Supplementary information - Prioritizing regionalization to enhance interpretation in consequential life cycle assessment: application to the alternative transportation scenarios using partial equilibrium economic modeling

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Context of the C-LCA case study

The case study is defined in the context of the French law on the energy transition (LTECV: *Loi relative à la Transition Energétique pour la Croissance Verte*, referred to as LTE here) published in August 2015 (Assemblée nationale and Sénat de France 2015). The law proposes a set of targets to tackle climate change, preserve the environment and enhance energy independence in France. In the transport sector, the main objective of the LTE is to "develop clean transports to enhance the air quality and protect the health of French people". Its implementation is done with two targets: (i) 15% renewable energy consumption in the transport sector and (ii) a reduction of 30% in fossil primary energy consumption by 2030 as compared to the 2012 level.

Foreground life cycle inventory based on a partial equilibrium economic model

To model the foreground inventory model, we use a TIMES-based model, called MIRET, which is developed by IFP Énergies nouvelles and represents the energy and transport sectors in France (Menten et al. 2015). The partial equilibrium model is techno-explicit with a high technological resolution level for transport and energy production in France, which makes it possible to minimize the uncertainty due to the variability of the technological representation of the transport and energy sectors in France (Mathiesen et al. 2009). The reference energy system of the model includes set of potential technologies to meet the exogenous trajectories for end-use energy demands (sectorial heat and electricity demands, fuel for water and rail freight transport) and for end-use energy service demands (air, rail and land transportation for passenger and freight). This set of technologies includes technologies providing final energy and services (power plants, heat plants, refineries, biofuel plants, cars, airplanes, etc.) and technologies providing primary energy from domestic sources and imports (fossil resources as oil, coal and natural gas; renewables resources as biomass, wind and sun, etc.). On these trajectories of demand basis, the equilibrium is computed by maximizing total surplus in one pass for the entire set of periods. In other words, this dynamic model helps determine which technologies (primary energy and final energy production and use) will be needed to meet the exogenous demands (mobility demand, energy demand, etc.) in each time slice by minimizing the total system cost under constraints (technological constraints, regulation constraints, etc.). Therefore, the identified technologies are cost-optimal and are limited by the structure of the model (technologies available, granularity chose) and the nature of the partial equilibrium model where demands are exogenous. The processes affected by the decision to implement alternative transportation scenarios in France by 2050 are identified by calculating the difference between MIRET results of two scenarios.

- Scenario without decision: A business as usual (BAU) scenario without the implementation of the LTE
- Scenario with decision: An LTE scenario that defines alternative transportation scenarios. The LTE scenario is based on the BAU scenario where the three following constraints are added simultaneously:
    - Introduction of 15% of renewable energy in the transportation sector by 2030
    - Constraints relative to the annual measures proposed by the government in its PPE[1] to implement previous LTE targets (specific incorporation rates for advanced biofuels, specific maximum contribution of conventional biofuels, specific incorporation rates for biogas, a minimum number of electrified vehicles)
    - Reduction of 30% in primary fossil energy consumption applied in the transportation sector by 2030

In each time slice of the MIRET model, the activity level of each process (how much of the process is used in the model) in the MIRET model is compared in both scenarios. The activity level of each process is then aggregated over time for the 2009 to 2050 horizon with a linear interpolation between a selection of time slices (2009, 2015, 2019, 2025, 2030, 2050). The complete list of the 97 affected processes from the MIRET model is available in SI.

<u>Adaptation for background life cycle inventory and links with the foreground</u>

To compute the C-LCI, each MIRET affected process was linked to a corresponding background process from a generic LCI database. The latter provides a dataset with the cradle-to-gate inventory to complete the life cycle of the affected process and model the affected process itself. Most of the background processes are from the ecoinvent database (version v3.3, cut off) (Wernet et al. 2016) and must be adapted for our case study (Yang 2016). The mapping and adaptation between ecoinvent processes and each MIRET affected process have been done as follows (more details are provided in the excel file in SI):

- The selection of the ecoinvent process follows the hierarchy: French technology (FR) whenever available, European (RER), Rest-of-the-World (RoW) or global (GLO) otherwise.
- MIRET affected processes belonging to domestic resources, imports and exports are linked to market processes in ecoinvent.
- Other MIRET affected processes are represented by transformation processes (not market processes) in ecoinvent which are adapted as follows:
    - To avoid double counting between ecoinvent background process and foreground processes already modelled in the MIRET model, we remove from the

[1] PPE : Programmation Pluriannuelle de l'Energie

    ecoinvent processes all economic flows inputs occurring in France and existing in MIRET, such as electricity production, fuel production, feedstock production, etc.
  - Ecoinvent vehicle use processes are modified to account for emissions from biofuel blended fuels. The biofuel share within each vehicle evolves dynamically based on the optimization result of the MIRET model.
  - Vehicle use processes from ecoinvent are adapted to account for the technological progress in energy efficiency. The tailpipe emissions related to fuel consumption are adapted year by year based on the prospective fuel consumption of each vehicle as described in the MIRET model.
- If no ecoinvent process fits with the affected process, we create a new dataset based on data available in the literature. It was the case for ethanol tailpipe emissions (Dardiotis et al. 2015), new generation biofuel plants (MIRET model data), some biofuel production inputs (enzyme production (French National Research Agency 2017), catalyst production (Colling et al. 1996; Bournay et al. 2005; Casanave et al. 2007; Monnier et al. 2010; Battiston et al. 2014)).
- Reference units from ecoinvent (kg, kWh, MJ, tkm, vkm, m^3, etc.) are converted to fit the MIRET units (kt, GJ, Mvkm) for each affected process.

Estimation of spatial uncertainty sources in the MIRET model

Input variables of the MIRET model that may be subject to spatial variability were selected based on expert judgment. The prices of five different biomass commodities were considered based on their geographic origins. Among them are (i) prices of imported products from undefined foreign countries to France and not dictated by a global market and (ii) prices of French domestic products influenced by territorial origin. We found prices for the commodities from different regions based on historical price data and forecasting studies for each time slice (IFP Énergies nouvelles 2010; Ben Fradj et al. 2016; FAO 2016). We calculated the relative minimum and maximum values of their spatial variability by dividing the minimum P_{min} and maximum P_{max} prices observed or forecasted in different regions by a reference price P_{ref} from the literature. P_{ref} are set as follows: (i) for domestic products, P_{ref} are set to the mean price from the literature since values in MIRET for exogenous prices of French domestic products are generally set to the mean prices from the literature; (ii) for imported products, P_{ref} are set to the maximum price from the literature. Indeed, values in MIRET for exogenous prices of imported biomass products are set to artificially inflated values from the literature, to favor the use of domestic products instead of imported products as a first optimal choice. It better depicts the fact that French policy for biofuel wants to favor the use of national biomass resources for biofuel production before importing biomass.

We calculated the relative extrema for spatial variability by dividing the minimum P_{min} and maximum P_{max} prices observed or forecasted in different regions divided by a reference price P_{ref} from the literature. The relative minimum price and relative maximum price are respectively defined as $\%P_{min} = \frac{P_{min}}{P_{ref}}$ and $\%P_{max} = \frac{P_{max}}{P_{ref}}$. P_{min}, P_{max} and P_{ref} are determined based on price datasets defined as follows:

- Price datasets for 2 biomass commodities produced in France (wood chips and perennial crop miscanthus): The mean price is the reference price for the calculation of a relative spatial range of variability of prices.
    - Prices for wood produced in France are extracted from the Valerbio project which provided observed and prospective scenarios for wood reserve and prices for each department in France (IFP Énergies nouvelles 2010). The mean price of wood in France is calculated based on a wood reserve weighted average.
    - Prices and yields for the perennial crop Miscanthus for different regions in France are results of a simulation from the AROPAJ model developed at INRA (Ben Fradj et al. 2016). The mean price of Miscanthus in France is calculated based on a yield weighted average.
- Price datasets for 3 commodities imported to France (wood chips, palm oil, and soybean oil): The maximum price is set as the reference price for the calculation of a relative spatial range of variability. Prices are estimated from FAOSTAT database which provides the monetary value and the quantity imported to France per import country for each commodity from 2000 to 2013 (FAO 2016).

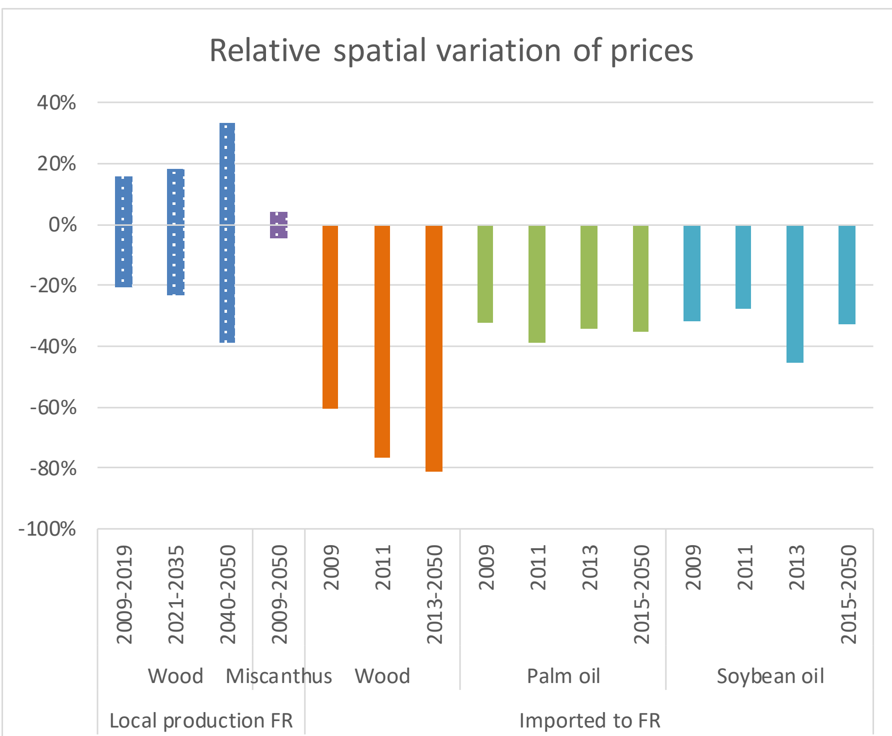


Figure 1 – Relative spatial range of variability used in the uncertainty analysis for prices of the five selected variables with a spatial variability in the foreground inventory for each time slice in the MIRET model (2009-2050 contains all time slices between 2009 and 2050).

Other uncertainty sources: LCIA data

Only spatial variability of global CFs for spatially-differentiated ICs is considered as the uncertainty source for the LCIA data as done in Patouillard et al (2019). This spatial variability is calculated based on the CF value of each native region weighted by the probability of the environmental intervention to occur in each native region as described in Bulle et al. (2019). It is represented with a four-parameter beta distribution using the moment method (Riggs 1989) to preserve at least the 4 parameters we knew for each CF: minimum and maximum values, variance and mean values. Four-parameter beta distribution is an alternative parametrization of the standard beta distribution (with 2 parameters) with a support of [min;max] instead of [0;1] and was the best fit we found compared to more classical distributions (normal, triangle, log-normal). Nevertheless, the fits were not perfect, and it would have been more representative to directly used sample values from the CF histogram. However, this implementation was not possible considering our means for this study. In addition, during the Monte Carlo simulation, we accounted for the LCIA spatial correlations between elementary flows produced by the same unit process only for the land transformation IC and for certain elementary flows. To do so, we sampled the value for CF "*from*" one type of land use to be spatially consistent with the sampled value for CF "*to*" the same type of land use. Other types of spatial correlation for regionalized ICs (spatial correlation at the product system level, spatial correlation between ICs, spatial correlation within IC between CFs, see Patouillard et al (2019) for more details) are not taken into account in this case study due to the challenge of implementing them in a reasonable amount of time.

Details on experimental design

A computer experimental design makes it possible to define sets of values for the selected inputs of a model within the space of their variation range (experimental region). The sets of values are not random, as they would be for a Monte Carlo sampling, but are chosen in a way to explore the experimental region while limiting the number of necessary runs.

GSA indicators based on Sobol variance decomposition

For the model $Y = m(X_1, \dots, X_k, \dots, X_K)$ where X_i are the uncertain (or random) variables of the model and Y is the output, the first-order sensitivity index ($SI1_{X_i}$) and total sensitivity index (SIT_{X_i}) for X_i are defined as follows (Saltelli et al. 2010):

$$SI1_{X_i} = \frac{Var(E(Y|X_i))}{Var(Y)} \quad (1)$$

$$SIT_{X_i} = SI1_{X_i} + \sum_{i \neq j} SI2_{X_i X_j} + \cdots + SIk_{X_i \dots X_k} \quad (2)$$

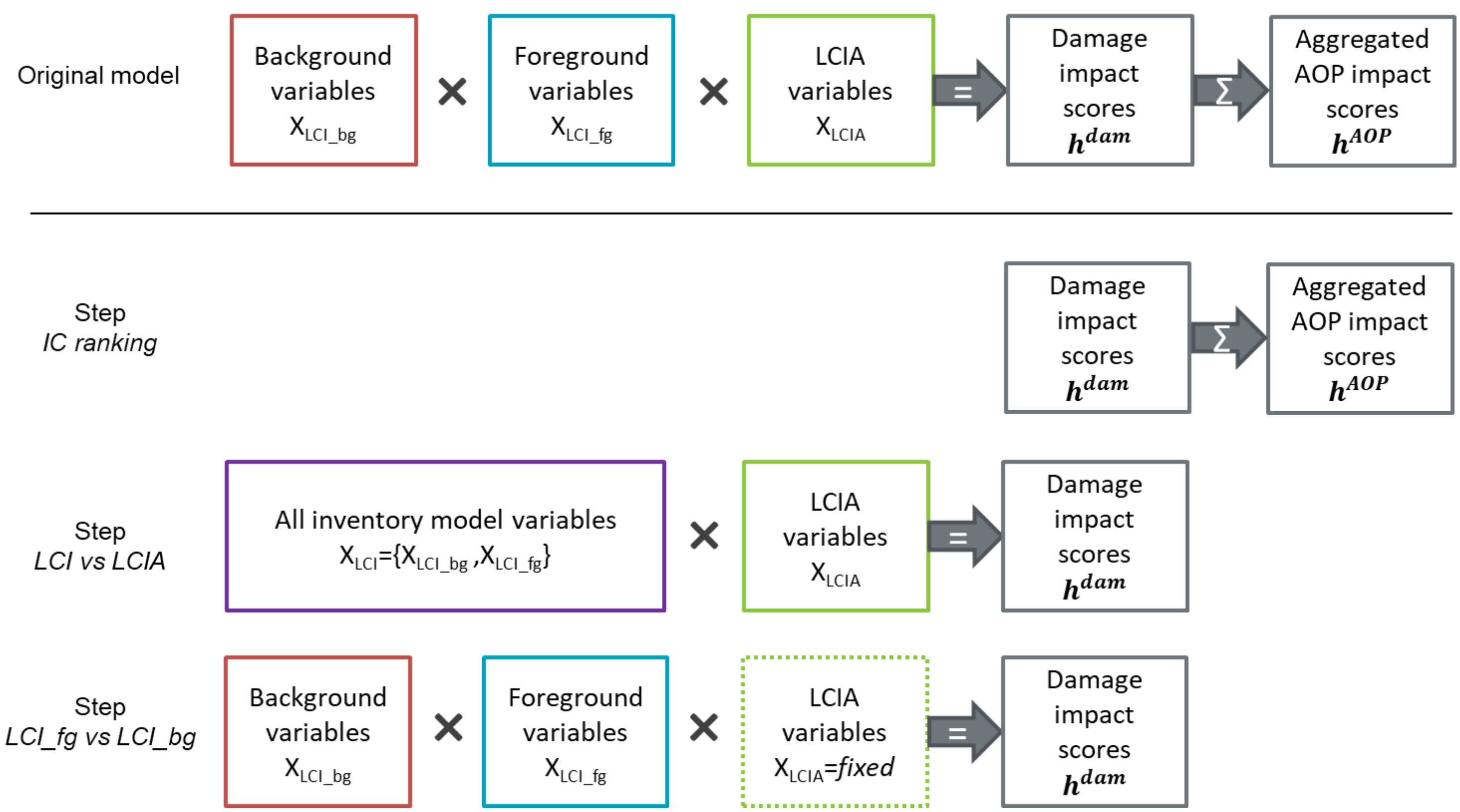
Where:

- $Var(Y)$ is the variance of Y;
- $Var(E(Y|X_i)) = E((E(Y|X_i) - E(E(Y|X_i)))^2)$. $Var(E(Y|X_i))$ is the variance of $E(Y|X_i)$ (the expectation of Y conditional on X_i). It represents "the expected reduction in variance that would be obtained if X_i could be fixed" (Saltelli et al. 2010).
- $SIk_{X_i \ldots X_k}$ is the k[th]-order sensitivity index which represents the sensitivity due to interactions between variables $X_i \ldots X_k$.

If $X_1, X_2, \ldots X_K$ are uncorrelated, the following equation can be written (Saltelli et al. 2010):

$$\sum_i SI1_{X_i} + \sum_i \sum_{j>i} SI2_{X_iX_j} + \cdots + SIk_{X_1 \ldots X_k} = 1 \ (3)$$

<u>Original C-LCA model and derived models for GSA</u>



A stepwise procedure to identify the main sources of uncertainty

Here, we describe the stepwise procedure used to identify the main sources of uncertainty for our case study. At each step, we performed a GSA on a specific model with the form $Y = m_{\mathrm{x}}(X_1, \dots, X_l, \dots, X_L)$ and estimated sensitivity indices as described in Patouillard et al (2019). The GSA interpretation to prioritize efforts for uncertainty reduction is explained at each step.

1. *IC ranking* step: determine which IC_j^{dam} is the main source of uncertainty for each IC_k^{AOP}.
   a. Model on which the GSA is performed: $\boldsymbol{h^{AOP}} = m_1\left(h_0^{dam}, \dots, h_j^{dam}, \dots, h_{J-1}^{dam}\right)$ based on the equation 5.
   b. Estimation of sensitivity indices
      i. m_1 is an additive model[2] so there is no interaction between variables. Therefore, only first-order sensitivity indices $SI1_{h_j^{dam}}$ are calculated.
      ii. h_j^{dam} are correlated in the model m_1, therefore $SI1_{h_j^{dam}}$ contains a correlated and uncorrelated part (Xu and Gertner 2008). We will not be able to distinguish the uncertainty contribution of each part but can still use $SI1_{h_j^{dam}}$ as an indicator for factor prioritization (Most 2012).
   c. Interpretation: For each IC_k^{AOP}, we ranked each IC_j^{dam} based on its $SI1_{h_j^{dam}}$ value. IC_j^{dam} with higher $SI1_{h_j^{dam}}$ are major contributors to the uncertainty of h_k^{AOP} and, therefore, should be prioritized for uncertainty reduction. This information is useful when the goal and scope of the LCA study do not focus on specific ICs.
2. *LCI vs LCIA* step: determine which group of variables between X_{LCI} and X_{LCIA} is the main source of uncertainty for each IC_j^{dam}.
   a. Model on which the GSA is performed: $\boldsymbol{h^{dam}} = m_2(X_{LCI}, X_{LCIA})$ based on the equation 4.
   b. Estimation of sensitivity indices
      i. $SI1_{X_{LCI}}$and $SI1_{X_{LCIA}}$are estimated based on mutated models, as described in Patouillard et al (2019).
      ii. As the model m_2 is a two-order[3] model where inputs are uncorrelated, the second-order sensitivity index $SI2_{X_{LCI},X_{LCIA}}$ can be calculated using the following equation $SI1_{X_{LCI}} + SI1_{X_{LCIA}} + SI2_{X_{LCI},X_{LCIA}} = 1$.
   c. Interpretation of sensitivity indices for this step makes it possible to prioritize efforts between inventory regionalization and inventory spatialization for IC_j^{dam} selected during the *IC ranking* step.
      i. if $SI1_{X_{LCI}}$ is the highest sensitivity index, the impact score uncertainty mainly comes from LCI variables, and the inventory should, therefore, be investigated for regionalization.
      ii. if $SI1_{X_{LCIA}}$ is the highest sensitivity index, the impact score uncertainty is mainly coming from LCIA variables, and the inventory should therefore be investigated for spatialization to use more regionalized CFs.
      iii. An $SI2_{X_{LCI},X_{LCIA}}$ (also refers as interaction sensitivity index) higher than other sensitivity indices indicates that the uncertainty mainly comes from

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[2] only addition signs between variables

[3] X_{LCI} and X_{LCIA} input variables of m_2 only interact each other with one multiplication sign and addition signs as defined in equation 4.

the interactions between both groups of variables. Therefore, no priority order may be drawn and both groups X_{LCI} and X_{LCIA} should be further studied.

3. *LCI_bg vs. LCI_fg* step: determine which group of variables between $X_{LCI_{bg}}$ and $X_{LCI_{fg}}$ is the main source of LCI uncertainty for each IC_j^{dam}.
    a. Model on which the GSA is performed: $\boldsymbol{h^{dam}} = m_3\left(X_{LCI_{bg}}, X_{LCI_{fg}}, \mu_{X_{LCIA}}\right)$ which is a derived model from m_2 where X_{LCIA} are set to their mean deterministic values ($\mu_{X_{LCIA}}$).
    b. Estimation of sensitivity indices
        i. SI1 for $X_{LCI_{bg}}$ and $X_{LCI_{fg}}$ are estimated based on mutated models, as described in Patouillard et al (2019).
        ii. As the model m_3 is a two-order model where inputs are uncorrelated, the second-order sensitivity index $SI2_{X_{LCI_{bg}},X_{LCI_{fg}}}$ are calculated using the following equation $SI1_{X_{LCI_{bg}}} + SI1_{X_{LCI_{fg}}} + SI2_{X_{LCI_{bg}},X_{LCI_{fg}}} = 1$.

Interpretation of sensitivity indices for this step makes it possible to prioritize inventory regionalization efforts between background and foreground LCI for IC_j^{dam} selected during the *IC ranking* step. Inventory regionalization efforts should be focused on: (i) the background LCI if $SI1_{X_{LCI_{bg}}}$ is higher than other sensitivity indices; (ii) the foreground LCI, i.e. the MIRET model here, if $SI1_{X_{LCI_{fg}}}$ is higher.

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