Takuma Ono tak.ono@dnv.com Veritasveien 1, 1363 Høvik, Norway

Abstract

A conventional approach to calculating environmental impacts is to use an emission factor, such as for Global Warming Potential (GWP). However, this approach may aggregate potentially important aspects such as which economic activity in the value chain produces the greenhouse gas (GHG), and what type of GHG. If there is a need to report Scope 1 through 3 per the Greenhouse Gas Protocol, a simple emission factor approach may be limiting. A publicly available life cycle assessment (LCA) dataset was modified to be compatible with the Stella system dynamics software. This allowed for calculating the direct (Scope 1) and indirect (Scope 2 and 3) requirements using the Leontief input-output matrix inversion. This was combined with the energy demands of the German buildings sector per DNV's Energy Transition Outlook (ETO) system dynamics model. The GWP calculation approach of the ETO model was compared with the SD-LCA approach proposed in this submission. The ETO building sector utilizes a diverse set of energy carriers, so the energy carrier demands from the ETO model resulted in an array of processes emitting GHG at different Scopes. The GHGs contributing to the overall GWP impact were predominantly CO2 and methane. Scope 3 contribution was higher than expected at more than 10%. Scope 3 emissions from coal decline, but emissions from natural gas remain prominent to upstream emissions.

Introduction and General Approach

A conventional approach to calculation environmental impacts is to multiply an activity level (e.g. kWh of electricity consumed) with an emission factor, such as for Global Warming Potential (GWP) per kWh of electricity consumption. However, this approach may aggregate potentially important aspects such as which economic activity produces the greenhouse gas (GHG), and what type of GHG. If there is a need to report the entirety of the value chain, Scope 1 through 3 per the Greenhouse Gas Protocol, a simple emission factor multiplication approach may be limiting (GHG Protocol, 2021).

Calculation methodology employed in *Life Cycle Assessment* (LCA) was integrated into the Stella software to seamlessly calculate the emissions and GWP of the total value chain. LCA is the practice of quantifying the impact of a product or service from production to disposal (Quist, 2025). Conventional LCA software such as SimaPro and OpenLCA leverages a calculation technique called Leontief input-output matrix, which calculates the total output of an economy comprised of interdependent sectors (Leontief, 1936; Wyss-Gallifent, 2023). Instead of monetary exchange between economic sectors, LCA employs the input-output technique to calculate the exchange of manufacturing process outputs between interdependent industrial processes (Heijungs et al., 2022).

While the described methodology is not *per se* a system dynamics technique, integrating it into the SD framework can be a valuable tool in dynamically quantifying industrial process and economic activities and the environmental emissions that occur. While the author does not recommend relying solely on the described technique to quantify Scope 2 emissions, it could be an essential technique to quantify total upstream activities and emissions (Scope 3). In this test case, it resulted in capturing an additional 10% of upstream environmental impacts that would otherwise be overlooked.

A freely available life cycle assessment (LCA) dataset called U.S. Life Cycle Inventory (USLCI) was modified to be compatible with the Stella system dynamics software (NREL, 2025). This allowed for calculating the direct (Scope 1) and indirect (Scope 2 and 3) requirements for 35 energy-relevant activities that emit 9 of the most common types of GHG. This was combined with the energy demands of the German buildings sector per DNV's Energy Transition Outlook (ETO) system dynamics model. The GWP calculation approach of the ETO model was compared with the ETO+LCA approach proposed in this submission.

Leontief Matrix and Life Cycle Assessment Description

LCA calculation based on Leontief matrix starts with a select number of interdependent industrial processes. Heijungs et al. (2022) discusses in great detail this approach. The complete matrix tables are available in the supporting material of this submission. The main Leontief equation is as follows:

$$X = (I - A)^{-1} \cdot Y$$ *Equation 1: Leontief matrix inversion*

Where A is the technology coefficient matrix, I is the identity matrix, Y is the final demand vector, and X is the total output vector.

As an example, hypothetical interdependence between four energy processes is summarized below (Table 1).

Table 1: Simple 4x4 table showing hypothetical interdependence between natural gas and electricity

	Electricity [1 kWh]	Natural gas [1 L]	Oil [1 L]	coal [1 kg]
Electricity [kWh]	0	0	0	0
Natural gas [L]	0	0	0	0
Oil [L]	1.2	2.5	0	0
coal [kg]	0.24	0.5	0	0

Table 1 summarizes how to produce a certain amount of a process, to what extent it is dependent on other processes. It can be considered a *matrix of coefficients*, or A matrix.

Takuma Ono tak.ono@dnv.com Veritasveien 1, 1363 Høvik, Norway

The identity matrix I is simply a matrix of the same dimension with 1's in a diagonal, and 0's everywhere else (Table 2).

Table 2: Identity matrix I of the corresponding technology coefficient matrix A

	Electricity [1 kWh]	Natural gas [1 L]	Oil [1 L]	coal [1 kg]
Electricity [kWh]	1	0	0	0
Natural gas [L]	0	1	0	0
Oil [L]	0	0	1	0
coal [kg]	0	0	0	1

Then, as per equation 1 the I matrix is subtracted by the A matrix, then a matrix inversion is performed, which results in the Leontief inverse matrix (Table 3).

Table 3: Leontief inversion matrix using the identify matrix I and technology coefficient matrix A

	Electricity [1 kWh]	Natural gas [1 L]	Oil [1 L]	coal [1 kg]
Electricity [kWh]	1	0	0	0
Natural gas [L]	0	1	0	0
Oil [L]	1.2	2.5	1	0
coal [kg]	0.24	0.5	0	1

If a certain industrial process hypothetically needs 10 L of natural gas and 100 kWh of electricity, this would be the demand, or the Y vector. As per Equation 1, when the Leontief matrix is multiplied by the final demand Y, it results in X, or the total output Table 4).

Table 4: FInal demand Y and the actual amount of processes needed shown by Total output X

	Final demand [Y]	Total output [X]
Electricity [kWh]	100	100
Natural gas [L]	10	10
Oil [L]	0	145
coal [kg]	0	29

Takuma Ono tak.ono@dnv.com Veritasveien 1, 1363 Høvik, Norway

After calculating the total output X, converting the values into the GHG emission and finally the GWP impact (notated as *h* in the equation) is simply a series of emission factor conversion using matrix multiplication (Table 5).

$$h = C \cdot B \cdot X$$

Equation 2: Matrix multiplication of emission matrix B and impact vector C

The X vector is multiplied by the emissions matrix B, which converts the industry process activity levels to a vector of their corresponding GHG emissions, which in LCA is referred to as *inventory*. This vector is then multiplied by the GWP emission factor vector C, to arrive at the final impact *h* (Table 6).

Table 5: Emission matrix B and impact vector C

B Matrix	Electricity [1 kWh]	Natural gas [1 L]	Oil [1 L]	coal [1 kg]
Carbon diodide [kg]	10	0.2	0.3	0.2
Methane [kg]	0	0.5	0.2	0.3
C Matrix	Carbon diodide [kg]	Methane [kg]		
GWP100 [$kgCO_2eq$]	1	25		

Table 6: Demand vector Y and their corresponding total output X, GHG emissions, and the final GWP100 impact [h]

	Demand Y	**Total Output X**	**Emission Inventory**		**Environmental Impact [h]**	
Electricity [kWh]	100	100	Carbon diodide [kg]	1051.3	**GWP100**	2118.8
Natural gas [L]	10	10	Methane [kg]	42.7		
Oil [L]	0	145				
coal [kg]	0	29				

Methodology Description

The ETO model is a system dynamics model that captures the major economic sectors: transportation, buildings, manufacturing, electricity generation, and fuels (DNV, 2024). The German ETO model is derived from the main global model by adjusting a wide variety of parameter inputs to be Germany-specific and simulated from years 1980 to 2050. The model calculates the type of energy demanded by the buildings sector by considering the type of equipment used for space and water heating, space cooling, and appliances. The amount of energy is calculated by considering the historical and projected population and GDP of Germany. The model calculates twelve *energy carriers*

Takuma Ono tak.ono@dnv.com Veritasveien 1, 1363 Høvik, Norway
of which this study considers the following five: electricity, oil, natural gas, coal, and biomass. The total energy demanded by the buildings sector for these five energy carriers will be the *reference flow*, or the final demand Y in Equation 1 (Scope 1). The reference flow will be used to calculate the *direct demand* (Scope 2), and *total demand* (Scope 1 – 3) by multiplying with the *technology matrix*, which is equivalent to the Leontief interdependent sectors matrix.

The technology matrix was derived from the freely available LCA database called U.S. Life Cycle Inventory (USLCI) provided by the National Renewable Energy Laboratory (NREL, accessed 2025). It is a database with a matrix of interdependencies for 587 of US industrial and economic activities and over 5000 associated emissions such as power generation, chemical manufacturing, and carbon dioxide emissions. Since the ETO model focuses on energy-specific activities and in climate-relevant emissions, the technology matrix was drastically reduced through filtering and aggregating—with 35 energy processes (Table 7).

Table 7: List of 35 energy processes considered in the reduced technology matrix

Process / Unit	**Process / Unit**
Ammonia, steam reforming, liquid, at plant	Ethanol average, 85%,/kg
Dummy_Electricity, at wind power plant, unspecified/kWh	Fuel grade uranium, at regional storage
Dummy_Electricity, geothermal, unspecified/kWh	Coal average, at mine
Dummy_Electricity, hydropower, at power plant, unspecified/kWh	Coal average, combusted in industrial boiler
Dummy_Electricity, photovoltaic, unspecified/kWh	Crude oil, at production
Electricity, at cogen, for natural gas turbine/kWh	Natural gas, at extraction site
Electricity, at grid, US, 2000 U	Natural gas, combusted in industrial equipment
Electricity, at grid, US, 2008 U	Natural gas, processed, at plant
Electricity, at grid, US, 2010/kWh	Oil average, at refinery/l
Electricity, at grid, US	Oil average, combusted in industrial equipment
Electricity, biomass, at power plant	Transport, aircraft, freight
Electricity, coal average, at power plant	Transport, barge, average fuel mix
Electricity, natural gas, at power plant	Transport, bus average/personkm
Electricity, nuclear, at power plant	Transport, combination truck, average fuel mix
Electricity, oil average, at power plant	Transport, motorcycle, gasoline powered/personkm
	Transport, ocean freighter, average fuel mix
	Transport, passenger car average/personkm
	Transport, pipeline, natural gas/tkm
	Transport, pipeline, unspecified petroleum products/tkm

The 35 x 35 technology matrix was implemented in the Stella software using the *array* function. Stella can accept the same array type multiple times in one variable; therefore, the two-dimensional technology matrix variable was implemented by adding the *process & emissions* array twice. Then, the Excel-calculated technology coefficient values were added in the appropriate positions. The identity matrix was also created similarly. Instead of the technology coefficient values, a value of 1 was placed among matching process or emissions, which results in a diagonal of 1's, with 0's for all other cells.

One of the limitations of a conventional LCA analysis is that the technology matrix is static, linear, and *time-neutral* (Heijungs, 2020). For example, impact of producing 1kWh of grid electricity in year 2000 is exactly the same as producing 1kWh from the same grid in 2020. Moreover, impact of producing the first widget in 1980 is the same as producing the billionth widget in 2020, with no ability to consider economies of scale or feedback loops. The data embedded in the technology coefficient must represent a single point in time or aggregated from a range of time and technologies into one data point. In other words, LCA is not equipped to capture dynamic changes over a time series. System dynamics is specifically oriented towards this task, so in this case study, the static electrical grid mix coefficient from USLCI was replaced by the dynamic grid mix calculations as performed by the ETO model (Figure 1).

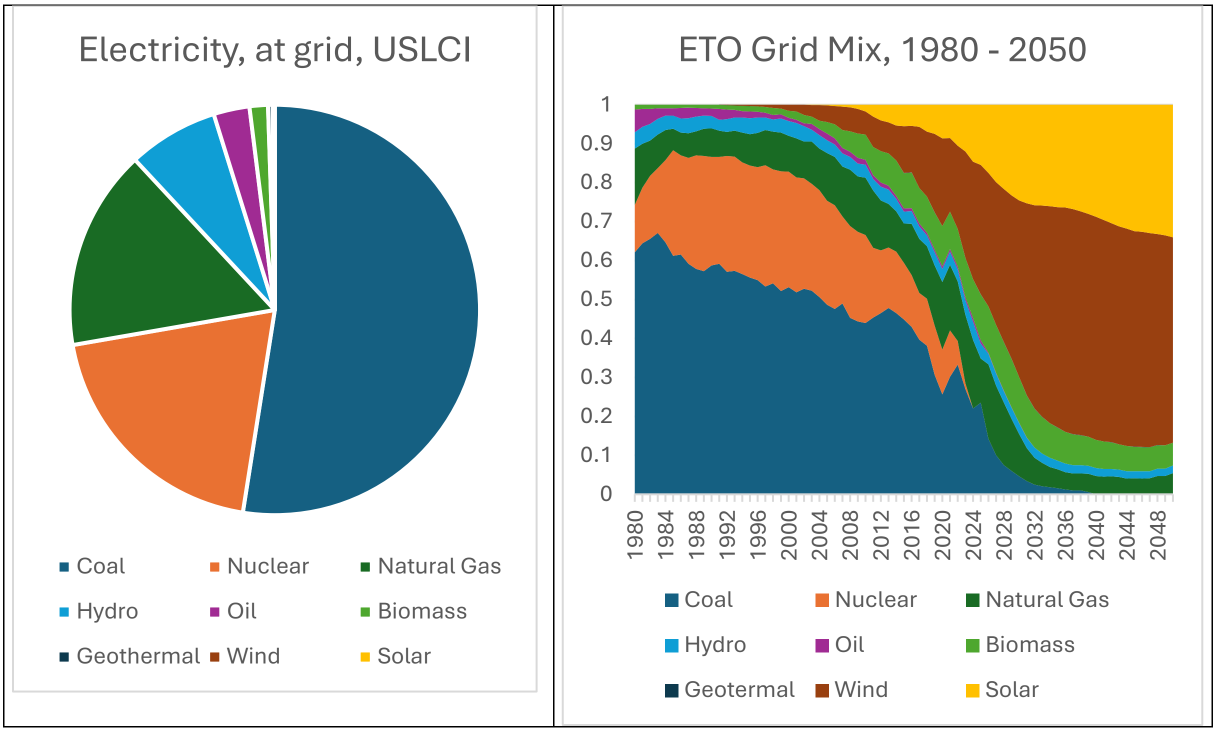

Figure 1: Static USLCI grid mix compared with dynamic ETO grid mix over years 1980 - 2050.

By connecting the technology matrix with the ETO grid mix in Stella, it is possible to test the implications of how the changing grid mix leads to difference in the total upstream demand when the building sector consumes electricity throughout the simulation years.

To replicate the Leontief inverse matrix in Stella (which is the $(I - A)^{-1}$ matrix formula), there was a need to perform the matrix subtraction first in one variable, then invert the resulting matrix with the *MATRIXINVERT* function. Note that since the technology matrix has been modified to be dynamic throughout the simulation, this leads to a dynamic Leontief inverse.

How do the components described so far—reference flow, technology matrix, identity matrix, and Leontief inverse—allow for calculating Scope emissions 1 through 3? Scope 1 is defined by GHG Protocol as “GHG emissions from sources located within the city [or regional] boundary" (GHG Protocol, 2021). In terms of the buildings sector, it is essentially fuel burned on site, presumably for cooking and heating. This is calculated by taking the energy demand reference flow *Y* from the ETO building sector, and multiplying by the emissions per process, or the *B matrix* in Equation 2.

Scope 2 emissions is defined as "GHG emissions occurring as a consequence of the use of grid-supplied electricity, heat, steam and/or cooling" (GHG Protocol, 2021). That is, the emissions because of using electricity or central heating/cooling. Scope 2, or the *direct demand,* can be calculated simply by a matrix multiplication of the reference flow Y and the *un-inverted* technology matrix A and then finally by the B matrix.

Scope 3 is a "catch all" category defined as "all other GHG emissions that occur outside the city[region] boundary as a result of activities taking place within the city boundary" (GHG Protocol, 2021). The Scope 3 is slightly more involved because the total output X must be first calculated by multiplying the reference flow Y vector with the Leontief inverse matrix $(I – A)^{-1}*Y$. Multiplying the total output X by the emission factor matrix B results in total emissions, Scopes 1 – 3. Then, the previously calculated Scopes 1 and 2 emissions are subtracted from this total value to infer the Scope 3 emissions.

To calculate the greenhouse gas emissions, as described in Equation 2, the emissions matrix B and then the impact vector C are multiplied in succession which results in the final impact h—h_{Scope1}, h_{Scope2}, and h_{Scope3}. All calculations will be made available in the supporting material.

Results and Discussion

Figure 2 shows the total climate change impacts as originally calculated by the ETO model. Note that impacts from electricity consumption have been attributed to the appropriate originating feedstock fuel, such as coal and natural gas. The most impactful energy carriers are coal, oil, and natural gas. Oil and coal are phase out over the course of the simulation, and natural gas remains the primary source of greenhouse gas.

Takuma Ono tak.ono@dnv.com Veritasveien 1, 1363 Høvik, Norway

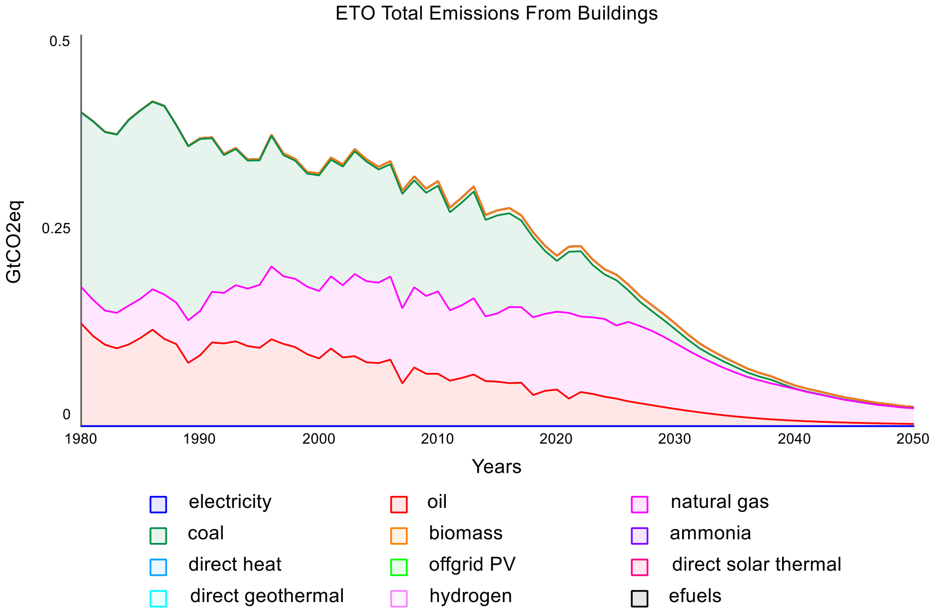

Figure 2: GHG impacts from the Buildings sector divided by energy carriers

In a similar vein, the proposed methodology can produce similar results, as shown in Figure 3. Here, coal is also phased out and natural gas remains virtually the sole fossil fuel emitter. However, biomass also has a small role in future greenhouse gas emission.

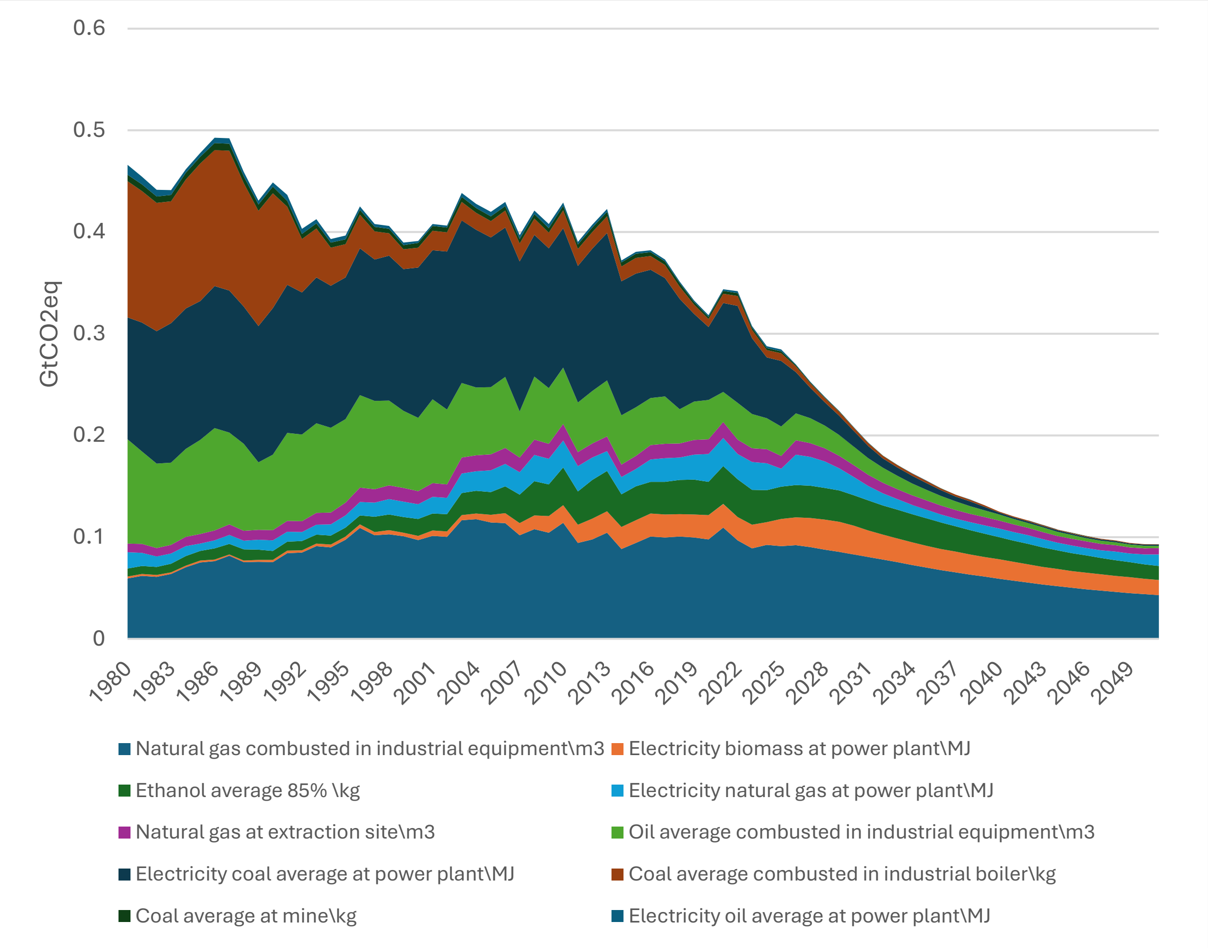

Figure 3: Results comparable to the original ETO results by the proposed LCA methodology

In addition to replicating the original results, the proposed methodology allows for multiple cross-sectional analyses that would not be possible with a simple emission factor multiplication. For example, Figure 4 shows that carbon dioxide is the predominant contributing greenhouse gas, but methane also plays a minor role in the total impacts. Applying the emissions matrix B allows for this type of analysis.

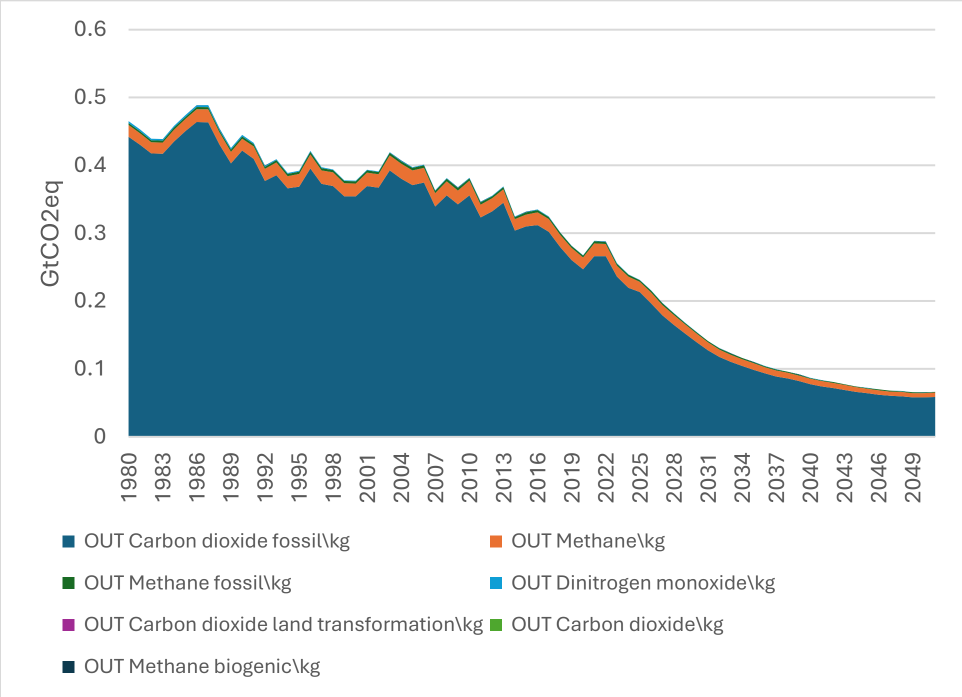

Figure 4: Total impacts seen as the contributing greenhouse gases

Moreover, using the approach described in the methodology section, it is possible to break out the total impacts by the scope of the life cycle (Figure 5). Here, it is possible to see that Scope 3—the "catch-all" upstream impacts—are approximately 10% of the total impacts that would not be captured without the Leontief inversion matrix. The results analysis pivot table will be made available in the supporting material.

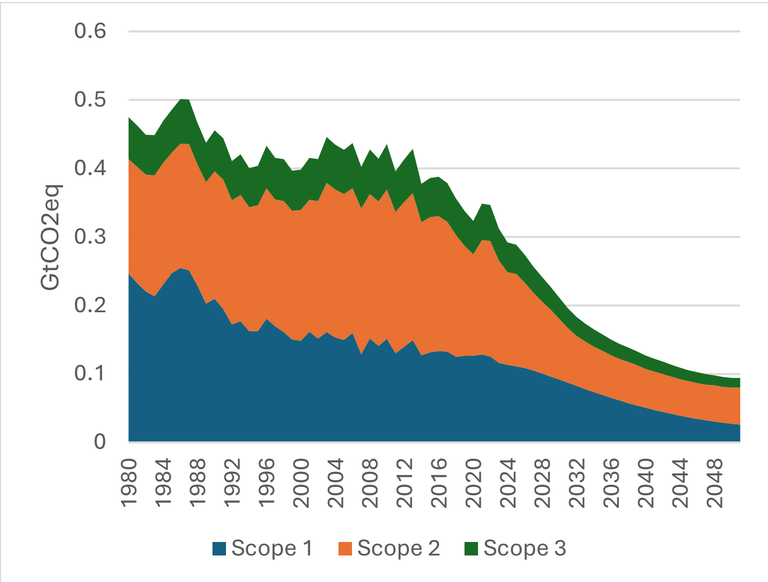

Figure 5: The supply chain scope contributions to the total GWP impacts

Takuma Ono tak.ono@dnv.com Veritasveien 1, 1363 Høvik, Norway

Conclusions, Limitations, and Next Steps

With the proposed methodology, it is possible to trace which energy process is emitting what greenhouse gas, and at which supply chain Scope, which timestep, and how the interdependency of the processes changes through the dynamic technology coefficient matrix. Depending on the reporting needs, this proposed methodology may prove to be highly valuable in capturing the Scope 3 "catch-all" emission sources.

There is a significant computational limitation when integrating matrix operations into the Stella model. In addition to filtering out non-energy process, one of the biggest motivations for reducing processes down to just 35 was that any matrices over 50 proved to be too slow for a standard personal computer. Number of datapoints to calculate grows exponentially with each new process (1 new process = 1 new row and 1 new column); therefore, it was prudent to minimize number of processes in the matrix.

The filtering and aggregating the USLCI was manually done to fit the needs of the study, and it is highly likely that the resulting coefficient matrix would not be useful for a different study. Therefore, there needs to be a generalizable and scalable approach to integrating existing LCA datasets like USLCI into the system dynamics framework.

Future work would include assessing how the matrix approach can be more endogenized. As noted in the introduction, this proposed methodology in of itself does not involve system dynamics techniques, although this paper demonstrates its value within the SD framework. In essence, calculating the Scope 2 and Scope 3 consumption is equivalent to calculating the instantaneous, *indicated* demand in a typical SD model. Therefore, the outputs of the Leontief operations can be incorporated in endogenous, feedback-rich system dynamic models as proposed by this study as well as past conference submissions (Braden, 1981; Yamashita, 2024).

Takuma Ono tak.ono@dnv.com Veritasveien 1, 1363 Høvik, Norway

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