Supplementary material: Human health and ecosystem impacts of deep decarbonisation of the energy system

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Review of the literature on the integration of LCA and ESOM.

**Number of technologies mapped:** Only two studies established an equivalent for all the technologies (i.e. complete mapping) in the ESOM\(^1\), and it was for simplified models, with less than 200 technologies. Several of the studies based on input-output approaches matched a larger number of technologies\(^3,4\) using on sector resemblance and acknowledged that this approach erodes representativeness.

Several studies limited the number of technologies to be mapped considering fewer sectors than those included in the original model. A majority of studies focused on the electricity sector. Limiting the boundaries of the system under study to a subcomponent of a wider model would miss all the effects occurring outside the sector under study, despite all being interconnected by energy vectors. It is especially unwarranted when analysing the effects of changes in the system, what is known as consequential assessments (CLCA) in the LCA literature. It is also problematic when LCA results are integrated into the optimisation problem, as it produces biased models.

The studies that introduced LCA coefficients but only for certain sectors acknowledge that this produces biased models whose results should be carefully interpreted\(^3\,5\). Moreover, addressing key policies, such as electrification of transport and heat services requires multisectoral approaches\(^1\). It also means “losing” the strength of large multisectoral models.

**LCA Scope:** Most of the studies are attributional (ALCA), and there are very few consequential ones (CLCA). However, the distinction is rarely stated and has been inferred from the objective and methodological approaches. Some of the CLCA assume that the use of TIMES model is inherently consequential\(^6\) because system expansion is used to deal with multifunctional processes inside the regions under study. However, what is important is how the allocation is solved when it cannot be avoided, for example with processes where only some co-products are outside the system boundary. A practical example is the expansion of second-generation biofuel based on residues. In CLCA versions of ecoinvent, by-products are considered to be constrained. Hence a rise in production cannot be based on co-products. Thus, the use of an attributional database on a consequential assessment wrongly assumes the expansion of production from by-products is a possibility.

**Parameter harmonisation:** Several of the previous studies have done harmonisation of ESOM and LCA parameters either at inventory or impact score level. However, the effect of harmonisation has not yet been assessed. Efficiencies appear to have been only adapted in one study and at impact score level\(^7\), which implies the assumption that the impact of a given technology is directly proportional to its efficiency. Harmonising at score levels means contribution analyses using the LCA matrix formulation cannot be done.

**Fuel switching:** An additional difficulty is how to model changes in fuel mixes. Many of the promising technologies to reduce GHG emissions involve using biofuels or hybrid electric powertrains. Taking these changes into consideration requires procedures to add new fuels and modify emissions accordingly. To the best of our knowledge, such a procedure has not yet been addressed in the literature.

**Reproducibility and documentation:** There is substantial room for improvement on how the integration studies are documented\(^8\). Integration procedures should be unambiguously described, ideally “codified” in a software program so they can be analysed, reproduced and reused\(^9\). Some good examples include the work of Rauner and Budzinski\(^1\) and Mendoza-Beltran and colleagues\(^10\).
<table>
<thead>
<tr>
<th>Ref.</th>
<th>Model scope</th>
<th>Sectors considered</th>
<th>N tech. mapped</th>
<th>Model</th>
<th>Substances modelled</th>
<th>Model paradigm</th>
<th>harmonisation</th>
<th>LCA Scope</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>Multisector</td>
<td>Electricity</td>
<td>21 tech x 9 regions</td>
<td>WEM</td>
<td>CO₂, CH₄, N₂O, HFCs, PFCs, SF₆, SO₂, NOₓ, PM₂.₅ (¹²)</td>
<td>Simulation &amp; bottom-up ESOM</td>
<td>CF from WEM</td>
<td>ALCA</td>
</tr>
<tr>
<td>13</td>
<td>Electricity</td>
<td>Electricity</td>
<td>21</td>
<td>REMix</td>
<td>Not documented</td>
<td>Bottom-up ESOM</td>
<td>CF and lifetime from REMix</td>
<td>ALCA</td>
</tr>
<tr>
<td>14</td>
<td>Electricity</td>
<td>Electricity</td>
<td>21</td>
<td>REMInd</td>
<td>CO₂, CH₄, N₂O, SO₂, BC, OC, NOₓ, CO, VOC, NH₃ (¹⁵)</td>
<td>Hard-linked bottom-up ESOM and macro-economic optimisation</td>
<td>CF, CO₂ EF and lifetime</td>
<td>ALCA</td>
</tr>
<tr>
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<td>Multisector</td>
<td>Electricity</td>
<td>11 tech. x 11 regions</td>
<td>REMInd</td>
<td>CO₂, CH₄, N₂O, SO₂, BC, OC, NOₓ, CO, VOC, NH₃ (¹⁵)</td>
<td>Bottom-up ESOM (TIMES)</td>
<td>Not done</td>
<td>CLCA</td>
</tr>
<tr>
<td>2</td>
<td>Multisector</td>
<td>Multisector</td>
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<td>MIRET</td>
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<td>Bottom-up ESOM (TIMES)</td>
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<td>ALCA</td>
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<td>Electricity</td>
<td>36</td>
<td>TIMES-SPAIN</td>
<td>CO₂, CH₄, N₂O, CO, NOₓ, SO₂, PM₂.₅, PM₁₀</td>
<td>Bottom-up ESOM (TIMES)</td>
<td>Not done</td>
<td>ALCA</td>
</tr>
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<td>Multisector</td>
<td>43</td>
<td>Swiss – Markal</td>
<td>CO₂</td>
<td>Bottom-up ESOM (TIMES)</td>
<td>Partial, based on other prospective LCI.</td>
<td>ALCA</td>
</tr>
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<td>Multisector</td>
<td>Multisector</td>
<td>203</td>
<td>Global Multi-regional Markal</td>
<td>CO₂</td>
<td>Bottom-up ESOM (Markal)</td>
<td>Indicators scaled to consider efficiency differences</td>
<td>ALCA</td>
</tr>
<tr>
<td>4</td>
<td>Multisector</td>
<td>Electricity</td>
<td>15</td>
<td>ETM-UCL</td>
<td>CO₂, CH₄ and N₂O</td>
<td>Bottom-up ESOM (TIMES)</td>
<td>Not done</td>
<td>ALCA</td>
</tr>
<tr>
<td>3</td>
<td>Multisector</td>
<td>Electricity</td>
<td>250</td>
<td>UK-TIMES</td>
<td>CO₂, CH₄, N₂O and HFCs</td>
<td>Bottom-up ESOM (TIMES)</td>
<td>Not done</td>
<td>ALCA</td>
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<tr>
<td>1</td>
<td>Electricity</td>
<td>Electricity</td>
<td>18</td>
<td>MOroSA</td>
<td>CO₂</td>
<td>Multi-objective optimisation</td>
<td>EF</td>
<td>ALCA</td>
</tr>
</tbody>
</table>

CF: capacity factors, EF: emission factors

Table S1: Summary of studies integrating LCA with energy system optimisation models
Methods

NATEM – Quebec

This section presents the most recent updates from the version presented in Astudillo et al. and extends the documentation.

Energy balance

NATEM is calibrated using the National Energy use database to ensure coherence with national statistics. The NEUD relies heavily on the report on energy supply and demand (RESD) among other sources. The NEUD provides values of energy use by fuel and by end-use, grouped by sector for each Canadian province. During calibration, the energy by end-use is disaggregated by technologies that provide those services using the stocks of each technology and explanatory variables such as efficiency. The calibration process allows characterizing current technologies with parameters related to their use (e.g. passengers per vehicle) and their efficiency (e.g. MJ of fuel per km). The parameters related to the use of technologies are kept constant during the whole simulation period.

The calibration is done in a way that the energy consumption and delivery of energy services in the year of reference in NATEM match the values of the NEUD. For coherence, we use the fuel properties reported in RESD. Biodiesel and ethanol are not reported in the RESD, and higher heating values of 35.82 and 23.49 MJ/l were considered. The energy needs are then projected until 2050 based on the expected evolution of a series of drivers (Fig. S1).
Fig. S1: Evolution of drivers for energy services in NATEM-Quebec. Values are normalised with respect to 2011 levels. Methods to estimate drivers are described in ref. 20.

**Greenhouse gas emissions balance**

GHG of fuel combustion are a function of the amount of fuel consumed and the emission factor (EF), that is, the amount of emissions per unit of fuel combusted. NATEM accounts for the CO₂, CH₄, and N₂O emissions from combustion. The EFs per unit of fuel use are derived from the National Inventory Report (NIR) on GHGe, which relies on the RESD for the energy commodities. The consistency of sources ensures a consistent accounting of GHG from energy commodities across the country and provinces. NIR considers different emission factors depending on the sector, as characteristics of fuel and combustion units vary. The CO₂ EF and CH₄ EF of transport have been updated for this study to the latest version of the report 21.

For fuels that are not covered in the inventory (wood pellets and biogas), EFs are derived from the LCA database ecoinvent (v3.5) 22. CH₄ and N₂O emissions from solid biomass in the NIR inventory (table A6-34) are very high, around 22 g CO₂eq/MJ LHV biomass, 25% of the CO₂ emissions of light fuel oil. The NIR EFs for biomass are based on a report from 2006 and are most likely outdated. Stoves built in 2004 had already emissions one order of magnitude lower 23.
Therefore we used values from the ecoinvent database, which are more in line with current wood stoves. Like in many other studies, “biogenic” CO$_2$ is assumed to have a global warming potential (GWP) of 0 (carbon neutrality assumption). While there is some delay in time between the absorption and release of bioderived CO$_2$, this period is very low in comparison with the residence time of CO$_2$ in the atmosphere.

Table S2: Sources of CH$_4$ and N$_2$O EF of biofuel combustion by sector

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Ecoinvent process</th>
<th>NATEM sectors</th>
</tr>
</thead>
<tbody>
<tr>
<td>Biomass burning (small scale)</td>
<td>heat production, mixed logs, at wood heater 6kW, state-of-the-art 2014</td>
<td>Residential</td>
</tr>
<tr>
<td>Biomass burning (large scale)</td>
<td>heat production, mixed logs, at furnace 100kW, state-of-the-art 2014</td>
<td>Electricity, industry, commercial, agriculture</td>
</tr>
<tr>
<td>Wood pellets (small scale)</td>
<td>heat production, wood pellet, at furnace 9kW, state-of-the-art 2014</td>
<td>Residential</td>
</tr>
<tr>
<td>Wood pellets (large scale)</td>
<td>heat production, wood pellet, at furnace 300kW, state-of-the-art 2014</td>
<td>Electricity, fuel supply</td>
</tr>
<tr>
<td>biogas</td>
<td>biogas, burned in micro gas turbine 100kWe</td>
<td>Electricity, residential, commercial,</td>
</tr>
</tbody>
</table>

To have coherent global warming mitigation pathways, aggregated CO$_{2eq}$ emissions for the reference year should be similar to emissions reported by the regions under study. The emissions included in NATEM correspond to the CO$_2$, CH$_4$ and N$_2$O emissions from stationary and transport fuel combustion as reported in the NIR. The total GHGs in the model are 58806 kt CO$_{2eq}$ in 2011, 1.3% lower than the reported emissions from Quebec in the same year $^{21}$. The discrepancy is low and considered valid. Differences could be due to slightly different EF for bioderived fuels.

Main scenarios

The study compares two scenarios, one with and one without GHG mitigation targets. GHG mitigation targets in the model are of 37.5% reduction by 2030 and 70% for 2050 with respect to 1990 levels, using linear interpolation to set up constraints for intermediate years. Provincial governments have an identical mitigation target for 2030, but higher (80%) for 2050. As explained in previous studies$^{17,20}$ the 80% mitigation target is not possible to achieve with the pool of technologies and constraints available in NATEM without changes in demand. Fig. S5 represents the GHG constraints per year compared with CO$_{2eq}$ emissions in 1990.

We note that emissions in 2011 were reported using GWP of the IPCC 4$^{th}$ assessment report, while the constraints for the future use GWP of the 5$^{th}$ assessment report. The updated GWP are slightly higher for methane and lower for N$_2$O. Nonetheless, combustion emissions are overwhelmingly dominated by CO$_2$, thus the differences in CH$_4$ and N$_2$O EFs are not expected to have a significant effect on the results.

Update of the transport sector

Previous work underlined the importance of the transport sector in the decarbonisation of Quebec energy system$^{17}$. Early iterations of the model also showed the relevance of the
transport sector in GHG reduction. In this study, the modelling of the transport sector has been revised and actualised to provide a more robust assessment of the mitigation options. Since this study does not consider modal shifts, the focus has been on the technologies that consume most of the energy (i.e. intra-modal improvements).

**Existing technologies**

The NATEM model is calibrated with statistics from the Canadian government. Aggregated data on fuel consumption by sector is reconciled with data on kilometrage, fuel consumption and stock to estimate the average load of different transport options. The load of a given energy service (i.e. average number of passengers or tonnes per vehicle) is estimated as the annual aggregated activity divided by the annual average distance travelled and kept constant during the whole period.

The average fuel consumption is derived from the average fuel consumption, converted to fuel consumption per unit of energy using HHV of the RESD report. Biofuels are assumed to have the same efficiency per unit of energy that the fossil fuel counterparts but their lower HHV is considered in the estimation of fuel consumption.

**New technologies**

**Powertrains**

With respect to previous versions of NATEM the heavy, medium and light freight, small car, large car, light passenger truck and urban buses have been updated. These technologies are the most energy-consuming, and therefore a priority for GHG mitigation. Table S2 details the powertrains that have been considered in road transport.

<table>
<thead>
<tr>
<th>Powertrains considered in different road transport segments</th>
<th>Heavy freight</th>
<th>Medium freight</th>
<th>Light freight</th>
<th>Small car</th>
<th>Large car</th>
<th>SUV</th>
<th>Urban bus</th>
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<td>ice-ci</td>
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<td>ice-cng-si</td>
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<td>Battery</td>
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<td>cat-ers</td>
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</table>

**Efficiency and costs**

**Cars**

In NATEM the passenger transport market is segmented in small cars, large cars and light trucks (i.e. SUV). The small and large car can provide long and short distance travel services. The efficiencies and costs of the technologies are based on data from the THELMA project, which assessed efficiencies and costs of current and future passenger transport powertrains under different driving cycles. The Thelma project estimated current and future efficiencies using...
backward facing simulation, that is, deducing the energy needs required to have a given speed profile. The analysis considered the principal forces involved in car dynamics (e.g. aerodynamic drag and rolling resistance) as well as the estimates of weight reduction over time. The technical details are provided in the final report of the Thelma project. The short distance energy consumption was estimated with the urban cycle and the long distance with the highway cycle as modelled in the THELMA project, which is based in the worldwide harmonized light vehicles test procedure (WLTP).

The matching between the technologies described in Thelma and those in NATEM required the following assumptions:

- Engines using ethanol are assumed to have the same efficiency (in passenger distance per unit of energy) than gasoline engines.
- Engines using biodiesel are assumed to have the same efficiency than diesel cars.
- GPL cars are assumed to have the same efficiency as CNG cars.
- Small cars (gross weight <1182 kg) approximated by the categories mini (830 kg, s= 80 kg) and small (988 kg, s=96 kg).
- Large cars (gross weight > 1182 kg) are approximated by the categories low-midsize (1191 kg, s=119), midsize (1371 kg, s=142) and up-midsize (1786 kg, s= 164 kg).
- Passenger light trucks are approximated by the cars in the category SUV.

Buses

Efficiency improvements for buses with different powertrains are derived from Cox et al. using the maxi-bus as the most suitable proxy (Cox, pers. Comm).

Freight transport

Freight road transport is considerably more complicated to model than passenger transport since much less data is available. For medium and heavy freight, efficiencies and costs come from a variety of sources. Electric road systems with catenaries are a promising technology, and here it is modelled as one of the alternative options. To our knowledge, this is one of the first assessments with ESOM considering this technology.

Light freight trucks have been modelled as light passenger trucks adapting fuel consumption due to higher loads. The increase of fuel consumption due to increased weight has been extrapolated using linear regression from THELMA data.

Airplanes

The efficiency of future passenger aircrafts is calculated from a recent prospective analysis of the Swiss commercial fleet. Fuel consumption has a strong non-linear relationship with flight distance. Hence average distance is an essential factor in the characterisation of the efficiency, particularly for short flights. For domestic flights efficiencies are based on the average distance of domestic flights in Canada (450km) (Statistics Canada, Pers. Comm.) For international flights, an average distance of 3000 km was assumed. Calculations are detailed on notebook 8.

Optimisation constraints

Constraints are used to represent technical or policy limitations to the space of potential solutions. We chose to limit constraints to the minimum, so results can be more easily

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interpreted. This means we do not introduce constraints to try to replicate non-optimising behaviour.

Transport

- Electric road systems are assumed to be viable only for 30% of the road heavy freight demand from 2030, as they are only cost-effective in routes with heavy traffic (IEA Future of trucks).
- Battery-based medium freight trucks are assumed to be viable for 30% of the traffic from 2030 when the technology becomes available.
- Battery electric cars can only cover 30% of the long-distance demand for passenger transport (small cars, large cars and light trucks).

Electricity (See 17 for details)

- The average and maximum share of annual electricity imports are assumed to do not increase above existing levels. This constraint represents energy security concerns (see Astudillo et al. 17 for details).
- The maximum and average share of intermittent renewable energy is limited to represent grid stability requirements.
- The resources available for renewable energy are limited.

Industry and agriculture (see 17 for details)

- Industry: The share of energy use in the form of electricity for each industrial sector is based on the maximum share of electrification of the same sector in other Canadian provinces. The minimum share of non-electric energy sources is fixed to 65% of the share at the start of the simulation period.
- Agriculture: The minimum share of energy coming from electricity is constant during the simulation period. The minimum share of other energy sources for 2050 is fixed at 50% of their market share in 2011.

Total Greenhouse gas emissions

GHG mitigation targets in the GW mitigation scenario are of 37.5% reduction by 2030 and 70% for 2050 with respect to 1990 levels, using linear interpolation to set up constraints for intermediate years.

The effect of constraints in the model can be analysed by the shadow price. Apart from the apparent effects of the constraint on GHG, other constraints of the model are affecting the solution. Constraints to electrification of road transport limit rates of electrification and further studies to refine assumptions would be of interest, particularly, to what extent road freight can be electrified. Other relevant constraints are the rate of electrification for energy demands of the industrial sector. There is a lack of detail on the statistics of energy consumption of the industrial sector 17 and this is hampering mitigation efforts.

Goal and scope

The formal definition of the study is framed using the “goal and scope” phase, the standard procedure used in LCA. The advantages of defining the study in a systematic manner using the “goal and scope” definition have also been recognised in the energy system model community31.
The goal of this study is to formalise the methods needed to quantify the potential environmental impact of broad changes in the energy system particularly, how to use the results of ESOM together with LCA to improve data quality. A secondary goal is to derive lessons for the energy transition of the region under study: the province of Quebec.

**Intended audience:** The intended audience can be divided between those who work either in LCA or ESOM, and those outside these fields of expertise. The use of jargon is avoided as much as possible, but a substantial amount of prior knowledge is required not to misinterpret the results. Therefore, an effort is made to underline the rationale and limitations of both LCA and ESOM.

**Functional unit:** The function of the system under study is to provide energy services to the province of Quebec for the period 2011-2050. On aggregate they represent the energy needs as quantified by the official statistics. These services are quantified for 2011 and projected until 2050 based on a series of exogenously defined drivers. The services as defined are considered independent (e.g. bus transport cannot substitute car transport). The model includes elasticities to the prices of energy services, meaning that the demand is to some extent dependent on its cost. The potential effects of the GW mitigation policy are studied comparing two alternative scenarios which fulfil the same energy services but one with the policy and a counterfactual scenario without. The study follows the CLCA paradigm, where studies attempt to assess the effects of changes in the system. CLCA attributes all the burden of the changes in the system to the origin of the change.

The demand (vector of demand in LCA) is composed of all processes that deliver ‘final’ energy services (as opposed to intermediate flows) and are identified as relevant by the screening algorithm plus the consumption of ‘non-relevant’ processes, consuming a commodity whose market is deemed relevant by the screening process. In our case, the electricity consumption of all final demands is considered because there are substantial changes in electricity supply.

**System boundary:** In line with the scope, the study aims to capture the most critical changes in the system. It does so with the help of a partial equilibrium optimisation model of the TIMES framework, probably the most widely used general-purpose ESOM. the model is described in detail in previous sections and publications\(^7\). TIMES models the market clearance (matching of supply and demand) on a defined market for energy services. The partial-equilibrium assumption means that markets outside the energy system can supply goods but do not see their clearance affected by what happens inside the system. These markets are defined by background LCA databases. Ideally, they would represent how the markets react to a change in demand during the studied period (2011-2050). The consequential version of Ecoinvent v 3.5, models only existing production of goods and services and not future ones\(^2\). Thus, results from our approach are as if the supply of services and goods from the “rest of the world” remains the same and as such should be interpreted. A potential future development would be to model how global supply chains may change with time, as partially done by Mendoza-Beltran et al.\(^10\).

### Table S4: Activities defining the demand vector and their respective proxy.

<table>
<thead>
<tr>
<th>NATEM process</th>
<th>name and location of ecoinvent proxy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Generic process of AGR sector</td>
<td>Non-existent, done from NATEM exchanges</td>
</tr>
<tr>
<td>Gasification</td>
<td>Non-existent, done from NATEM exchanges</td>
</tr>
<tr>
<td>Biodiesel from transesterification</td>
<td>Non-existent, done from NATEM exchanges</td>
</tr>
<tr>
<td>Ethanol from fermentation</td>
<td>Non-existent, done from NATEM exchanges</td>
</tr>
<tr>
<td>Ethanol from enzymatic hydrolysis</td>
<td>Non-existent, done from NATEM exchanges</td>
</tr>
<tr>
<td>Service Description</td>
<td>Details</td>
</tr>
<tr>
<td>------------------------------------------------------------------------------------</td>
<td>-------------------------------------------------------------------------</td>
</tr>
<tr>
<td>HFO used by auxiliary equipment (2015) (COM) (impr)</td>
<td>heat production, heavy fuel oil, at industrial furnace 1MW (CA-QC)</td>
</tr>
<tr>
<td>HFO used by auxiliary equipment (2025) (COM) (impr)</td>
<td>heat production, heavy fuel oil, at industrial furnace 1MW CA-QC</td>
</tr>
<tr>
<td>LFO used by auxiliary equipment (2025) (COM) (impr)</td>
<td>heat production, light fuel oil, at industrial furnace 1MW CA-QC</td>
</tr>
<tr>
<td>Generic process for other services in the COM sector</td>
<td>Non-existent, done from NATEM exchanges</td>
</tr>
<tr>
<td>Space heating by natural gas in COM sector (std.)</td>
<td>heat production, natural gas, at industrial furnace low-NOx &gt;100kW CA-QC</td>
</tr>
<tr>
<td>Coal use by cement manuf. (2012)</td>
<td>heat production, at hard coal industrial furnace 1-10MW CA-QC</td>
</tr>
<tr>
<td>Coal use in cement manuf. (2025)</td>
<td>heat production, at hard coal industrial furnace 1-10MW CA-QC</td>
</tr>
<tr>
<td>Heavy fuel oil used by other mining industries (2012)</td>
<td>heat production, heavy fuel oil, at industrial furnace 1MW CA-QC</td>
</tr>
<tr>
<td>Heavy fuel oil used by other mining industries (2025)</td>
<td>heat production, heavy fuel oil, at industrial furnace 1MW CA-QC</td>
</tr>
<tr>
<td>Coal used by non-ferrous metals industry (2025)</td>
<td>heat production, at hard coal industrial furnace 1-10MW CA-QC</td>
</tr>
<tr>
<td>Space heating in apartments by oil furnaces (impr)</td>
<td>heat production, light fuel oil, at boiler 10kW condensing, non-modulating RoW</td>
</tr>
<tr>
<td>Space heating in apartments by oil furnaces (med)</td>
<td>heat production, light fuel oil, at boiler 10kW condensing, non-modulating RoW</td>
</tr>
<tr>
<td>Space heating in detached houses by oil furnaces (impr.)</td>
<td>heat production, light fuel oil, at boiler 10kW condensing, non-modulating RoW</td>
</tr>
<tr>
<td>Space heating in detached houses by oil furnaces (med.)</td>
<td>heat production, light fuel oil, at boiler 10kW condensing, non-modulating RoW</td>
</tr>
<tr>
<td>Space heating in mobile homes by oil furnaces (impr.)</td>
<td>heat production, light fuel oil, at boiler 10kW condensing, non-modulating RoW</td>
</tr>
<tr>
<td>Domestic Passenger air transport (std.) (existing)</td>
<td>transport, passenger, aircraft, intracontinental RoW</td>
</tr>
<tr>
<td>Domestic passenger air transport (impr.) (2030)</td>
<td>transport, passenger, aircraft, intracontinental RoW</td>
</tr>
<tr>
<td>Domestic passenger air transport (std.) (2012)</td>
<td>transport, passenger, aircraft, intracontinental RoW</td>
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<tr>
<td>Domestic passenger air transport (impr.) (2015)</td>
<td>transport, passenger, aircraft, intracontinental RoW</td>
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<tr>
<td>International passenger air transport (impr.) (2030)</td>
<td>transport, passenger, aircraft, intercontinental RoW</td>
</tr>
<tr>
<td>Electricity exports to US-NPCC (existing)</td>
<td>electricity production, natural gas, combined cycle power plant US-NPCC</td>
</tr>
<tr>
<td>Electricity exports to US-NPCC (new)</td>
<td>electricity production, natural gas, combined cycle power plant US-NPCC</td>
</tr>
<tr>
<td>Marine freight transport (generic)</td>
<td>Non-existent done from NATEM exchanges</td>
</tr>
<tr>
<td>Heavy truck freight transport (diesel) (2012)</td>
<td>transport, freight, lorry &gt;32 metric ton, EURO6 RoW</td>
</tr>
<tr>
<td>Heavy truck freight transport (hybrid) (2012)</td>
<td>transport, freight, lorry &gt;32 metric ton, EURO6 RoW</td>
</tr>
</tbody>
</table>

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| Medium truck freight transport (diesel) (2012) | transport, freight, lorry 7.5-16 metric ton, EURO6 RoW |
| Light truck freight transport (diesel) (2012) | transport, freight, lorry 3.5-7.5 metric ton, EURO6 RoW |
| Light truck freight transport (hybrid) (2012) | transport, freight, lorry 3.5-7.5 metric ton, EURO6 RoW |
| Large car passenger transport (diesel) (2012) | transport, passenger car, large size, diesel, EURO 5 RoW |
| Large car passenger transport (gasoline hybrid) (2012) | transport, passenger car, large size, petrol, EURO 5 RoW |
| Large car passenger transport (gasoline) (2012) | transport, passenger car, large size, petrol, EURO 5 RoW |

**Cut-off criterion:** In theory, all the processes that change their production volume should be included in the analysis. However, since more than 600 processes change their emissions, we implement an screening algorithm to include only those that contribute more than 0.8% to the absolute changes in CO2eq emissions, the exception being the refinery process (responsible of 1.62% of changes in CO2eq emissions). Refining is a significant contributor but refinery emissions are entirely based on LCA assumptions and not updated by NATEM results. Refinery is an extremely complex process, with more than 8 products, and not major technological breakthroughs are modelled in NATEM, therefore we decided to skip the inclusion of this process and include others to compensate. The implementation reduces the number of processes exponentially to be considered, setting a balance between completeness and study feasibility. The procedure is documented in the electronic notebooks of the study, and it is the method we propose to simplify the mapping problem.

**Allocation:** How to allocate the burdens of multifunctional processes has long been debated in the LCA field. For processes within the energy system, allocation can be avoided by means of system expansion. Multifunctional processes, namely biodiesel and electricity autothermic gasification have to be simplified to single-output unit processes using an allocation factor. Nonetheless, the aggregated results, (i.e. the effects of the change under study) are independent of these factors since all the co-products are used within the system. However, care should be taken in the contribution analysis during the interpretation phase, since knowing the life cycle impact of a specific observation in NATEM (e.g. the increase in the electrification of cars) requires the use of allocation factors. Several transport processes provide long and short distance travel, which is also problematic to model in LCA. The results of NATEM take into account the different fuel efficiency and technical constraints between both services. However, for simplicity, the LCA component aggregates both long and short distance travel in one single transport service. The process delivering the aggregated service has an efficiency based on NATEM, reflecting the total distance and total fuel consumption. The study uses the consequential version of ecoinvent 3.5, which is consistent with the scope of the study: the effects of changes induced by the GW mitigation policy.

**Data representativeness:** We consider the data quality, as assessed in LCA, to be adequate for a prospective analysis. Efficiencies and CO2 emission factors for the main contributors are based on NATEM, which is more representative of future technologies than ecoinvent. The selection of suitable proxies from ecoinvent is based on name resemblance. Usually, the same process is available in different regions. Priority was given to the version of the region under study (Quebec). If it did no exist “Rest of the World” or “Global” datasets were chosen. We note that there can be substantial regional differences in the environmental impact of a product or...
Efficiency values from NATEM are used to scale fuel use and airborne emissions. It is assumed that all airborne emissions of the adapted ecoinvent processes are due to fuel consumption. This is clearly the case for cars, where non-exhaust emissions are modelled separately. For other processes we considered it to be a reasonable assumption.

Efficiencies of a process in TIMES are defined differently than in LCA. The same process can have efficiency improvements over time. Thus, efficiencies are scenario specific. Therefore, different versions of the same process exist, one for the business as usual scenario, and another for the GW mitigation scenario.

Fuel inputs are adapted to represent the values of the TIMES model according to the following decision tree.

**Fig. S2:** Procedure to adjust the fuel mix and associated emissions of a process

**LCI Consistency:** NATEM quantifies energy commodities in energy terms, while ecoinvent usually uses mass. Thus, heating values for fuels are used in the conversion. The current version of ecoinvent rarely references the heating value considered in each process. This study uses values reported in ecoinvent v2, from which most of the datasets are derived. In transport processes, the function can be expressed in pkm/Tkm or km. In cases where the definition differed between NATEM and ecoinvent, occupancy values of NATEM derived from the calibration were used. See notebook 1 for the details.
NATEM and ecoinvent model CO₂, CH₄ and N₂O emissions from combustion. CO₂ emissions are by far the most relevant emission from GW perspective (Fig. S3). Thus the harmonisation only affects CO₂ emission factors.

Fig. S3: Combustion emission factors of fuels per unit of energy in CO₂eq units. Emission factors are averaged per sector. Some fuels are just present in specific sectors.

For processes using blends of fossil and bio-derived fuels, only the CO₂ emissions are adjusted, reducing the CO₂ emissions by the % of bio-derived fuels. CH₄ emissions in natural gas and liquified natural gas are particularly high in the transport sector, although the relation is not apparent due to sector-averaging. For emissions that are included in ecoinvent but not in NATEM, ecoinvent values are used.

LCI Completeness: The inventory includes many changes in different parts of the energy system foreseen by changes in the market, improving completeness. The data sources of the main contributing processes (e.g. transport), as well as emission factors, are documented. Transparency is improved by documenting the use of times2lca in electronic notebooks.

Some processes required specific adaptations. For instance, hybrid electric vehicles do not exist in ecoinvent. Values from THELMA and the literature were used to include battery needs on them. Conveniently, LCI of be cars is also based on THELMA, increasing consistency. Other processes did not exist in ecoinvent and were created from zero. For those, the inputs and emissions come from NATEM. The process is documented in notebook 3.
Most of the processes are adaptations of Ecoinvent processes, which consider a wide range of emissions, therefore the account of emissions is considerably complete.

**Impact assessment method:** The study uses the impact assessment method Impact World+, the state of the art in LCA. The study report impacts to human health and ecosystem quality, referenced as “areas of protection” in the LCA literature as well as the contribution to different mechanisms to environmental damage. For specific flows which had a high contribution to impact scores and were occurring in a localised region, regional instead of global characterisation factors were used. An indicator on global warming emissions is also reported, because it is widely used in climate change mitigation studies. Additionally reporting global warming emissions allows to understand which emissions are neglected if only emissions from combustion in the region of interest are considered.

Impact World+ as well as alternative methods consider the impact of climate change in ecosystem quality and human health. For the calculation of CO$_2$eq emissions, global warming potentials developed by the IPCC were used. For consistency, we have chosen to keep the GWP of GHG as implemented by the ecoinvent database and LCA software such as Brightway2 or Simapro. However, this implementation does not include the effect of climate change feedbacks, as recommended by the UNEP-SETAC initiative and the IPCC. The reason argued is that the feedbacks are only accounted for some GHG and consistency was preferred instead of precision. As far as CH$_4$ and N$_2$O are not significant contributors to the GHG budget, the differences in implementation of GWP are not likely to affect the results significantly.

**Additional results**

![Fig. S4 Contribution of global warming to ecosystem quality or human health for energy-related processes of the ecoinvent database (ReCIPE, Impact world + method).](image-url)
In the BAU scenario, there are some emission reductions that occur purely by economic reasons. They are mainly driven by the introduction of road freight electric road systems and the substitution of heating oil by electric heating in commercial and residential sectors.

**Fig. S5:** NATEM CO$_{2eq}$ emissions per scenario

**Fig. S6:** Changes in supply chain-related CO$_{2eq}$ emissions grouped by sector (isic division). Most of them are directly related to the energy sector.
Fig. S7: Effects of LCI adaptations on CO$_{2eq}$ score (fuel efficiency, emission factors and fuel switching). Relative scores between adapted process and initial proxy.

Fig. S4 represents the relative CO$_{2eq}$ emissions between the final process and the initial proxy from ecoinvent, once the efficiency, emission factors and fuel mix is updated. Each proxy process is used at least two times (bau and mitigation scenario). In the higher end, much more efficient processes are found in vehicles with hybrid powertrains and airplanes. Hybrid vehicles are modelled from conventional ones, hence the difference in efficiency. For airplanes, the difference originates from fuel efficiency improvements in aviation.

In the lower end, heavy road freight diesel trucks are less efficient in NATEM. The differences in road freight are due to the low payloads result from the calibration. The low payloads are the consequence of an underestimation of freight service demand (MTkm) in the NEUD database. Activity levels are based on a subset of the road freight sector (CANSIM table 403-0004), which only partially covers the heavy freight activity. We decided not to modify payloads, because the final demand of freight truck is also based in the activity estimates. Hence results are overall correct. This example highlights how soft-linking can help to improve the quality of both models.
Fig. S8: Comparison of CO₂ combustion emission factors in the LCA database and NATEM.

The ecoinvent database and the Canadian National Inventory report use similar CO₂ emission factors for fossil fuels.

Fig. S9: Use-phase CO₂eq emissions per process included in the demand vector: comparison of NATEM and LCA model. Each process had its efficiency, CO₂ emission factor and production volume harmonised with NATEM, therefore ‘direct’ CO₂eq are expected to be very similar.

The comparison is grounded in the idea of ‘common measurement points’ where both models should render comparable results. Direct combustion emissions are indeed very similar, and we attribute minor differences to differences in non-CO₂ GHG emission factors.

References


