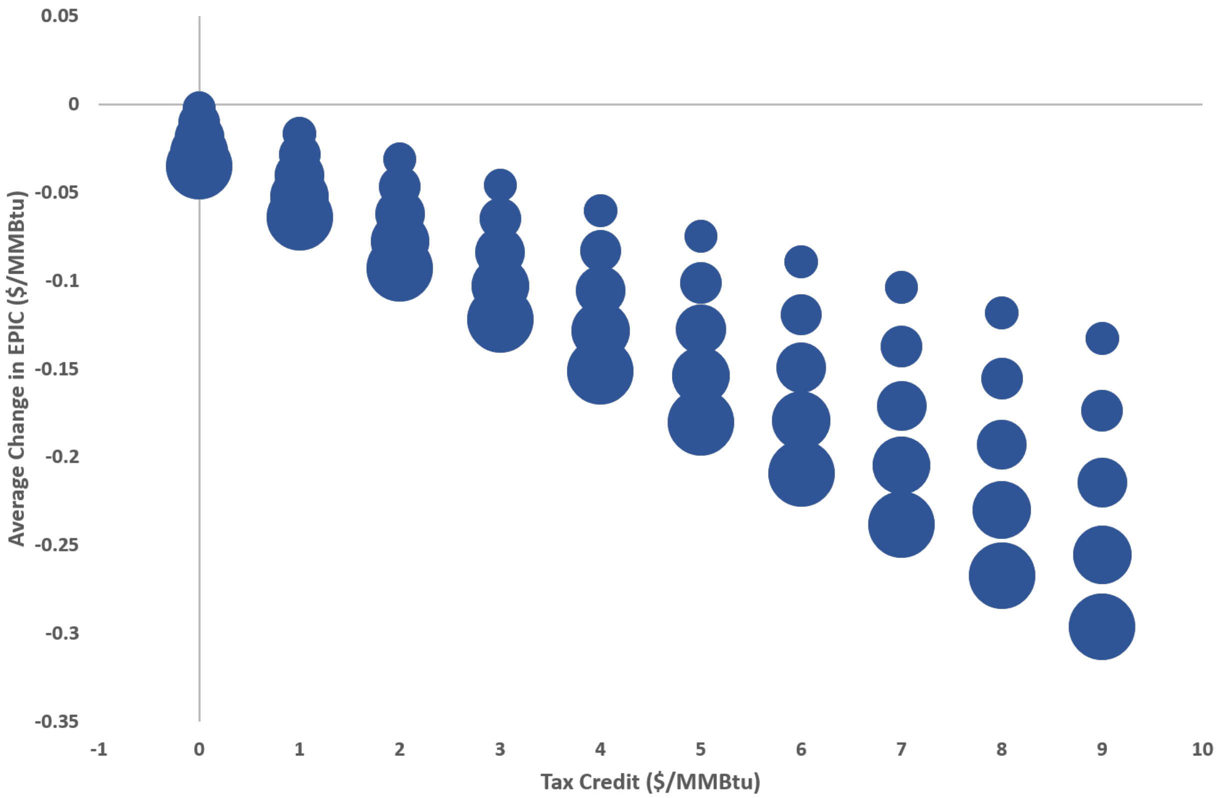


Figure G.5: Hydroelectric Power at different Target Weights & Tax Credits, 2020-2024

The grid of results for hydroelectric power at different target weights and tax credits from 2020 to 2024 is shown in this figure. Due to the low levelized cost of hydroelectric power, EPIC tends to decrease even without tax credit levels. At maximum weight (16%) and without tax credit, EPIC decreases by 0.198% with no budget required, whereas at maximum weight (16%) and maximum tax credit ($9/MMBtu), EPIC decreases by 1.672% requiring more than $20.0 billion annually from the government's budget.

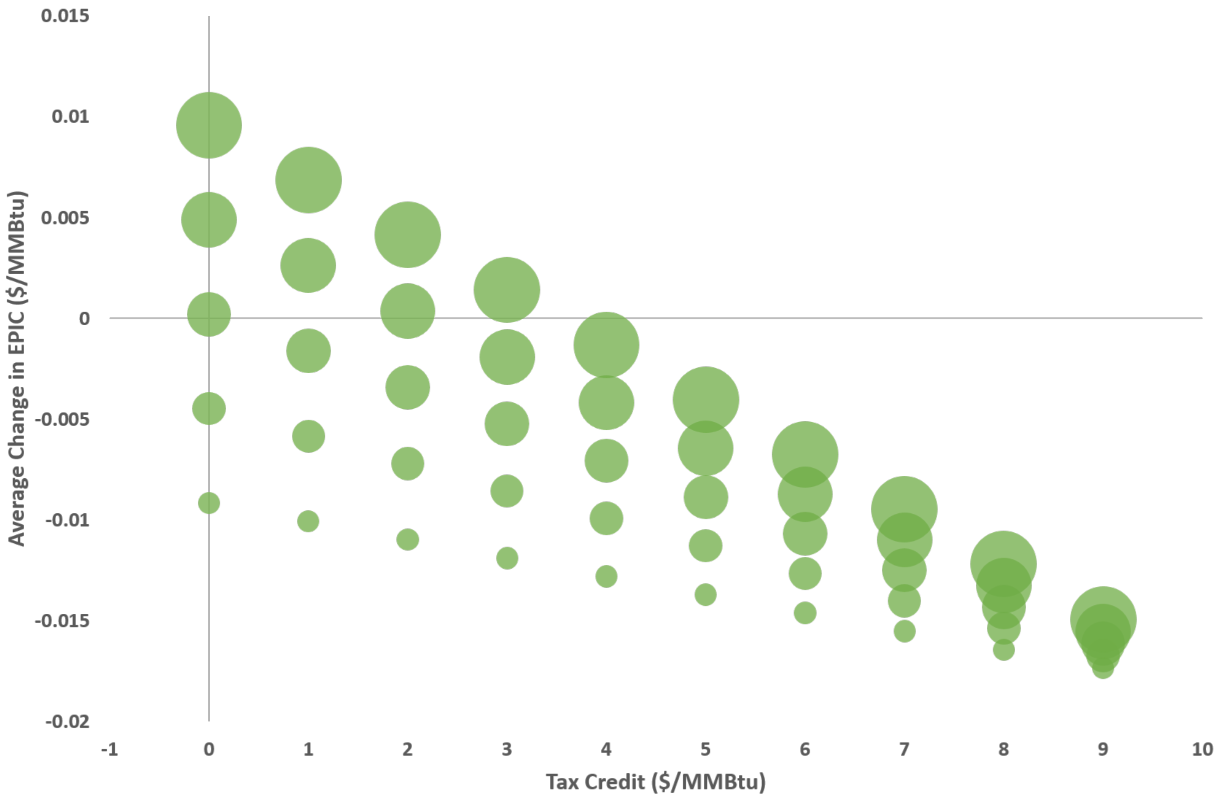


Figure G.6: Biomass Power at different Target Weights & Tax Credits, 2020-2024

The grid of results for biomass energy at different target weights and tax credits from 2020 to 2024 is shown in this figure. The contribution of biomass into the electric power sector is rather low, even at the maximum weight target (1.5%). Due to the relatively higher levelized cost of biomass energy, EPIC decreases at higher tax credit. At maximum weight (1.5%) and without tax credit, EPIC increases by 0.054% with no budget required, whereas at maximum weight (1.5%) and maximum tax credit ($9/MMBtu), EPIC decreases by 0.084% requiring around $1.9 billion annually from the government's budget.

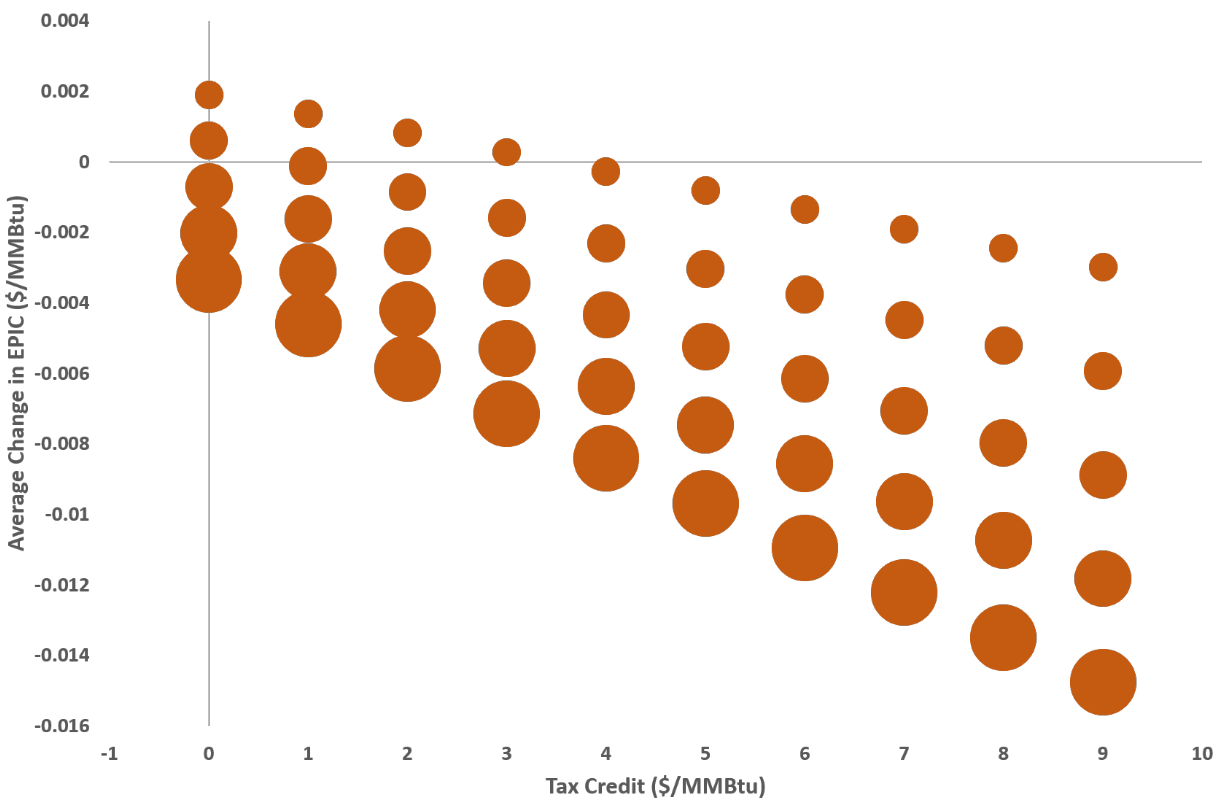


Figure G.7: Geothermal Power at different Target Weights & Tax Credits, 2020-2024

The grid of results for geothermal energy at different target weights and tax credits from 2020 to 2024 is shown in this figure. The contribution of geothermal into the electric power sector is limited, even at the maximum weight target (0.7%). Despite the fact that the levelized cost of geothermal energy is quite low, it has minimal effects on EPIC due to its limited availability as a source of energy in the power sector. At maximum weight (0.7%) and without tax credit, EPIC decreases by 0.019% with no budget required, whereas at maximum weight (0.7%) and maximum tax credit ($9/MMBtu), EPIC decreases by 0.083% requiring $887 million annually from the government's budget.

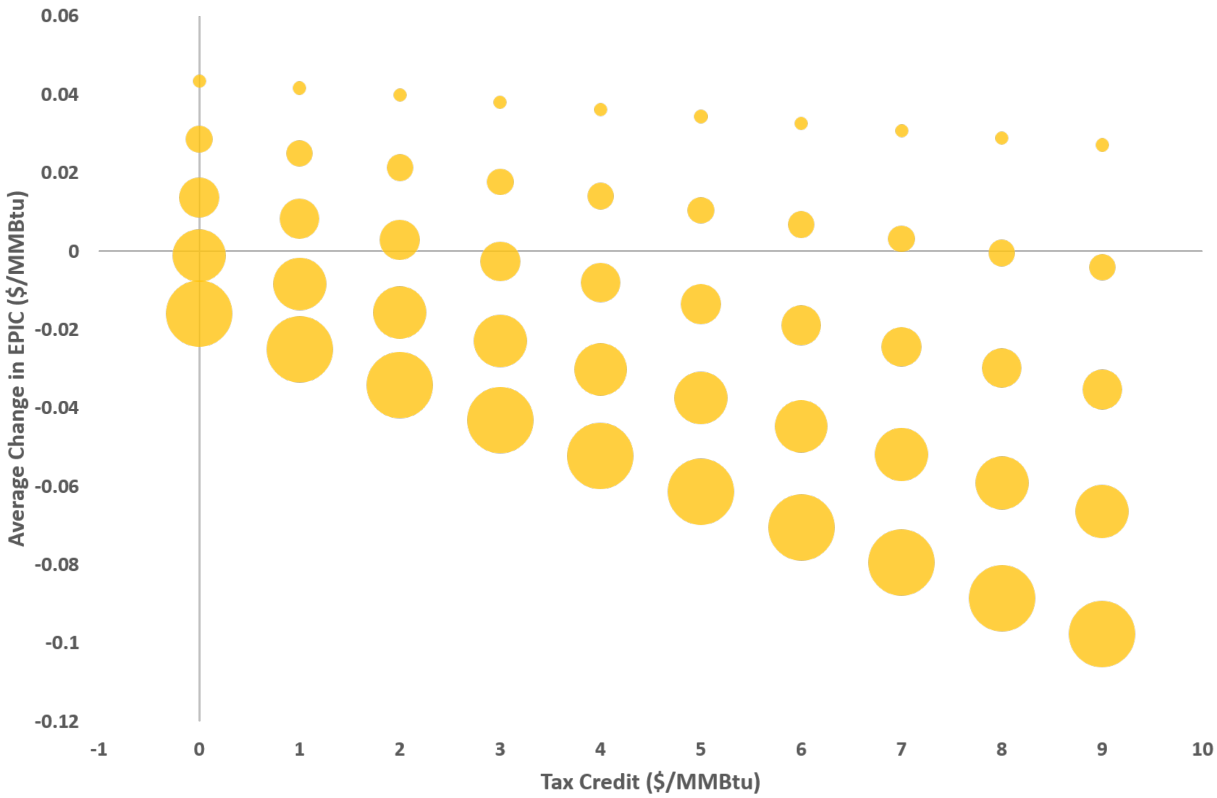


Figure G.8: Solar Power at different Target Weights & Tax Credits, 2020-2024

The grid of results for solar power at different target weights and tax credits from 2020 to 2024 is shown in this figure. The levelized cost of solar energy has decreased considerably over the years, resulting in decreasing EPIC even at low tax credit values. At maximum weight (5%) and without tax credit, EPIC decreases by 0.09% with no budget required, whereas at maximum weight (5%) and maximum tax credit ($9/MMBtu), EPIC decreases by 0.551% requiring more than $6.3 billion annually from the government's budget.

Table G.1: Weights and Levelized Cost of Energy Feedstocks for the Electric Power Sector

Feedstock	Average weight (%)	Minimum weight (%)	Maximum weight (%)	LCOE (2020$/MMBtu)
Coal	40.95	15.29	54.97	22.40
Natural Gas	25.21	11.72	43.12	15.34
Petroleum Liquids	1.26	0.42	4.45	67.78
Nuclear	20.45	17.27	22.93	21.95
Hydroelectric	7.03	4.28	10.68	15.47
Wind	3.51	0.19	11.24	11.71
Biomass	0.71	0.54	0.95	27.79
Solar	0.48	0.00083	3.32	9.71
Geothermal	0.40	0.31	0.50	10.38

The weights of the different energy feedstocks are taken from the EIA Monthly Energy Review [77] for the period from January 2003 to June 2020. The levelized cost of the energy feedstocks is taken from the Lazard's Levelized Cost of Energy Analysis report for the period from 2008 to 2013 [169, 170, 171, 172, 173, 174] and the EIA Annual Energy Outlook for the period 2014 to 2020 [175, 176, 177, 178, 179, 180, 181] apart from the figures for the petroleum liquids which are also taken from the Lazard's Levelized Cost of Energy Analysis reports. The data from 2008 are used for the period from 2003 to 2007.

APPENDIX H

CIRCULAR ECONOMY SYSTEMS ENGINEERING*

H.1 Introduction

The concept of CE has captured the interest of governmental and inter-governmental organizations, decisions makers, academia and industry during the last years, however a recent review of over 114 definitions for CE illustrates a vagueness with regards to the definition as well as with regards to the actual perception of people working on this concept [252]. The same review highlights that only 40% of the CE definitions use a systems perspective to conceptualize it while another review suggests that a non-holistic approach could lead to ambiguous and contradicting conclusions [384]. Similar findings were made from another review which considers CE as an evolving as well as an umbrella concept which needs to unify definitions, principles, and boundaries [385] as well as metrics for monitoring framework [332]. This fact could explain the lack of robust mathematical and engineering methodology, even though someone would expect that such an approach is indispensable not only for the transformation of the corresponding processes and business models but also for the effective evaluation towards CE implementation/fulfillment.

H.2 Origin and Definition of Circular Economy

The origins of the CE concept cannot be easily traced back to a single author or date, but due to its potential applications to the modern economic and industrial world, the concept has gained momentum since the 1970s [27]. According to the same report [27], CE is based on 3 principles: a) design out waste, b) build resilience through diversity, c) rely on energy from renewable sources. However, and despite the fact that it seems a rather straight forward and easy to conceive term, in reality, it creates confusion among the involved parties including researchers, policymakers and practitioners. In particular, a review of 114 definitions for CE, revealed ambiguity on the framework and the principles which if not addressed promptly could potentially crash the concept [252]. Similar findings were reported in a review of 327 articles, where

*Reprinted from "Circular Economy-A challenge and an opportunity for Process Systems Engineering" by S. Avraamidou, S.G. Baratsas, Y. Tian, E.N. Pistikopoulos, Computers & Chemical Engineering, 2020, 133, p.106629, with permission from Elsevier and Copyright Clearance Center. A summary of the work is given in Chapter 5, with additional details provided here.

a lack of consensus and convergence on the terminologies and definitions was pointed out [386]. In the same review, an analysis of a sample of 35 definitions was presented and a "CE sample-based definition" was proposed. In an attempt to unify these definitions, Saidani et al. (2018) [323] proposed the following definition: "CE is an economic system that replaces the 'end-of-life' concept with reducing, alternatively reusing, recycling and recovering materials in production/distribution and consumption processes. It operates at the micro-level (products, companies, consumers), meso-level (eco-industrial parks) and macro-level (city, region, nation and beyond), with the aim to accomplish sustainable development, thus simultaneously creating environmental quality, economic prosperity and social equity, to the benefit of current and future generations".

H.3 The Key Features and Goals of Circular Economy

The goals and features of a CE can differ for different systems (e.g. organic vs non-organic cycles), but similar principles can be applied. The key features of CE have been recently identified and are listed below along with a description [182]:

1. *Reduction of material losses/residuals:* Waste and pollutants minimization through the recovery and recycle of materials and products.

2. *Reduction of input and use of natural resources:* The reduction of the stresses posed on natural resources through the efficient use of natural resources (e.g. water, land, and raw materials).

3. *Increase in the share of renewable resources and energy:* Replacement of non-renewable resources with renewable ones, limiting the use of virgin materials.

4. *Reduction of emission levels:* The reduction in direct and indirect emissions/pollutants.

5. *Increase the value durability of products:* Extension of product lifetime through the redesign of products and high-quality recycling.

Even though the economic and financial aspects do not appear as one of the main goals of the CE, the transition to such an economic model is expected to be economically sustainable. The elimination of waste could lead to significant cost savings in the production processes, create new sources of revenue from the distribution of the waste to new markets, as well as reduction in the resource dependency.

Moreover, the economic and financial objectives are not limited to the traditional approach of the cost minimization or profit maximization but has a wider and holistic objective. As per Ellen MacArthur Foundation, the transition to circularity has the potential to reveal an economic opportunity with a positive impact to all involved parties i.e. economies, companies, consumers and customers [27]. In particular, the significant net material and energy cost savings, the effective implementation of recycling that will reduce the volatility between the supply and demand and the relevant risks, along with the resilient economic growth through the minimization of the externalities will greatly benefit the economies.

Similarly, the companies will benefit from new profit pools in the reverse value cycles, the improved logistic services that put high emphasis in the material recycling systems and refurbishment of products as well as the new venues of financing and capital that will be required from the shift towards the tertiary sector. The transition to the CE will force the improvement of service quality, durability and reliability of the products which would eventually assist the appearance of new emerging trends of sharing, lending, swapping etc. that will benefit the end users and consumers. At the same time, increasing competitiveness among the companies will lead to greater variety of products and services, less hassles from obsolescence, as well as an overall improved company - customer interaction and loyalty that will benefit both of them.

H.4 Literature Review Process Systems Engineering and Circular Economy

This section focuses on tools and methods developed or widely used in the PSE community, such as modeling & optimization, life cycle assessment, and process integration and intensification and their potential in assisting in the transition from linear to circular supply chains H.1. The goal of this section is to highlight the relevant literature and identify research gaps and possible PSE research opportunities.

H.5 PSE Tools and Methods towards CE

H.5.1 Multi-Scale Modeling

CE supply chains are multi-spacial and multi-temporal (Section H.6.1), similar to other problems encountered by the PSE community. Process engineering could play a significant role in the growing CE, by utilizing in a multi-scale approach its key principles i.e. basic laws of mass and energy, entropy, mathematics, and system science, towards an integrated environmental, economic and social sustainable plan [387]. To this respect, the positive impact from the usage of multi-scale systems engineering into energy and environment has been already identified in the literature [73], without though referring to the CE term. A more

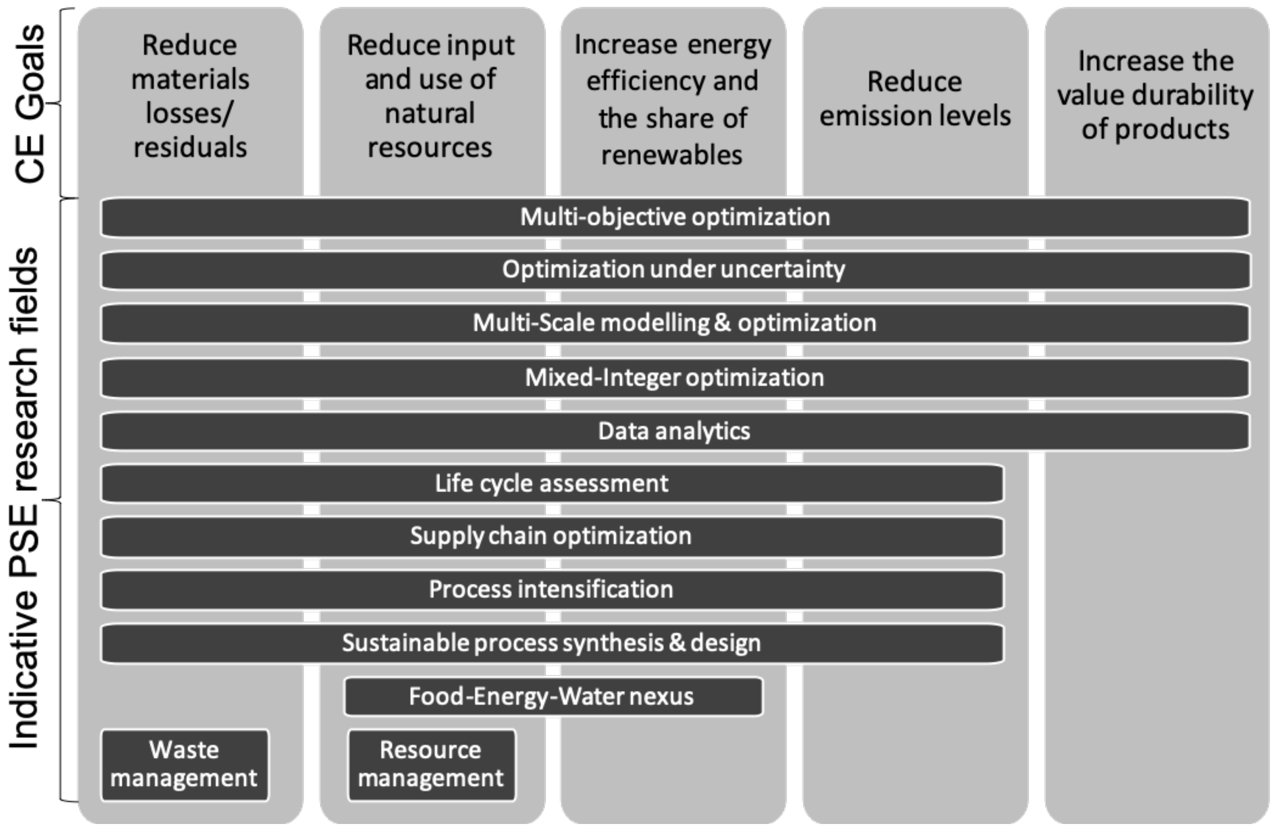


Figure H.1: Indicative PSE Research Fields with Potential Use in Achieving Different CE Goals

recent study presents a multi-scale framework for the optimized production of bio-gas and fertilizer from residues conducting a techno-economic as well as a supply chain network evaluation [197]. Moreover, the concept of Circular Integration as a unified methodology towards the sustainable development of processes, industries, and economies by applying a multi-dimensional, multi-scale approach for the minimization of the resource and energy consumption has been also proposed [198]. However, the social aspect of the CE should not be overlooked and must be integrated along with economic and ecological dimensions. Such an attempt was conducted through a multi-scale integrated analysis of societal metabolism in China, revealing a need for a more balanced development strategy and sector structure, combining the economic progress with the social welfare of the people [388]. This result is of particular interest since China was one of the pioneer's in adopting and promoting the CE terminology.

H.5.2 Life Cycle Assessment (LCA)

Any attempt towards analysis, modeling, implementation and/or assessment of the CE requires a holistic and structured approach that has Life Cycle Assessment (LCA) as an inherent attribute. Being an internationally standardized method, LCA quantifies all relevant emissions and resources consumed and the related environmental and health impacts and resource depletion issues that are associated with any goods or services [389], and has recently emerged as the main tool to evaluate sustainable development. Different researchers [390, 391] model processes and properly judge different options towards the implementation of CE [392]. As illustrated in Table 5.1, the PSE community has been using LCA approaches extensively and has been developing tools and methodologies around it. Extensions that would allow the consideration of the value durability of products in an LCA assessment would make this tool extremely useful for CE decision making and assessment.

H.5.3 Process Intensification

Process intensification (PI) have been gaining increasing momentum from the chemical engineering research community and the chemical/energy industry during the past several decades [393, 394]. Although there is also a significant lack of clarity on the scope and definitions of PI (see [395] and [396] for the summary and evolution of PI definitions), insights on the synergy between CE and process integration and intensification can still be gained through some representative definitions. One of the early definitions for PI refers to PI as "a methodology for making remarkable reductions in equipment size, energy consumption, or waste generation while achieving a given production goal" [397]. In another well-accepted definition, PI is recognized as "the development of novel apparatuses and techniques that are expected to bring dramatic improvements in manufacturing and processing, substantially decreasing equipment-size/production-capacity ratio, energy consumption, or waste production, and ultimately resulting in cheaper, sustainable technologies" [393]. From these definitions, it is obvious that process integration and intensification along with the CE share commonalities in reducing energy consumption, minimizing waste production, improving sustainability performance, reducing capital/operating costs, etc.

Moreover, PI aims to "substantially" improve chemical processes. For example, the Rapid Advancement in Process Intensification Deployment (RAPID) Manufacturing Institute has set as one of the evaluation metrics for the intensified process modules the achievement of 10x reduction in capital cost, 20%

improvement in energy efficiency, and 20% lower emissions/waste related to commercial state of the art. It is also worth noting the unique nature of process integration and intensification for innovation (i.e., novel process schemes and equipment), which renders PI an enriched design space to discover "out-of-the-box" process solutions [398]. Specifically from PSE's perspective, the development of systematic strategies and advanced computer-aided tools to assist quantitative decision making in PI applications has been the topic of many academic works, with considerations on energy savings [211], sustainability [216], waste minimization [210], emission reduction [222], etc.

H.6 Scientific Needs and Challenges in Circular Economy Research

Several challenges and scientific needs for PSE to assist in the convergence towards a CE have been identified. Major challenges arise in the modeling, optimization and decision making for supply chains and their transition from a linear to a CE. These challenges include: i) interconnected supply chains, ii) boundary selection, iii) multi-scale issues, iv) multiple stakeholders and objectives, v) uncertain and dynamic conditions and vi) no widely accepted assessment criteria among others. This section is focused on the discussion of some of those challenges.

H.6.1 Interconnected Supply Chains, Boundary Selection and Multi-Scale Issues

Product supply chains are highly interconnected making the selection of system boundary conditions very challenging. Similarly to LCA studies, system boundary definition plays a critical role in the context of the results from such an analysis. Circularity, in terms of CE, is a property of entire interconnected supply chain that includes the micro (consumers, companies), the meso (eco-industrial parks) and macro (city, nation) levels, therefore system boundaries should be greatly expanded beyond the traditional process boundaries the PSE community is currently exploring.

The extension of the boundaries introduces multiple scales, both spacial and temporal, with each level having the potential to impact the rest of the levels. For example, the operation of an industrial process unit (e.g. reactor, separator, etc.) can impact the operation of the whole industrial plant, and sequentially any other industry or consumer down the supply chain using the products of the first plant. The interaction between the different special and temporal scales introduces high complexities in the modeling and optimization of CE supply chains. Modeling and optimization of some of the individual scales have been widely explored by the PSE community (e.g. process units and industrial plants), although the consideration of individual levels neglects the connectivity between them and can lead to sub-optimal or even infeasible solutions.

Although multi-scale approaches have been developed in the PSE community (Section H.5.1), they were mainly applied to industrial case studies, that did not involve all scales relevant to CE, such as consumers at the household level or diplomatic relations at the global scale. Gaining knowledge for the modeling of such scales that have not yet being explored by the PSE community is a vital step for multi-scale modeling and optimization of CE supply chains.

Furthermore, highly interconnected CE supply chains, with expanded boundaries and multiple scales would consist of large-scale mixed-integer problems that are challenging to solve. Even though many tools and algorithms have been proposed for the solution of this class of problems [399, 400, 401] more efficient approaches must be explored.

H.6.2 Multiple Players and Objectives

Product supply chains are often managed by different companies, governments, and consumers. Figure H.2 shows that different stakeholders in a CE supply chain have competing interest and objectives. Furthermore, each entity can affect the actions and outcomes of the other entities; for example, a governmental policy can change the behavior of societies, such as their energy consumption patterns or diet preferences, affecting the demand of these utilities and products, and subsequently affecting the industries and businesses supplying those. In turn, the industries can lobby against these new policies and affect the governmental decision-making process. These multiple interconnected stakeholders and their differing or conflicting objectives introduce major challenges in modeling and decision making, requiring game theoretic approaches, such as multi-agent hierarchical optimization that require a Stackelberg equilibrium for their solution [402, 403, 404].

Even though the economic objectives of companies have been widely studied by the PSE community, the consideration of the interest of the wider range of the stakeholders involved in a CE supply chain, such as consumers, regulators and local authorities has not being explored by the PSE community yet, making the modeling of such supply chains even more challenging.

H.6.3 Dynamic and Uncertain Conditions

In the existing unstable environment, with constantly changing market conditions and customer needs and expectations along with climate change, it is of high importance to consider the effect of uncertainties

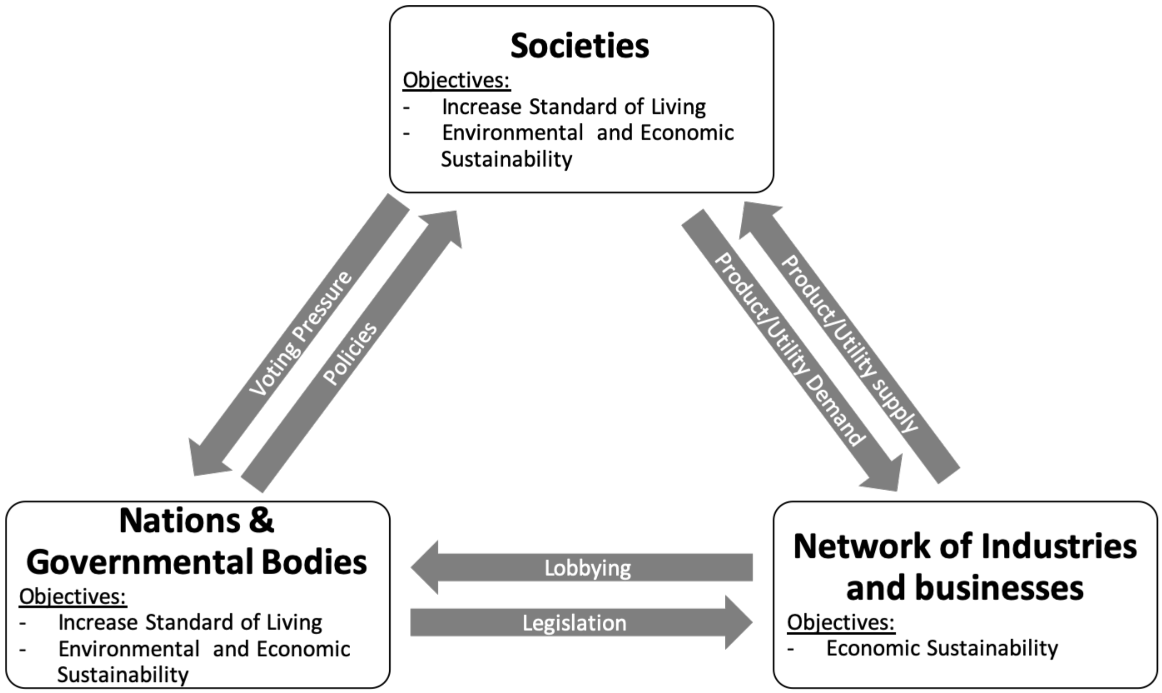


Figure H.2: CE Stakeholders, their Interconnections and Conflicting Objectives

when modeling a CE supply chain. Sources of uncertainty in a CE supply chain may include variations in processing rates, canceled or rushed orders, equipment failure, raw material, final product or utility price fluctuations, demand variations and climate changes [405]. Failure to consider these uncertainties can lead to unsatisfied costumer's demands and loss of market share by the industries and businesses involved along with environmental costs. Therefore, considering these uncertainties and their effect appropriately in the modeling of CE supply chains is critical but can result in new technical challenges as the size and complexity of the models is increased.

A number of publications have been devoted to studying supply chain planning under demand uncertainty or price fluctuations in the PSE community [406, 405, 407, 378], although not the same attention has been given to other sources of uncertainties, such as population growth or raw material depletion. Climate change has also received a lot of attention as many researchers focus on the development of inherently safer processes and network designs that can withstand extreme weather events, thus reducing the human, economic, and environmental costs [408, 409].

Key methodologies behind the approaches listed above are robust and stochastic programming [410, 411]. These fields have been widely explored by PSE and other communities with the development of approaches for the solution of different classes of optimization problems under uncertainty such as adjustable robust optimization [381, 412, 413], and multi-stage stochastic optimization [414, 415].

H.6.4 Assessment Criteria

A method for evaluating and comparing different CE pathways and scenarios is vital for effective decision making. In the literature, a selection of metrics relevant to CE has been collected and evaluated [332]. These metrics were developed for measuring different aspects of CE but not CE holistically, i.e. a CE metric limited to the flow of materials [416]. Tools have also been developed that can be used to track the transition of nations towards a CE and circularity of materials [417, 334, 335, 28, 418, 348]. Despite the availability of metrics, CE has only been measured at national or material levels with the main focus on material flows, while no metric is currently applicable at the product supply chain level or company level, therefore efforts for the development of a CE metric that can be effectively used in decision making should be made.

H.7 Motivating Case Study - The Supply Chain of Coffee

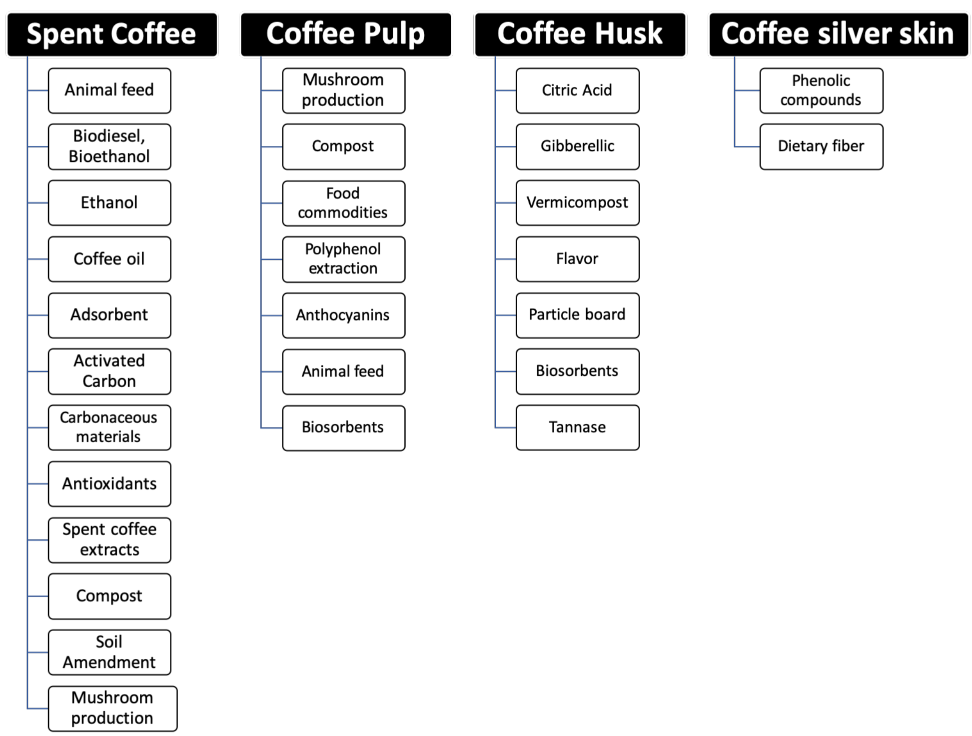


Figure H.3: Alternative Product Pathways from Organic Coffee Waste [3, 4]

H.7.1 Challenges and Opportunities for PSE

The transition of the coffee supply chain from a linear to a CE consists of many challenges but at the same time many opportunities for PSE. This section summarizes some of these challenges and the corresponding research opportunities for PSE.

Assessment of Multiple Pathways. As discussed in section 5.4.1.1, there are a lot of different pathways developed for the utilization of organic waste created along the supply chain of coffee (Figure H.3). The huge amount of waste generated annually in the production of coffee along with the large number of alternative pathways available for waste utilization requires sophisticated waste management plans for optimal operation. Furthermore, many of the illustrated pathways have been reviewed and demonstrated mainly at a lab scale [3, 4, 297], making them not reliable on a larger meaningful scale. Modeling and optimization can be used to predict the technical and economic feasibility of these pathways at a larger scale. A techno-economic analysis of the different pathways will require collaborative work between PSE and experimental scientist working on the different utilization pathways, in conjunction with industry to identify which of these processes are technically and economically viable and can add value to both the industries and the environment.

Similarly to waste management, there are different pathways for coffee harvesting, processing, and packaging. Process integration and intensification may be able to develop further integrated and intensified processes for the processing of coffee that are more energy and resource efficient. A methodology to holistically evaluate these different pathways is of great importance. CE assessment metrics along with superstructure representations and optimization of the alternative coffee supply pathways would be necessary tools for preliminary screening of the different technologies. Using these as the first step, more detailed models can be built for further and more reliable assessment of the most promising coffee supply chain pathways.

Multiple Stakeholders. The coffee supply chain involves different stakeholders, small and bigger coffee farmers, coffee bean processing industries, exporters and importers, coffee roasting industries, coffee waste management companies, coffee shops, beverage companies, and other vendors along with consumers at different demand centers, different governments, and nations (Figure H.4). Farmers and industries are focusing on increasing their profits, while regulators and policymakers can have multiple objectives including the minimization of environmental impact in their nation, the cost of coffee for their societies and the maximization of profit for their farmers and industries (Figure H.2). Consumers, on the other hand, are focusing on enjoying the best cup of coffee at the most 'reasonable' price, although the brand loyalty should not be overlooked. Studies in different industries have shown that loyal customers are less price sensitive, they are frequent buyers of current products and willing to try new products and services, while at the same time they bring in new customers [419]. Another study [420], revealed that loyal customers can boost company's revenues since a 5% increase in customers' retention leads to a surge of 25-75% in profit. Moreover, the cost to attract a new customer is 5 times higher than to maintain an existing one [421]. In the coffee industry, the brand loyalty has emerged as a crucial factor for the sustainability and growth of the coffee organizations in today's extremely competitive, international business environment. In particular, brand satisfaction was indicated as the most important contributor to building brand loyalty, while cognitive and affective factors such as brand awareness, brand image, pleasure and arousal, along with relationship commitment are the rest of the key drivers towards building brand's loyalty.

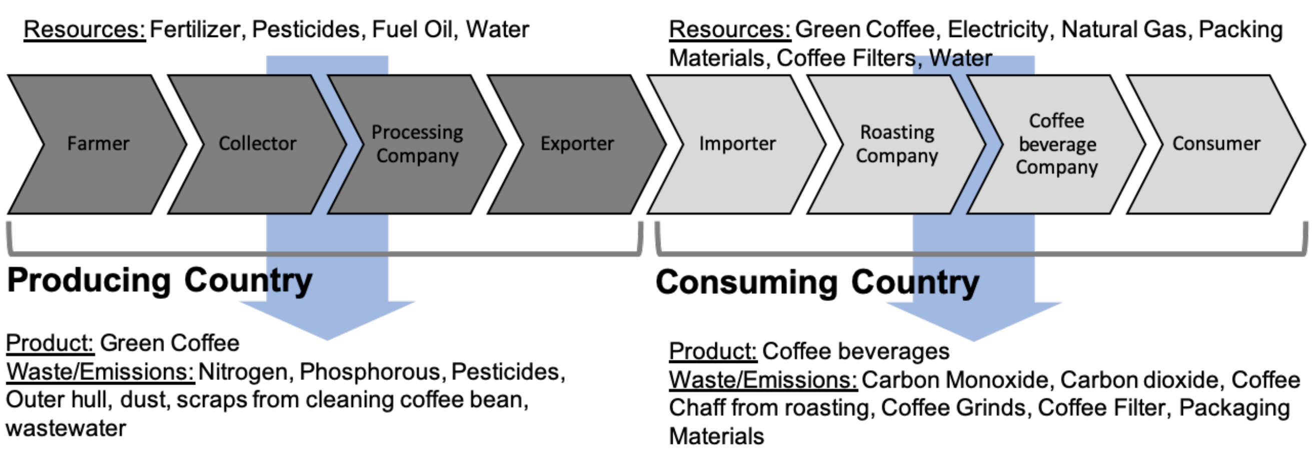


Figure H.4: Example of the Chain of Stakeholders in a Coffee Supply Chain

Besides that, there is a hierarchy in the decisions taken by the different stakeholders. For instance, policymakers can come up with a new policy on the type of fertilizers allowed for coffee farming. Then, the farmers can increase the price of the coffee beans if the new fertilizers are more expensive, and eventually this change in coffee bean price will gradually climb up the ladder, potentially reaching the consumers. On the other hand, importers might choose to import more coffee from another nation that has cheaper coffee beans. Coffee brands might not be willing to switch to different coffee beans unless it becomes absolutely mandatory since this is going to affect their final product and potential harm their brand loyalty. Consumers might potentially not like the new coffee or do not want to pay more for the coffee they were used to having, and as a result the fluctuating demand for the different types of coffee will affect all stakeholders involved.

Consequently, a global shift from the current linear, throwaway model to a circular, restorative/recycle model is necessary and shall be viewed from all parties involved as a pioneering and rewarding opportunity in the 21st century. The scarcity of resources and the environmental standards have become a reality and will continue to be on the top of the agenda. At the same time, a shift in the consumers' behavior in the direction of a greener and more environmentally friendly ecosystem of products and services has taken place.

Both public and private sectors though should closely collaborate making this a smooth transition. Governments and policy makers shall adjust the rules, advance the taxation and regulatory environment, setting the direction to a circular and international model and at the same time provide incentives that promote innovation and entrepreneurship. Furthermore, the private firms shall take advantage of the quickly altering business environment, and advance their recycling technologies, redesign their business models, optimize their supply chain networks, minimize their dependence in depleted resources, re-brand their products and services so as to attract new customers and eventually re-position themselves in the global market [27]. In a recent report, the U.S. Chamber of Commerce Foundation Corporate Citizenship Center along with the Ellen MacArthur Foundation illustrated an extensive list of companies that utilize the principles of CE in a profitable and rewarding way [422]. Apparently, the adoption and incorporation of the CE could generate an estimated of over 1 trillion US dollar annually by 2025, create 100,000 new jobs and prevent 100 million tonnes of materials waste within five years [324].

Therefore, hierarchical and multi-objective optimization will be needed to model this highly interconnected supply chain. Such formulations would make both modeling and solving the coffee supply chain problem very challenging. Multi-objective strategies developed and used in the PSE community can be directly applied to this problem. PSE community has focused on the solution of two or three level hierarchical optimization systems [423, 383, 424, 382], thus a focus on extending the methodologies developed for problems with more hierarchical levels and decision players is of great importance.

Multi-scale modeling. The coffee supply chain is spanning different countries as most of the coffee in the market is produced in a different country than the one that it is consumed (Figure H.4). Based on the UN Comtrade Database, in 2017 more than 30% of the total production of coffee was produced in Brazil and it was exported and consumed in 108 different countries.

The multi-spacial and multi-temporal nature of the coffee supply chain introduces challenges in modeling and optimization. Multi-scale modeling approaches that would allow multi-spacial and multi-temporal considerations in supply chain modeling need to be further developed. Effective decomposition methods for the large scale models that will be created will also be vital for the solution of the optimization problems.

APPENDIX I

CIRCULAR ECONOMY FOOD SUPPLY CHAIN FRAMEWORK

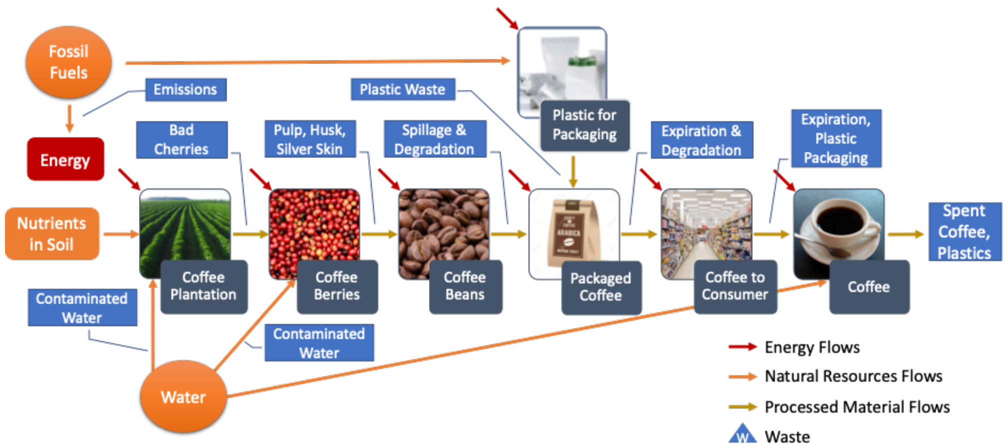


Figure I.1: Simplified Linear Supply Chain of Coffee

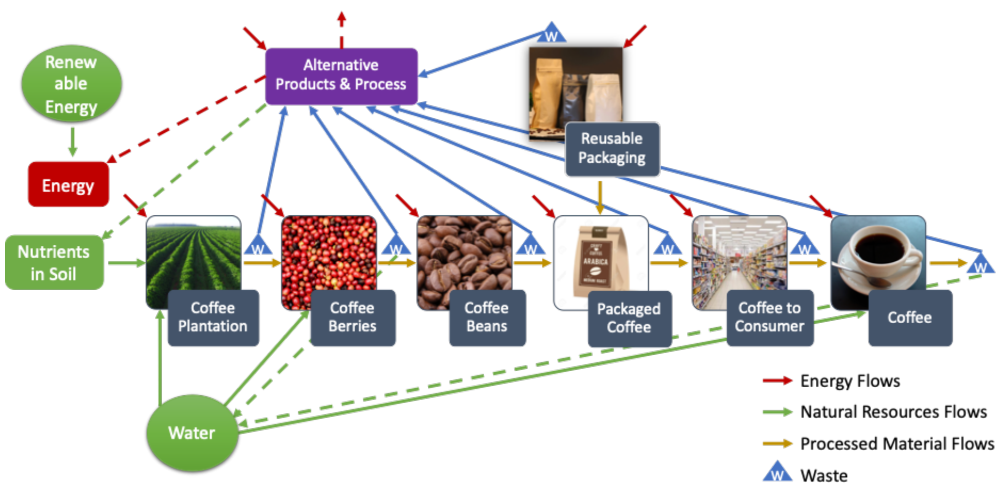


Figure I.2: Simplified Circular Supply Chain of Coffee. Dashed lines refer to the energy and resource flows that return to the supply chain.

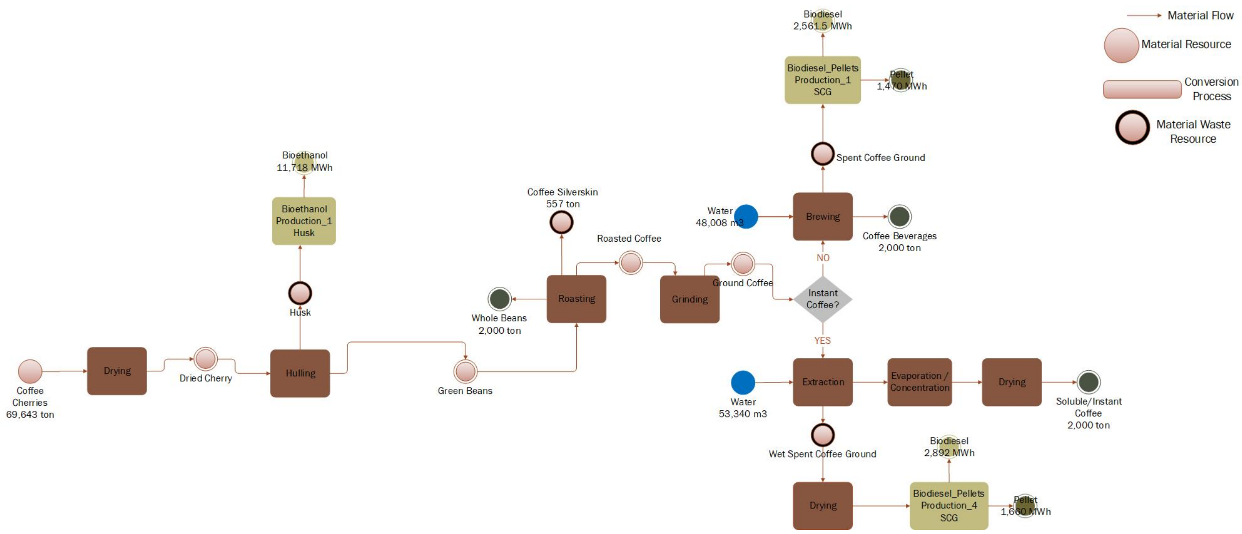


Figure I.3: Optimal Solution of Single Objective Problem 1: Min Waste Generation (CWG) of the supply chain under Scenario 1.
[5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19]

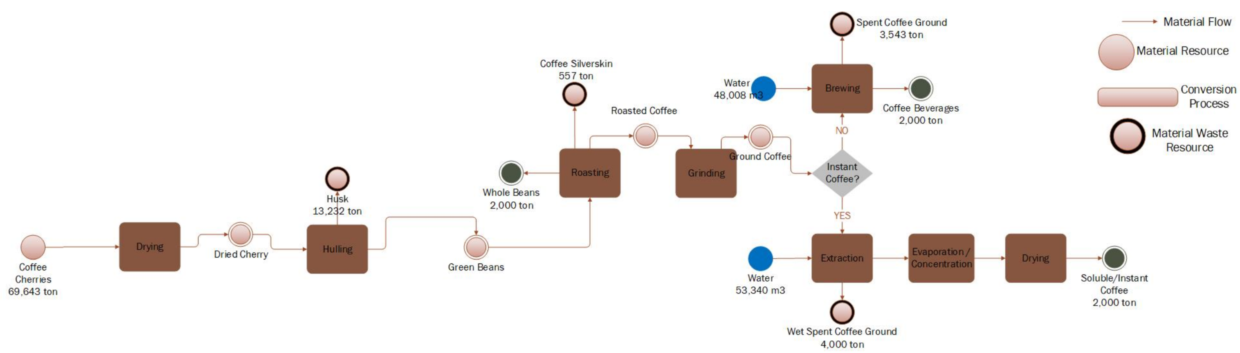


Figure I.4: Optimal Solution of Single Objective Problem 2: Min Coffee Cherries Consumption (CCC) of the supply chain under Scenario 1.
[5, 6, 7, 10, 13, 14, 16, 17, 19]

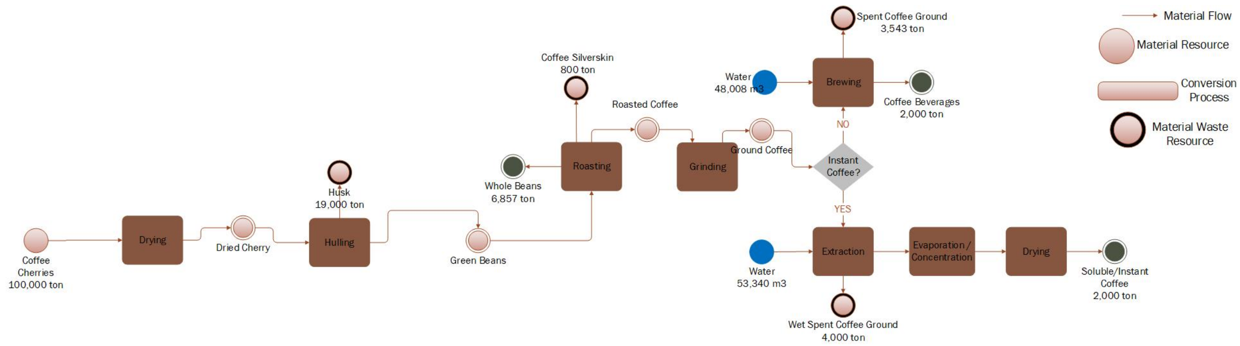


Figure I.5: Optimal Solution of Single Objective Problem 3: Min Water Consumption (CWC) of the supply chain under Scenario 1.
[5, 6, 7, 10, 13, 14, 16, 17, 19]

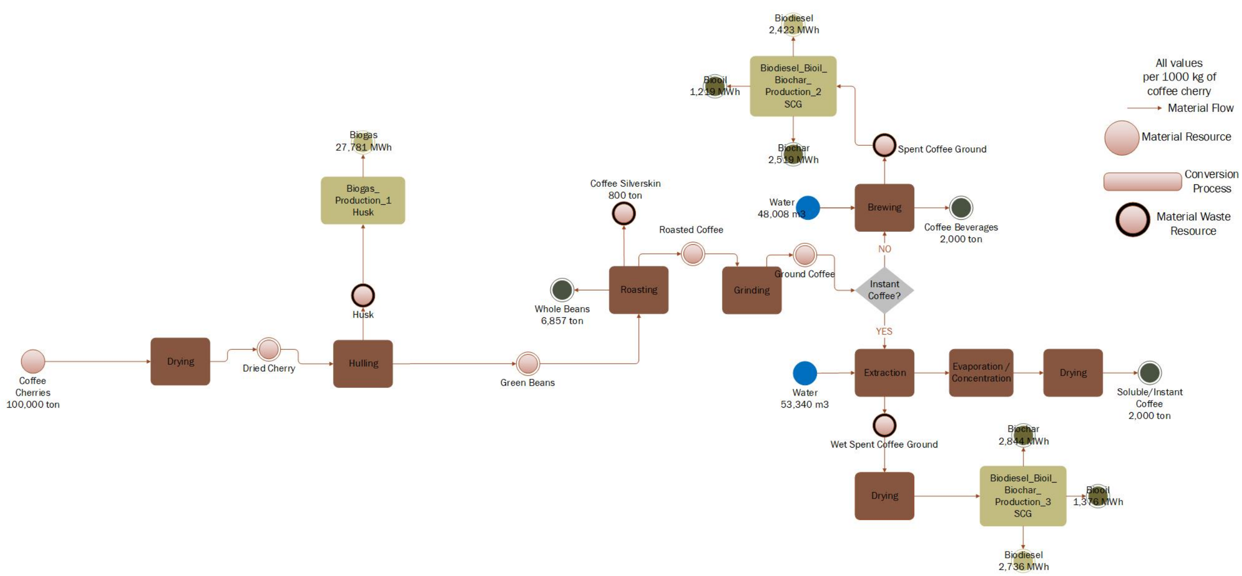


Figure I.6: Optimal Solution of Single Objective Problem 4: Max Energy Output (CEO) of the supply chain under Scenario 1.
[5, 6, 7, 20, 8, 9, 10, 11, 21, 12, 13, 14, 15, 16, 17, 18, 19]

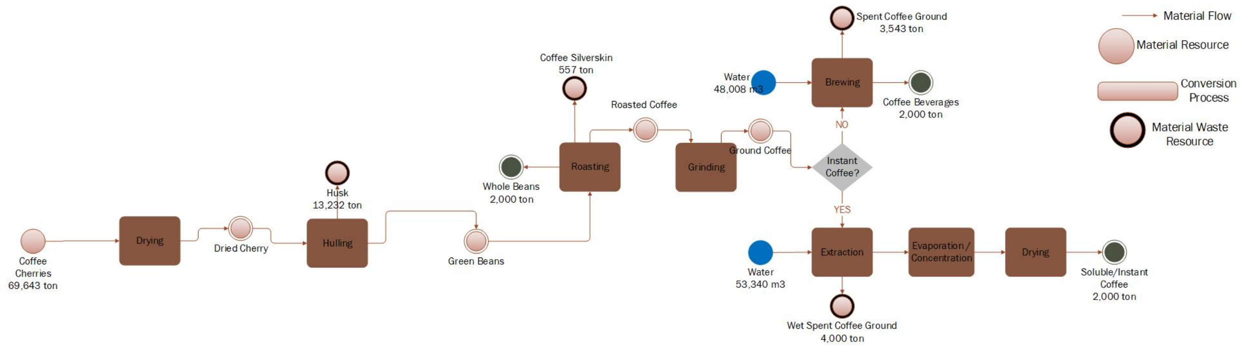


Figure I.7: Optimal Solution of Single Objective Problem 5: Min CO_2 Emissions (CEM) of the supply chain under Scenario 1.
[5, 6, 7, 10, 13, 14, 16, 17, 19]

Figure I.8 reveals the results of a trade-off analysis for the multi-objective problem 2 (Eq. (9)) (Chapter 6) of minimizing the coffee cherries consumption while minimizing the waste generation (minCCC & minCWG), subject to the constraints of the coffee supply which are described by Eqs. (1) - (2).

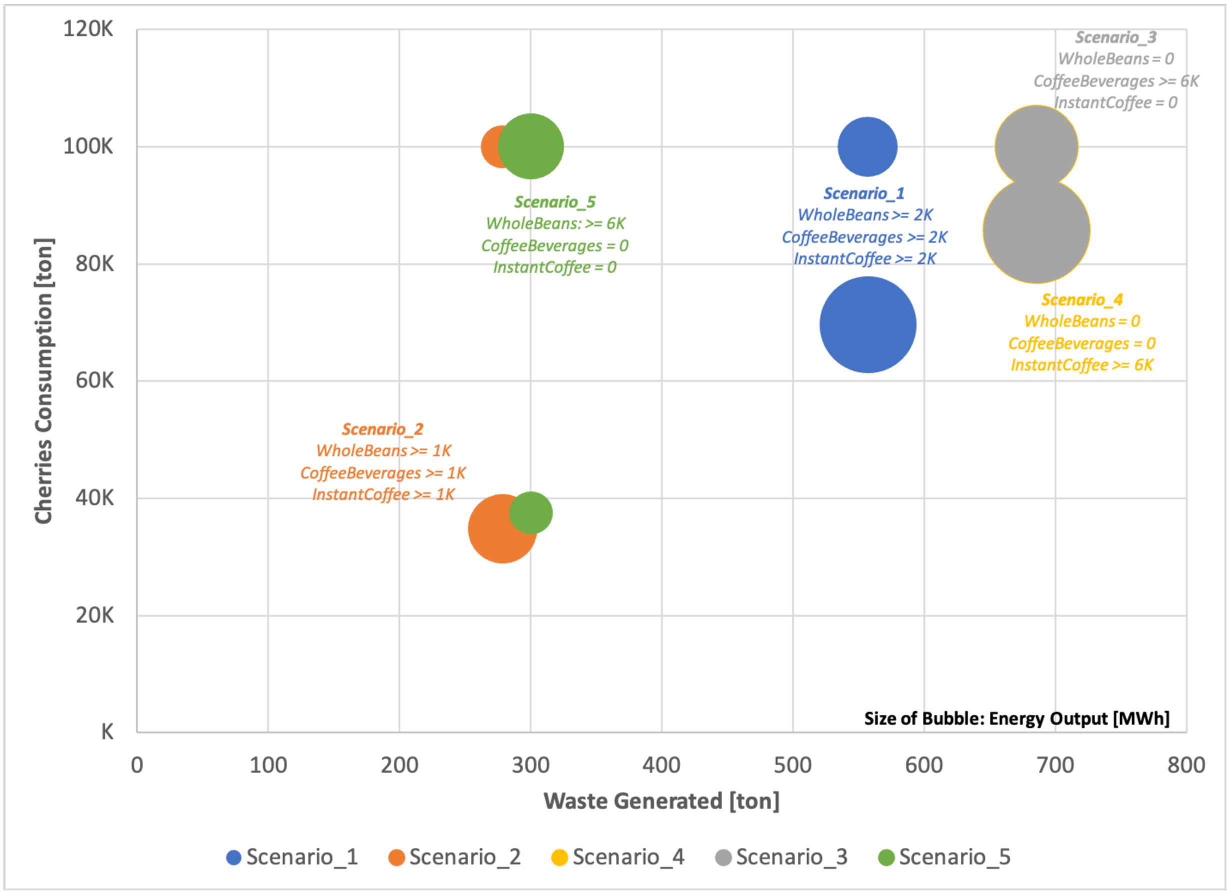


Figure I.8: Pareto Analysis for Problem 2: Min Coffee Cherries Consumption (CCC) & Min Waste Generation (CWG) & Energy Output

Figure I.9 reveals the results of a trade-off analysis for the multi-objective problem 3 (Eq. (10)) (Chapter 6) of minimizing the waste generation while maximizing the total energy output (min CWG & max CEO), subject to the constraints of the coffee supply which are described by Eqs. (1) - (2).

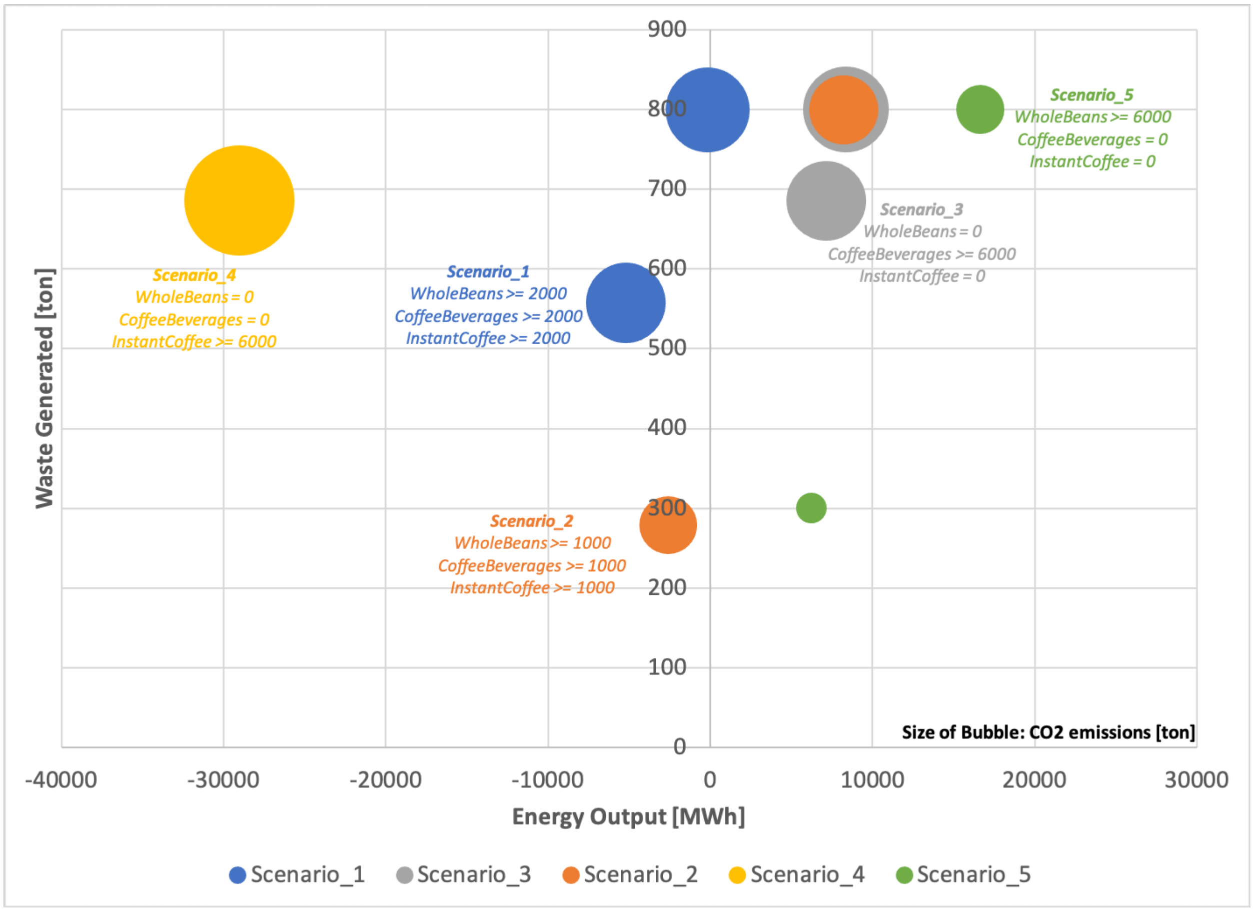


Figure I.9: Pareto Analysis for Problem 3: Min Waste Generation (CWG) & Max Energy Output (CEO) & CO_2 Emissions

Figure I.10 reveals the results of a trade-off analysis for the multi-objective problem 5 (Eq. (12)) (Chapter 6) of minimizing the emitted CO_2 emissions while maximizing the total energy output (min CEM & max CEO), subject to the constraints of the coffee supply which are described by Eqs. (1) - (2).

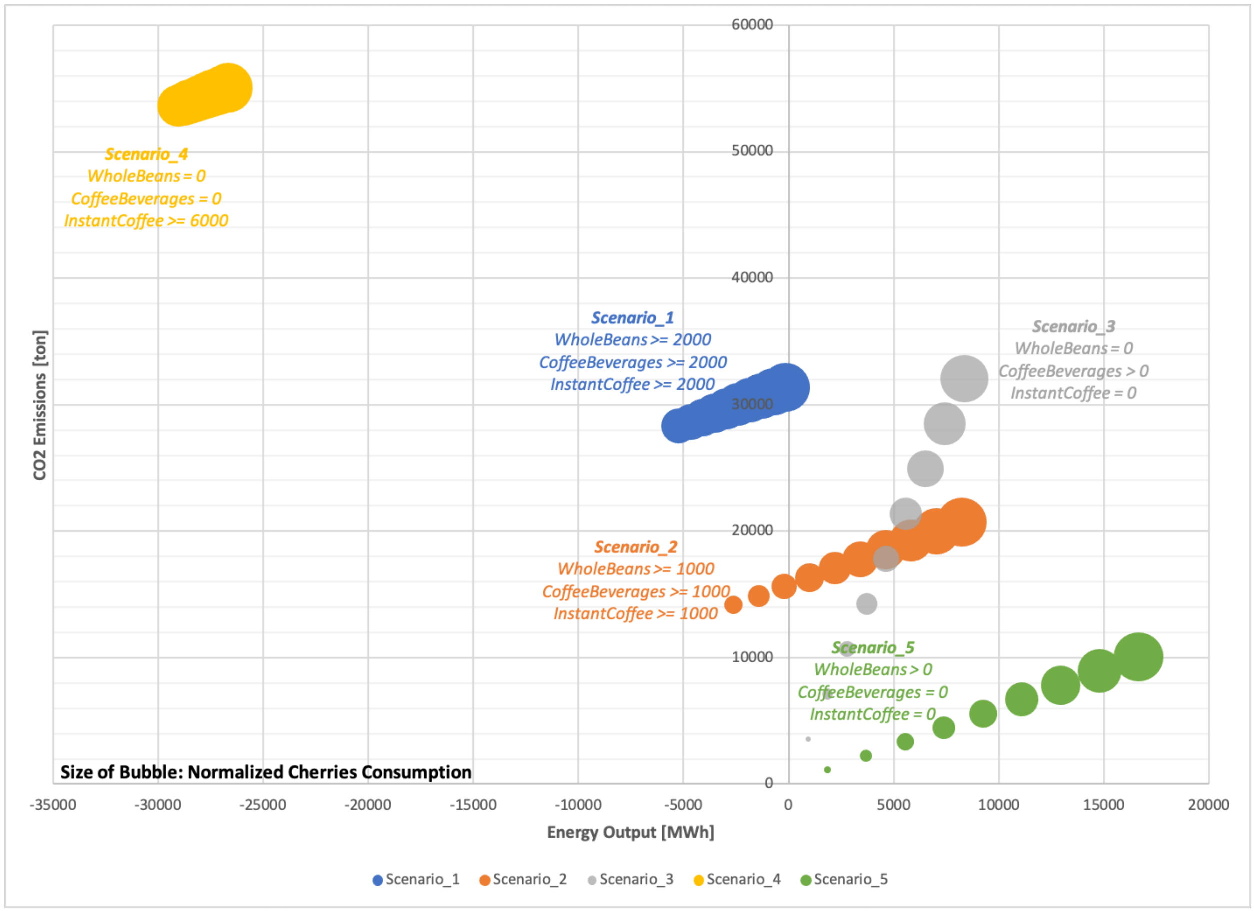


Figure I.10: Pareto Analysis for Problem 5: Min CO_2 Emissions (CEM) & Max Energy Output (CEO) & Normalized Coffee Cherries Consumption

Figure I.11 expands the results of a trade-off analysis for the multi-objective problem 1 by incorporating three different values (low, average, high) for the parameters of the drying process [19, 306]. As the values of parameters in the drying process increase, the optimal solutions require more energy to meet the demand scenarios. For the scenarios 1 and 2 where demand for all three final products must be met, the higher values of parameters in the drying process result into just one optimal point since the consumption of more cherries will deteriorate the energy balance.

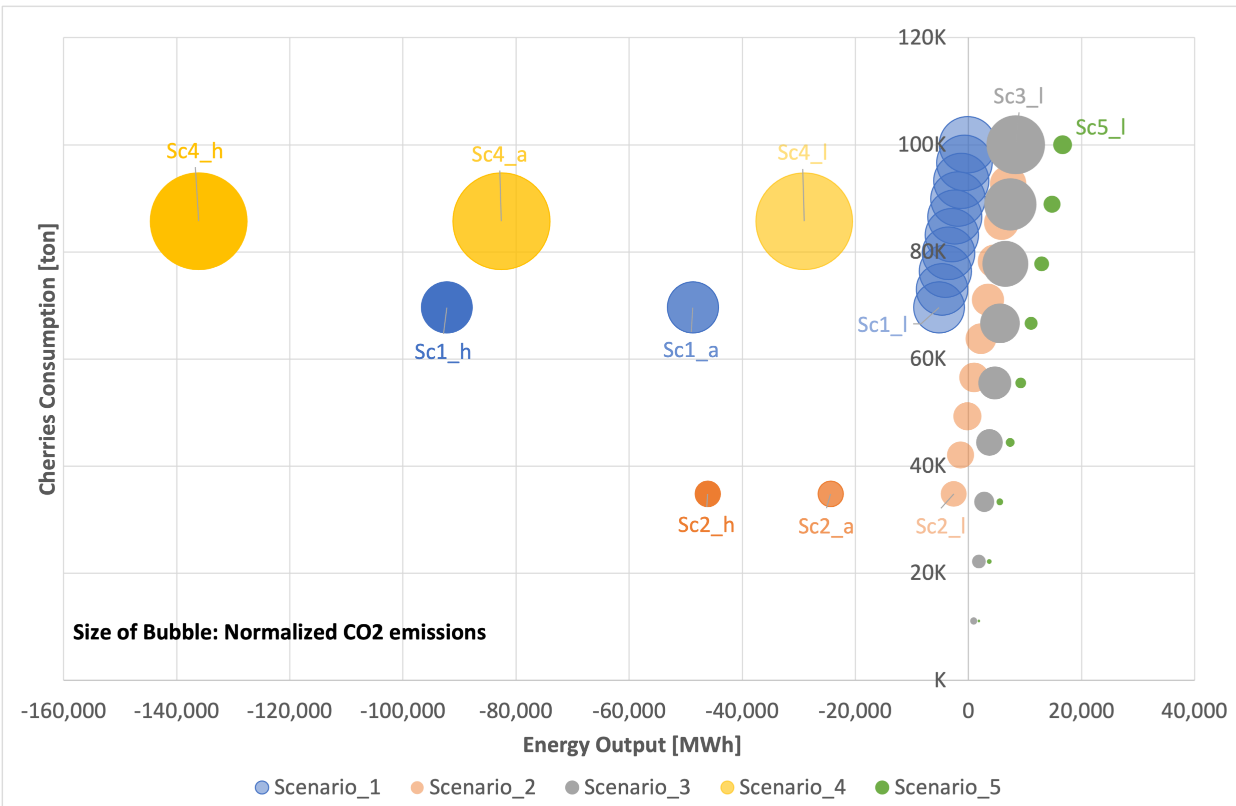


Figure I.11: Pareto Analysis for Problem 1 with Uncertain Parameters for the Drying Process: Min Coffee Cherries Consumption (CCC) & Max Energy Output (CEO) & Normalized CO_2 Emissions

Figure I.12 expands the results of a trade-off analysis for the multi-objective problem 3 by incorporating three different values (low, average, high) for the parameters of the drying process [19, 306]. Similar findings with the previous analysis hold true. Thus, as the values of drying parameters increase, more energy is needed to meet the demand scenarios. Since the objectives refer to the minimization of waste and maximization of energy output, the higher values of drying parameters result in single optimal points for scenarios 1, 2 and 4 because the consumption of more coffee cherries will only increase the waste generation and reduce the energy output.

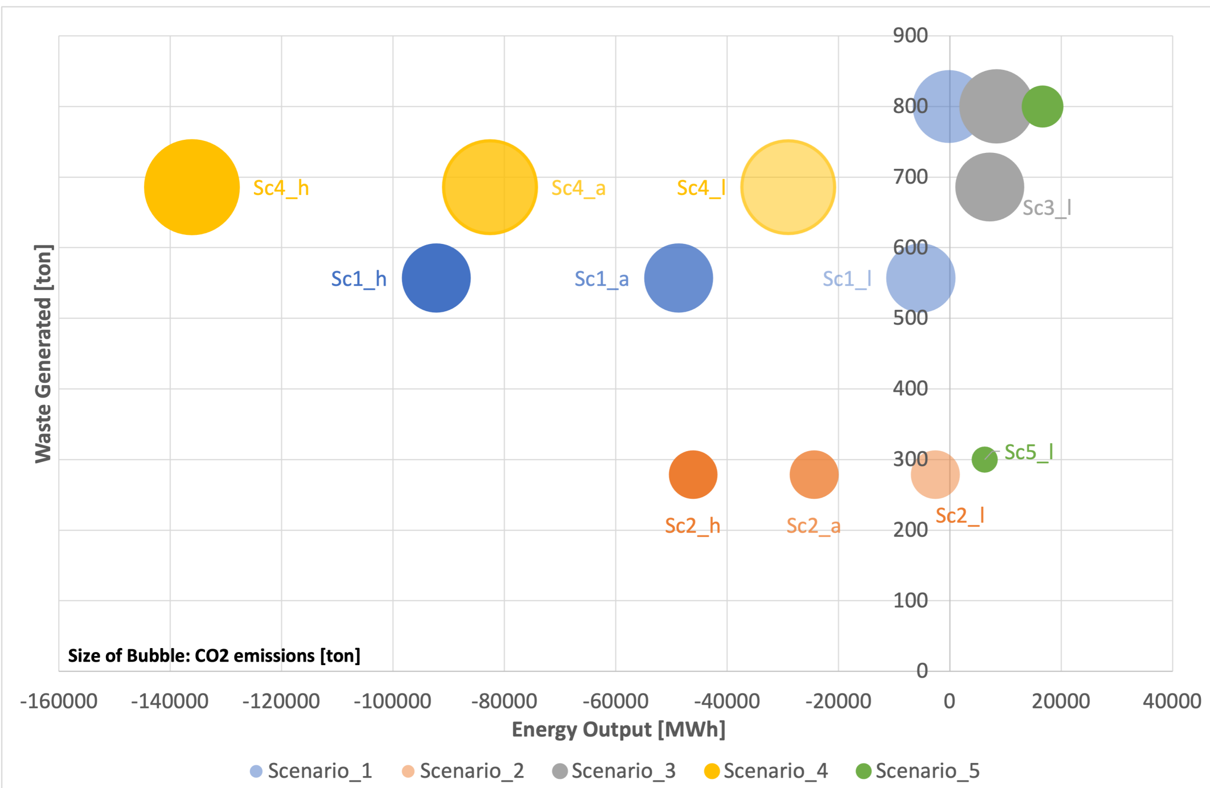


Figure I.12: Pareto Analysis for Problem 3 with Uncertain Parameters for the Drying Process: Min Waste Generation (CWG) & Max Energy Output (CEO) & CO_2 Emissions

Table I.1: Coffee Cherries Supply and Final Coffee Products Demand Scenarios

	Units	Scenario 1	Scenario 2	Scenario 3	Scenario 4	Scenario 5
Coffee Cherries	**ton**	$\leq$ 100,000	$\leq$ 100,000	$\leq$ 100,000	$\leq$ 100,000	$\leq$ 100,000
Whole Beans	**ton**	$\geq$ 2,000	$\geq$ 1,000	0.00	0.00	$>$ 0.00
Coffee Beverages	**ton**	$\geq$ 2,000	$\geq$ 1,000	$>$ 0.00	0.00	0.00
Instant Coffee	**ton**	$\geq$ 2,000	$\geq$ 1,000	0.00	$\geq$ 6,000	0.00

Note: For the multi-objective optimization problems 2 and 3, the demand of coffee beverages in scenario 3 is higher or equal to 6,000 ton, while the demand of whole beans in scenario 5 is higher or equal to 6,000 ton.

APPENDIX J

CIRCULAR ECONOMY ASSESSMENT FRAMEWORK

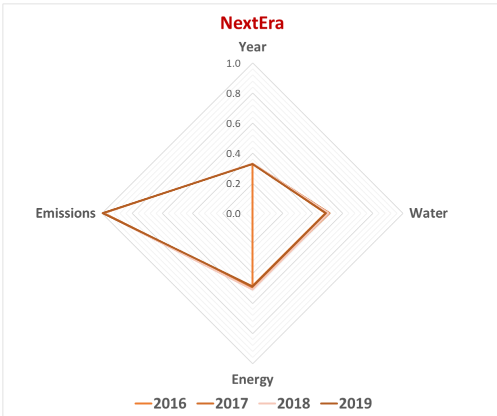


Figure J.1: NextEra Category-based Circularity Sub-Indices for 2016-2019

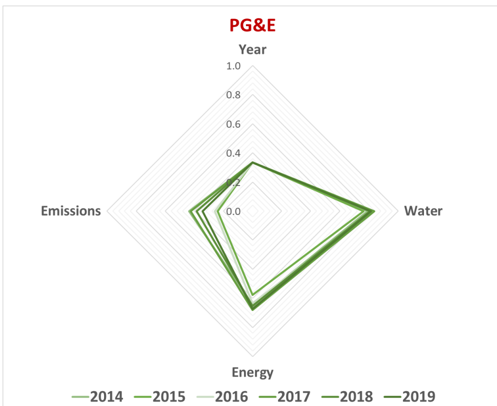


Figure J.2: PG&E Category-based Circularity Sub-Indices for 2014-2019

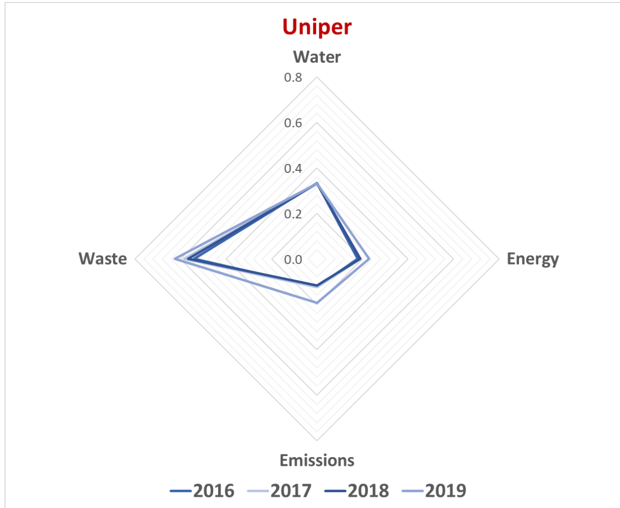


Figure J.3: Uniper Category-based Circularity Sub-Indices for 2016-2019

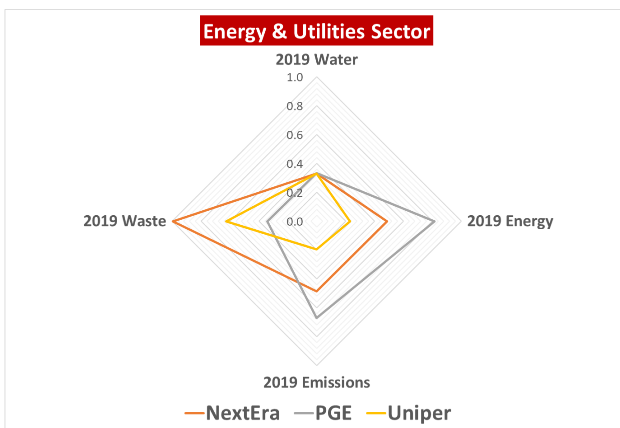


Figure J.4: Energy & Utilities Category-based Circularity Sub-Indices for 2019

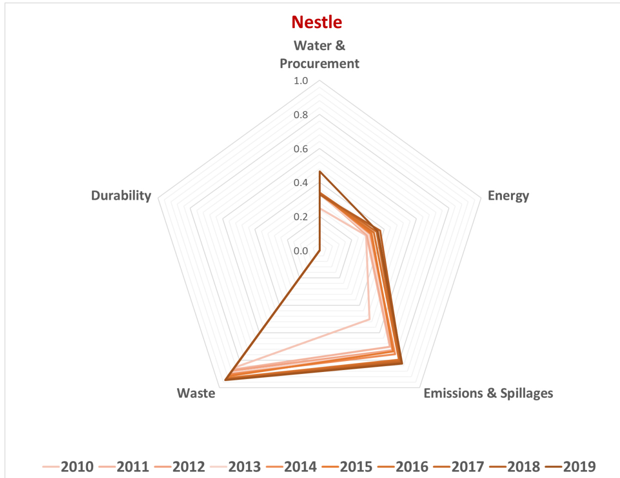


Figure J.5: Nestle Category-based Circularity Sub-Indices for 2010-2019

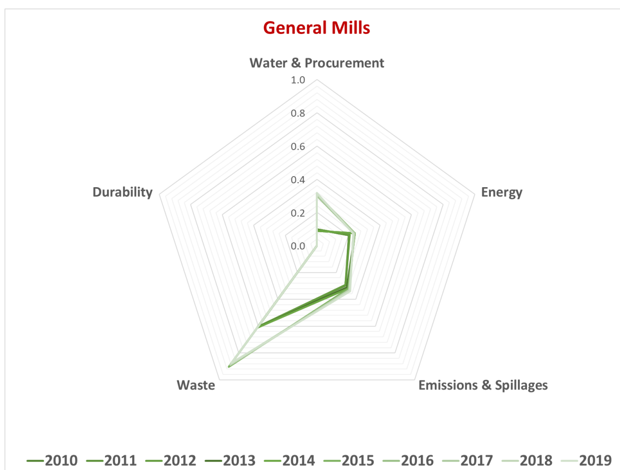


Figure J.6: General Mills Category-based Circularity Sub-Indices for 2010-2019

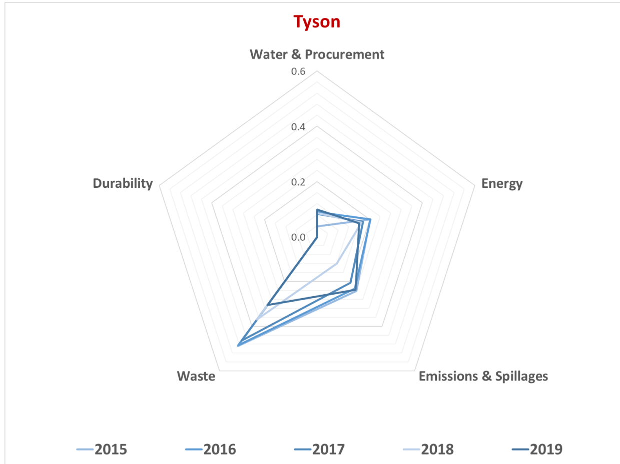


Figure J.7: Tyson Category-based Circularity Sub-Indices for 2015-2019

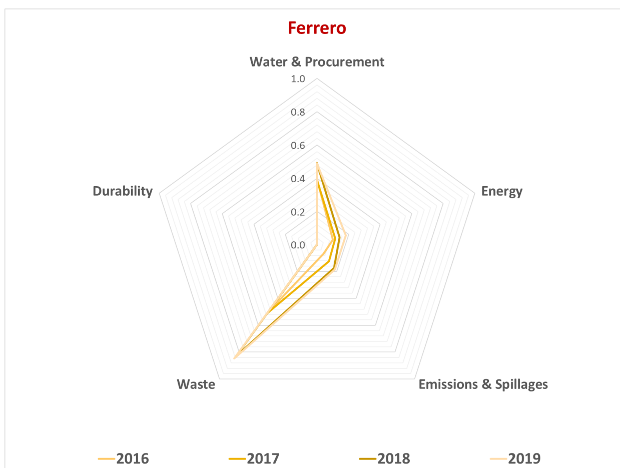


Figure J.8: Ferrero Category-based Circularity Sub-Indices for 2016-2019

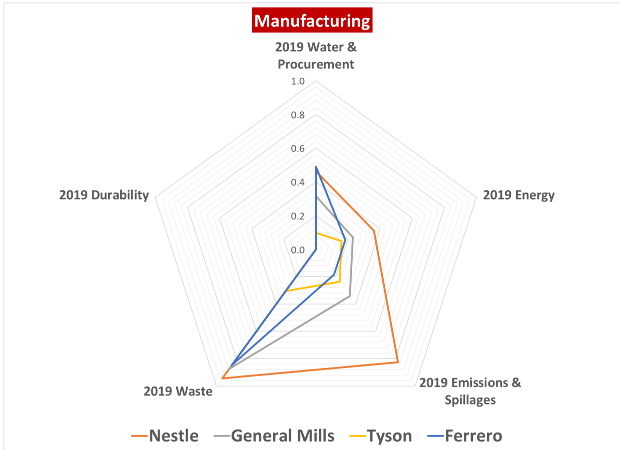


Figure J.9: Manufacturing Category-based Circularity Sub-Indices for 2019

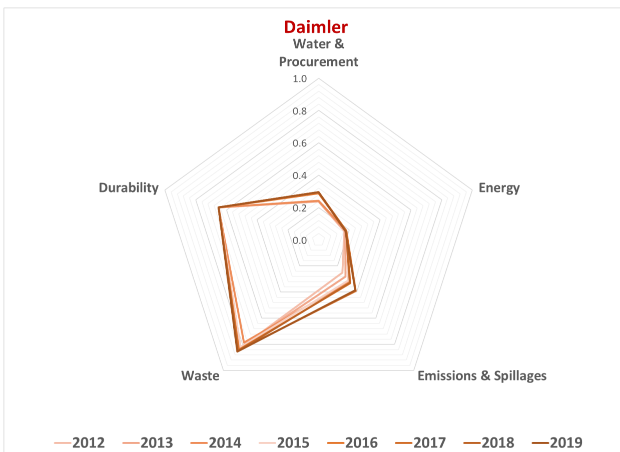


Figure J.10: Daimler Category-based Circularity Sub-Indices for 2012-2019

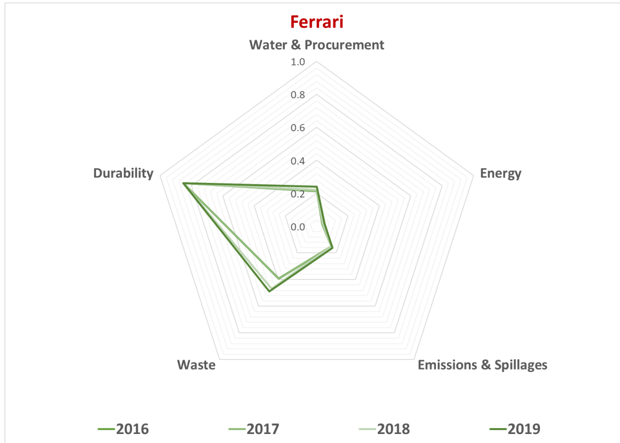


Figure J.11: Ferrari Category-based Circularity Sub-Indices for 2016-2019

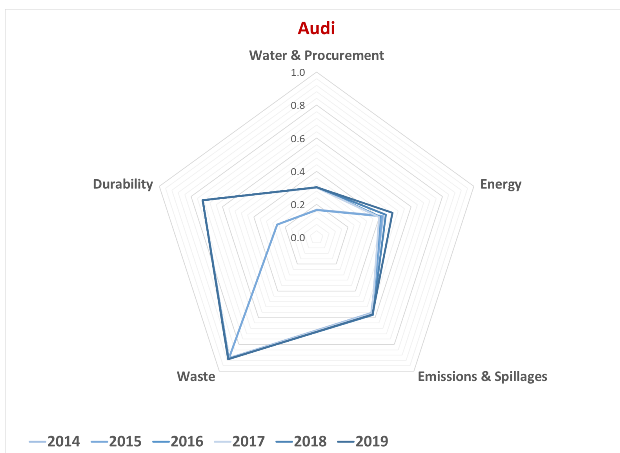


Figure J.12: Audi Category-based Circularity Sub-Indices for 2014-2019

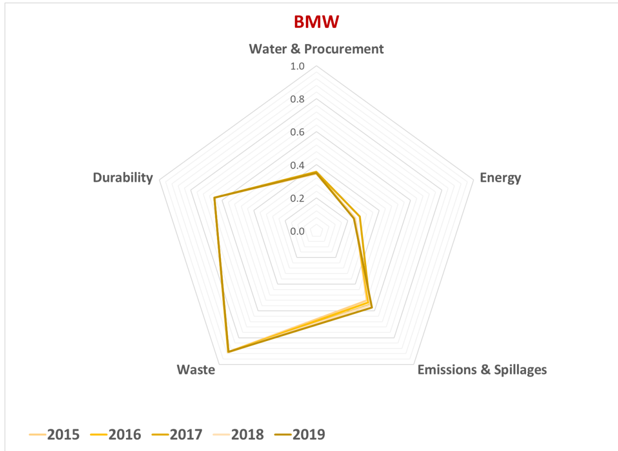


Figure J.13: BMW Category-based Circularity Sub-Indices for 2015-2019

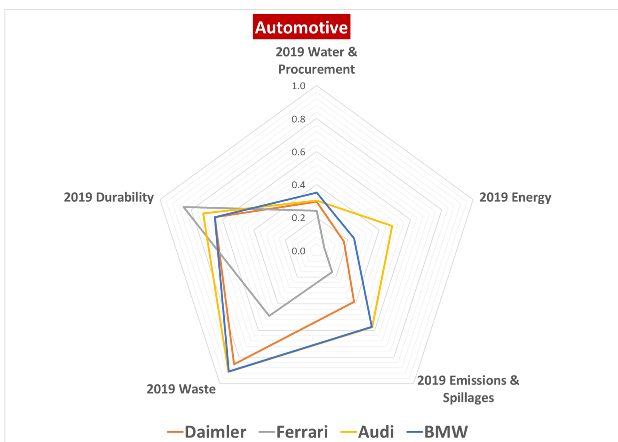


Figure J.14: Automotive Category-based Circularity Sub-Indices for 2019

Table J.1: CE Indicators for the Energy and Utilities Sector

Principal Categories	Indicators	GRI Standards Correspondence
Organization	Revenues [million $]	GRI-201-1
	Total social investment for environmental sustainability and circular economy [million $]	GRI-203-1
Waste	Waste generated - Hazardous [weight]	GRI-306-3
	Waste generated - Non Hazardous [weight]	GRI-306-3
	Diverted waste from disposal (reused, recycled, recovered) [weight]	GRI-306-4
Water	Water withdrawal [volume]	GRI-303-3
	Fresh water discharge (<= 1,000mg/L TDS) [volume]	GRI-303-4
	Other water discharge (>= 1,000mg/L TDS) [volume]	GRI-303-4
	Water recycled or reused [volume]	GRI-303-3 (2016)
Energy	Total energy generated [joules or multiples]	GRI-302-1
	Total non fossil fuel energy generated [joules or multiples]	GRI-302-1
GHG Emissions	Direct GHG emissions (Scope 1) [tCO2e]	GRI-305-1
	Energy indirect GHG emissions (Scope 2) [tCO2e]	GRI-305-2
	Total use of products (Scope 3) [metric tons CO2 equivalent (tCO2e)]	GRI-305-3
	Emissions neutralized by carbon offset projects [tCO2e]	GRI-305-5
	Emissions of ozone-depleting substances (ODS) [metric tons of CFC-11 equivalent]	GRI-305-6
	Nitrogen oxides [NOx], sulfur oxides [SOx] and other significant air emissions [kg or multiples]	GRI-305-7
Spillages and Discharges	Environmental fines [$]	GRI-307-1
	Volume of flared hydrocarbon [tCO2e]	GRI-306-3
	Volume of vented hydrocarbon [tCO2e]	GRI-306-3

Table J.2: CE Indicators for the Manufacturing Sector

Principal Categories	Indicators	GRI Standards Correspondence
Organization	Revenues [million $]	GRI-201-1
	Total social investment for environmental sustainability and circular economy [million $]	GRI-203-1
	Products sold [weight or volume]	GRI-301-3
Waste	Waste generated - Hazardous [weight]	GRI-306-3
	Waste generated - Non Hazardous [weight]	GRI-306-3
	Diverted waste from disposal (reused, recycled, recovered) [weight]	GRI-306-4
Water	Water withdrawal [volume]	GRI-303-3
	Fresh water discharge (<= 1,000mg/L TDS) [volume]	GRI-303-4
	Other water discharge (>= 1,000mg/L TDS) [volume]	GRI-303-4
	Water recycled or reused [volume]	GRI-303-3 (2016)
Procurement: Production and Packaging	Non-renewable packaging material used [volume or weight]	GRI-301-1
	Renewable packaging material used [volume or weight]	GRI-301-1
	Recycled packaging material used [volume or weight]	GRI-301-2
	Reusable, compostable or recyclable packaging material [%]	GRI-301-3
Energy	Total energy consumed [joules or multiples]	GRI-302-1
	Renewable energy consumed [joules or multiples]	GRI-302-1
GHG Emissions	Direct GHG emissions (Scope 1) [tCO2e]	GRI-305-1
	Energy indirect GHG emissions (Scope 2) [tCO2e]	GRI-305-2
	Total use of products (Scope 3) [metric tons CO2 equivalent (tCO2e)]	GRI-305-3
	Emissions neutralized by carbon offset projects [tCO2e]	GRI-305-5
	Emissions of ozone-depleting substances (ODS) [metric tons of CFC-11 equivalent]	GRI-305-6
	Nitrogen oxides [NOx], sulfur oxides [SOx] and other significant air emissions [kg or multiples]	GRI-305-7
Spillages & Discharges	Environmental fines [$]	GRI-307-1
Durability	Packaging Material to be reclaimed/recovered [# of products or %]	GRI-306-2

Table J.3: CE Indicators for the Automotive Sector

Principal Categories	Indicators	GRI Standards Correspondence
Organization	Revenues [million $]	GRI-201-1
	Total social investment for environmental sustainability and circular economy [million $]	GRI-203-1
	Number of products sold [# of products]	GRI-301-3
	Full time employees (FTE) [# of people]	GRI-401-1
Waste	Waste generated - Hazardous [weight]	GRI-306-3
	Waste generated - Non Hazardous [weight]	GRI-306-3
	Diverted waste from disposal (reused, recycled, recovered) [weight]	GRI-306-4
Water	Water withdrawal [volume]	GRI-303-3
	Fresh water discharge (<= 1,000mg/L TDS) [volume]	GRI-303-4
	Other water discharge (>= 1,000mg/L TDS) [volume]	GRI-303-4
	Water recycled or reused [volume]	GRI-303-3 (2016)
Procurement: Production and Packaging	Non-renewable material used [volume or weight]	GRI-301-1
	Renewable material used [volume or weight]	GRI-301-1
	Recycled input material used [volume or weight]	GRI-301-2
	Reusable, compostable or recyclable material [%]	GRI-301-3
Energy	Total energy consumed [joules or multiples]	GRI-302-1
	Renewable energy consumed [joules or multiples]	GRI-302-1
GHG Emissions	Direct GHG emissions (Scope 1) [tCO2e]	GRI-305-1
	Energy indirect GHG emissions (Scope 2) [tCO2e]	GRI-305-2
	Total use of products (Scope 3) [metric tons CO2 equivalent (tCO2e)]	GRI-305-3
	Average specific CO2 emissions [gCO2/km]	GRI-305-4
	Emissions neutralized by carbon offset projects [tCO2e]	GRI-305-5
	Emissions of ozone-depleting substances (ODS) [metric tons of CFC-11 equivalent]	GRI-305-6
	Nitrogen oxides [NOx], sulfur oxides [SOx] and other significant air emissions[kg or multiples]	GRI-305-7
Spillages & Discharges	Environmental fines [$]	GRI-307-1
Durability	Material to be reclaimed/recovered [%]	GRI-306-2
	Average lifespan of product or Warranty provided [years]	GRI-306-2

Table J.4: CE Indicators for the Service Sector

Principal Categories	Indicators	GRI Standards Correspondence
Organization	Revenues [million $]	GRI-201-1
	Total social investment for environmental sustainability and circular economy [million $]	GRI-203-1
	Full time employees (FTE) [# of people]	GRI-401-1
	Operational building/facilities space	GRI-302-3
Waste	Waste generated - Hazardous [weight]	GRI-306-3
	Waste generated - Non Hazardous [weight]	GRI-306-3
	Diverted waste from disposal (reused, recycled, recovered) [weight]	GRI-306-4
Water	Water withdrawal [volume]	GRI-303-3
	Fresh water discharge (<= 1,000mg/L TDS) [volume]	GRI-303-4
	Other water discharge (>= 1,000mg/L TDS) [volume]	GRI-303-4
	Water recycled or reused [volume]	GRI-303-3 (2016)
Procurement: Production & Packaging	Non-renewable material used [volume or weight]	GRI-301-1
	Renewable material used [volume or weight]	GRI-301-1
	Recycled input material used [volume or weight]	GRI-301-2
	Paper consumption [weight]	GRI-301-1
	Single-use plastics consumption [weight]	GRI-301-1
Energy	Total energy consumed [joules or multiples]	GRI-302-1
	Renewable energy consumed [joules or multiples]	GRI-302-1
	Certified buildings and facilities i.e LEED [%]	GRI-302-3
GHG Emissions	Direct GHG emissions (Scope 1) [tCO2e]	GRI-305-1
	Energy indirect GHG emissions (Scope 2) [tCO2e]	GRI-305-2
	Total use of products (Scope 3) [metric tons CO2 equivalent (tCO2e)]	GRI-305-3
	Emissions neutralized by carbon offset projects [tCO2e]	GRI-305-5
	Emissions of ozone-depleting substances (ODS) [metric tons of CFC-11 equivalent]	GRI-305-6
	Nitrogen oxides [NOx], sulfur oxides [SOx] & other significant air emissions [kg or multiples]	GRI-305-7
Spillages & Discharges	Environmental fines [$]	GRI-307-1

Table J.5: CE Metrics for the Energy and Utilities Sector

Principal Categories	Metrics		Upper Bound	Formula Used
Waste	1a	% of Hazardous waste over Total waste generated	100%	100%-1a
	1b	% of Diverted waste over Total waste generated	100%	1b
Water	2a	% of Recycled/reused water over Total water withdrawal	100%	2a
	2b	% of Other water discharge over Total water discharge	100%	100%-2b
	2c	% of Water consumed over Total water withdrawal	100%	100%-2c
Energy	3aa	% of Non fossil fuel energy generated over Total energy generated	100%	3aa
GHG Emissions	4aa	Net total emissions over Total energy delivered [tCO2e over joules or multiples]	600	1-norm[4aa]
	4ba	Emissions of ODS over Total energy delivered [metric tons of CFC-11 eq. over joules or multiples]	0.1	1-norm[4ba]
	4ca	NOx, SOx, and other significant air emissions over Total energy delivered [metric tons over joules or multiples]	1.0	1-norm[4ca]
Spillages and Discharges	4da	Environmental fines over Total energy delivered [$ over joules or multiples]	1.0	1-norm[4da]

Table J.6: CE Metrics for the Manufacturing Sector

Principal Categories	Metrics		Upper Bound	Formula Used
Waste	1a	% of Hazardous waste over Total waste generated	100%	100%-1a
	1b	% of Diverted waste over Total waste generated	100%	1b
	1ca	Waste generated over Products sold [kg waste over tons of product]	200	1-norm[1ca]
Water	2a	% of Recycled/reused water over Total water withdrawal	100%	2a
	2b	% of Other water discharge over Total water discharge	100%	100%-2b
	2c	% of Water consumed over Total water withdrawal	100%	100%-2c
	2da	Water withdrawal over Products sold [m3 water over tons of product]	10	1-norm[2da]
Procurement: Production and Packaging	2pab	% of Recycled packaging material used	100%	2pab
	2pbb	% of Renewable packaging material used	100%	2pbb
	2pcb	% of Reusable, compostable or recyclable packaging material used	100%	2pcb
Energy	3ab	% of Renewable energy consumed over Total energy consumed	100%	3ab
	3ba	Total energy consumed over Products sold [joules or multiples over tons of product]	10	1-norm[3ba]
GHG Emissions	4ab	Net total emissions over Products sold [tCO2e over tons of product]	500	1-norm[4ab]
	4bb	Emissions of ODS over Products sold [metric tons of CFC-11 eq. over tons of product]	0.1	1-norm[4bb]
	4cb	NOx, SOx, and other significant air emissions over Products sold [metric tons over tons of product]	1	1-norm[4cb]
Spillages and Discharges	4db	Environmental fines over Products sold [$ over tons of product]	10	1-norm[4db]
Durability	5a	% of Packaging material to be reclaimed/recovered	100%	5a

Table J.7: CE Metrics for the Automotive Sector

Principal Categories	Metrics		Upper Bound	Formula Used
Waste	1a	% of Hazardous waste over Total waste generated	100%	100%-1a
	1b	% of Diverted waste over Total waste generated	100%	1b
	1cb	Waste generated over Number of products sold [kg waste over # of products]	1500	1-norm[1cb]
Water	2a	% of Recycled/reused water over Total water withdrawal	100%	2a
	2b	% of Other water discharge over Total water discharge	100%	100%-2b
	2c	% of Water consumed over Total water withdrawal	100%	100%-2c
	2db	Water consumption over Number of products sold [m3 water over # of products]	30	1-norm[2db]
Procurement: Production and Packaging	2paa	% of Recycled input material used	100%	2paa
	2pba	% of Renewable material used	100%	2pba
	2pca	% of Reusable, compostable or recyclable material used	100%	2pca
Energy	3ab	% of Renewable energy consumed over Total energy consumed	100%	3ab
	3bb	Total energy consumed over Number of products sold [joules or multiples over # of products]	15	1-norm[3bb]
GHG Emissions	4ac	Net total emissions over Number of products sold [tCO2e over # of products]	2,000	1-norm[4ac]
	4bc	Emissions of ODS over Number of products sold [metric tons of CFC-11 eq. over # of products]	0.1	1-norm[4bc]
	4cc	NOx, SOx, and other significant air emissions over Number of products sold [metric tons over # of products]	10	1-norm[4cc]
	4d	Average specific CO2 emissions [gCO2/km]	200	1-norm[4d]
Spillages and Discharges	4dc	Environmental fines over Number of products sold [$ over # of products]	10	1-norm[4dc]
Durability	5b	% of Material to be reclaimed/recovered	100%	5b
	5c	Average lifespan of product or Warranty provided [years]	20	norm[5c]

Table J.8: CE Metrics for the Service Sector

Principal Categories	Metric		Upper Bound	Formula Used
Waste	1a	% of Hazardous waste over Total waste generated	100%	100%-1a
	1b	% of Diverted waste over Total waste generated	100%	1b
	1cc	Waste generated over Full Time Employees [kg waste over # of FTE]	1000	1-norm[1cc]
Water	2a	% of Recycled/reused water over Total water withdrawal	100%	2a
	2b	% of Other water discharge over Total water discharge	100%	100%-2b
	2c	% of Water consumed over Total water withdrawal	100%	100%-2c
	2dc	Water consumption over Full Time Employees [m3 water over # of FTE]	100	1-norm[2dc]
Procurement: Production & Packaging	2paa	% of Recycled input material used	100%	2paa
	2pd	Paper consumption over Full Time Employees [kg over # of FTE]	365	1-norm[2pd]
	2pe	Single-use plastics consumption over Full Time Employees [kg plastic over # of FTE]	50	1-norm[2pe]
Energy	3ab	% of Renewable energy consumed over Total energy consumed	100%	3ab
	3bc	Total energy consumed over Operational space [joules or multiples over surface area]	1	1-norm[3bc]
	3bd	% of Certified buildings and facilities i.e LEED	100%	3bd
GHG Emissions	4ad	Net total emissions over Operational space [tCO2e over surface area]	300	1-norm[4ad]
	4bd	Emissions of ODS over Operational space [metric tons of CFC-11 eq. over surface area]	1	1-norm[4bd]
	4cd	NOx, SOx, and other significant air emissions over Operational space [metric tons over surface area]	0.05	1-norm[4cd]
Spillages & Discharges	4dd	Environmental fines over Operational space [$ over surface area]	0.5	1-norm[4dd]

APPENDIX K

LIST OF PUBLICATIONS AND PRESENTATIONS

At the time of writing, the journal publications, the conference proceedings, and the presentations produced during my graduate studies are listed below.

K.1 Journal Publications

- S. Avraamidou, **S.G. Baratsas,** Y. Tian, E.N. Pistikopoulos, "Circular Economy-A challenge and an opportunity for Process Systems Engineering," *Computers & Chemical Engineering*, vol. 133, p.106629, 2020.

- **S.G. Baratsas,** A.M. Niziolek, O. Onel, L.R. Matthews, C.A. Floudas, D.R. Hallermann, S.M. Sorescu, E.N. Pistikopoulos, "A framework to predict the price of energy for the end-users with applications to monetary and energy policies," *Nature Communications*, vol. 12, no. 1, pp. 1-12, 2021.

- **S.G. Baratsas,** E.N. Pistikopoulos, S. Avraamidou, "A systems engineering framework for the optimization of food supply chains under circular economy considerations," *Science of The Total Environment*, vol. 794, p. 148726, 2021.

- **S.G. Baratsas,** A.M. Niziolek, O. Onel, L.R. Matthews, C.A. Floudas, D.R. Hallermann, S.M. Sorescu, E.N. Pistikopoulos, "A novel quantitative forecasting framework in energy with applications in designing energy intelligent tax policies," *Applied Energy*, vol. 305, 2022.

- **S.G. Baratsas,** E.N. Pistikopoulos, S. Avraamidou, "A quantitative and holistic circular economy assessment framework at the micro level," *Computers & Chemical Engineering*, 2021. In Review.

- R. Kokodkar, G. He, C.D. Demirhan, M. Arbabzadeh, **S.G. Baratsas,** S. Avraamidou, D. Mallapragada, I. Miller, R.C. Allen, E. Gençer, E.N. Pistikopoulos, "A review of analytical and optimization methodologies for transitions in multi-scale energy systems," *Renewable & Sustainable Energy Reviews*, 2021. In Review.

- R.C. Allen, **S.G. Baratsas,** R. Kokodkar, S. Avraamidou, C.D. Demirhan, C.F. Heuberger, M. Klokkenburg, E.N. Pistikopoulos, "A Mode Based Formulation for Solving Multi-Period Integrated Planning and Scheduling Problems," *Optimal Control Applications and Methods*, 2021. In Review.

- **S.G. Baratsas,** R.C. Allen, E.N. Pistikopoulos, "A hybrid forecasting framework with statistical and machine learning methods for the energy sector," *Computers & Chemical Engineering*, 2021. In Review.

K.2 Conference Proceedings

- **S.G. Baratsas,** E.N. Pistikopoulos, S. Avraamidou, "Circular economy systems engineering: A case study on the coffee supply chain," *Computer Aided Chemical Engineering*, vol. 50, p. 1541-1546, 2021.

- **S.G. Baratsas,** N. Masoud, V.A. Pappa, E.N. Pistikopoulos, S. Avraamidou, "Towards a Circular Economy Calculator for Measuring the “Circularity” of Companies," *Computer Aided Chemical Engineering*, vol. 50, p. 1547-1552, 2021.

- R. C. Allen, **S.G. Baratsas,** R. Kokodkar, S. Avraamidou, J.B. Powell, C.F. Heuberger, C.D. Demirhan, E.N. Pistikopoulos, "An optimization framework for solving integrated planning and scheduling problems for dense energy carriers," *IFAC-PapersOnLine*, vol. 54, no. 3, p. 621-626, 2021.

K.3 Conference Presentations

- Towards a novel energy financial security: The Texas A&M Energy Spot Price Index

  - TAMU Energy Conference 2019, AIChE Meeting 2019.

- Towards a novel energy price predictive framework: The Texas A&M Energy Price Index

  - TAMU Energy Conference 2019, AIChE Meeting 2019.

- A novel energy price predictive framework, and its energy and monetary applications

  - TAMU ChESGA Symposium 2020

- A novel energy financial security: The Texas A&M Energy Spot Price Index (ESPIC)

  - TAMU ChESGA Symposium 2020

- Circular Economy systems engineering for food supply chains: A case study on the coffee supply chain

  - International Conference on Sustainable Development (ICSD) Conference 2020

- Forecasting prices of energy feedstocks & commodities using advanced statistical & machine learning methods

  - AIChE Meeting 2020

- Designing and optimizing energy policies through a novel energy price predictive framework

  - AIChE Meeting 2020

- Circular economy systems engineering: A case study on the coffee supply chain

  - AIChE Meeting 2020, ESCAPE-31 2021

- Towards a Circular Economy Calculator for measuring the "Circularity" of Companies

  - ESCAPE-31 2021

- An optimization framework for solving integrated planning and scheduling problems for Dense Energy Carriers

  - 11th IFAC International Symposium - ADCHEM 2021

- A quantitative framework for the optimization of food supply chains under Circular Economy considerations

  - III Sustainable Supply Chains Conference 2021

K.4 Commercial Presentations

- A Novel Energy Financial Security: The Energy Spot Price Index (ESPIC)

  - Texas A&M New Ventures Competition 2021 - (TNVC2021), TEES Advisory Board Meeting September 2021