# DIGITAL SUPPLEMENTARY MATERIAL

The work synthesized in this article reports and analyzes GHG emissions from the chemical industry sector, including the manufacturing of chemical products (NAICS 325) and plastic and rubber products (NAICS 326), while proposing effective electrification solutions. The segment studied includes 19 plants, specifically for the chemical manufacturing subsector:

- two petrochemical manufacturing plants,
- one resin and synthetic rubber manufacturing plant,
- one synthetic dye and pigment manufacturing plant,
- one alkali and chlorine manufacturing plant,
- three industrial gas manufacturing plants,
- three other basic inorganic chemical manufacturing plants,
- two other basic organic chemical manufacturing plants,
- one other miscellaneous chemical product manufacturing plant,
- one plastic sheet, plate, and laminate manufacturing plant (excluding packaging),
- one tire manufacturing plant,
- three polystyrene foam product manufacturing plants.

The processes analyzed involve the use of natural gas primarily to produce heat through combustion, which will be replaced in the scenarios by direct and/or indirect heating technologies (e-gas, hydrogen). Natural gas is also used as a reactant to produce hydrogen through steam reforming, with the decarbonized process being water electrolysis. Additionally, one process uses petroleum coke as a reducing agent, with the potential replacement process using biochar. Fossil CO_2 is used as an input in processes, with future supply potentially coming from biogenic CO_2. To complete, HFC is used as a blowing agent input in processes. According to regulations, the preferred route is the transition to HFO blowing agents with a lower environmental impact.

This study is a preliminary analysis of decarbonization scenarios based on public data and assumptions, with data not validated in the field and with the concerned plants. Additionally, the technical feasibility and techno-economic potential of the scenarios are not considered in this study and remain to be validated in future work. This study is based on "What-If?" scenarios. In this initial analysis, GHG emissions related to transport equipment assigned to the various industrial sites have been neglected. The results of the scenarios are subject to change. The main objective of this study is to primarily initiate reflections to start projects of interest with a vision of carbon neutrality.
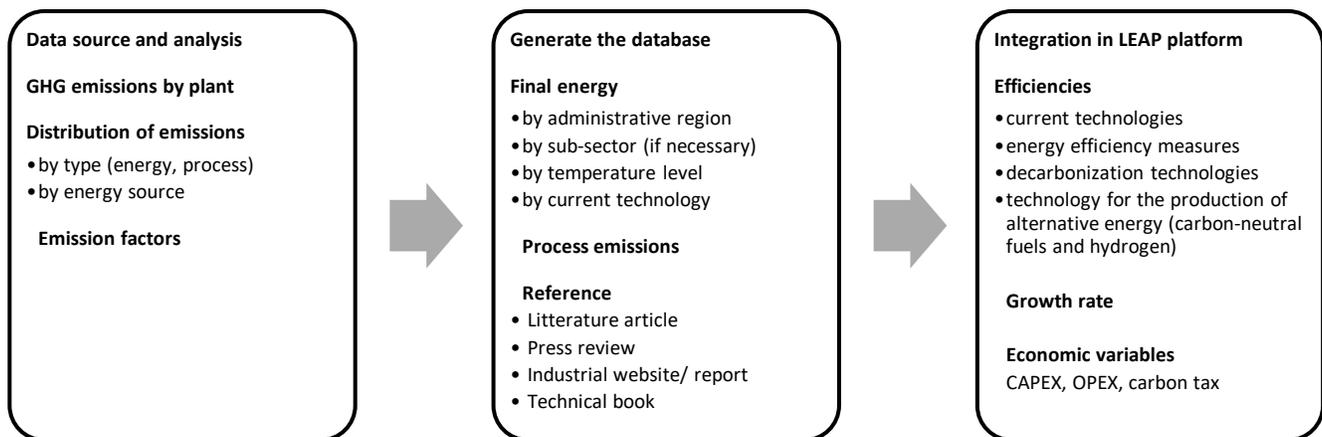
Figure S1. Methodology for data import and model parameters

Table S1. Process by range of temperature

ID	Temperature	Process
LT	100-300°C	vapor, dryer
MT	300-500°C	vapor, dryer, thermal oil reheater
HT	500-1500°C	heater, calcinator
Prod.	raw materials	hydrogen

Table S2. Emission source in 2020 for chemical industries in Quebec [1]

Emission Source	GHG emissions (Mt CO_2e)	Share of GHG total
Stationary Fuel Combustion	0,534	43,1%
Low temperature (LT)	0,353	28,5%
Medium temperature (MT)	0,109	8,8%
High temperature (HT)	0,053	4,3%
Raw materials (Prod.)	0,019	1,6%
Industrial Processes (fossil CO_2)	0,218	17,6%
Industrial Processes (biogenic CO_2)	0,062	5,0%
Industrial Processes (HFC)	0,425	34,3%

Estimation and analysis of public data for each industry and/or similar industry to make some hypothesis about energy share by level of temperature (sensibility analysis will be made in future work to mitigate risk of this value) and could be validate with another source.

Equation S1. Estimated energy demand based on GHG by energy source

$$E_{j,k} = \frac{x_{j,k} \cdot \text{GHG}}{EF_j} \qquad (S1)$$

Where E is the final useful energy demand in MWh, j is fuel consumed (like natural gas, petroleum coke, biomass and other), k is the level temperature range, x is the share rate, GHG is the total energy source emission (t CO2e), EF is the average emission factors [2] for upstream emissions per unit of consumption (t CO_2e/MWh)

Table S3. Energy source by level of temperature in 2020 for chemical industries in Quebec based on hypothesis and public database (the share of different energy sources used can change based on the integrated processes within each industry, and each industrial setup is unique)

Energy source (TWh)	Low temperature (LT)	Medium temperature (MT)	High temperature (HT)	Raw materials (Prod.)
Biomass and biogas	0,009	0,000	0,026	0,000
Natural gas	2,002	0,210	0,301	0,214
Distillate gas/pet. coke	0,000	0,217	0,000	0,000
LPG	0,000	0,018	0,000	0,000
Total	2,011	0,446	0,327	0,214

Table S4. Efficiency of technology by process integration (assumption based on analysis of the reference)

Temperature level	End-use technology	Efficiency	Ref
[LT & MT] Low and medium-grade heat	Fossil fuel boiler	75%	[3]
	Electric boiler	99%	[4]
	Biomass boiler	70%	[3]
	Heat pump (HTHP)	250%	[5]
[HT] High-grade heat	Fossil fuel	75%	[6]
	Hydrogen	85%	[7]
	Plasma-based	75%	[8]
[Prod] Raw materials	Electrolysis H_2	64%	[7]

The efficiency of technologies varies according to several parameters as well as their integration into the process. The efficiencies used in this article are approximate values and will vary in future studies to evaluate the sensitivity of each assumption on the results.

Equation S2. Decarbonization Efficiency Coefficient (DEC)

$$\text{DEC} = \frac{E_{j,baseline} - E_j}{E_i - E_{i,baseline}} \qquad (S2)$$

Where E is the primary energy demand in MWh, j is non-renewable resource (like natural gas, petroleum coke and other), i is the renewable resource of interest (electricity, biomass or both).

Equation S3. GHG Performance Indicator (GPI)

$$GPI_i = \frac{E_i - E_{i,baseline}}{GHG_{baseline} - GHG} \qquad (S3)$$

Where GHG is quantified as the product of the 100-year global warming potential coefficient (GWP) and the emissions (GHG units in t CO_2e).

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