

Evaluation of energy transition pathways for the instant coffee industry: Supplementary materials

S1. OSMOSE tool

S1.1. General description of the workflow

OSMOSE ('OptimiSation Multi-Objectifs de Systèmes Énergétiques intégrés', i.e. Multi-Objective Optimization of Integrated Energy Systems) is a tool developed by the IPESE group of Ecole Polytechnique Fédérale de Lausanne (EPFL). The OSMOSE tool provides a combined mass, heat, and power integration and is able to optimize simultaneously environmental, economic, and thermodynamic targets. OSMOSE is a research tool coupling databases, optimization methods and solvers, simulation tools, as well as post-analysis methods (Flórez-Orrego, Ribeiro Domingos and Maréchal, 2022). The OSMOSE workflow is depicted in Figure S1.

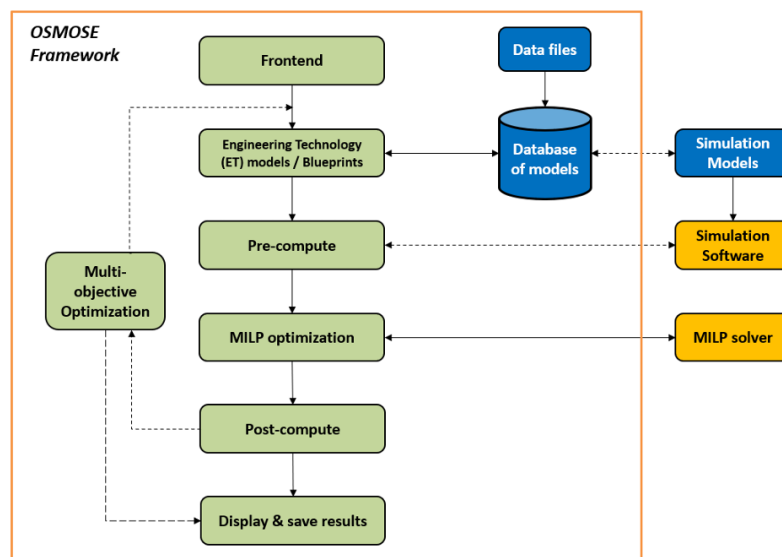


Figure S1: OSMOSE workflow.

The **frontend** is the routine launched for the execution of the OSMOSE workflow. In this file is defined the problem: the objective function, the choice of the solver and its settings, the choice of the decision variables and their value range in case of a multi-objective optimization, the loading of models and the definition of the superstructure (i.e. assembling of several ET models), the values of model parameters, the post-compute functions.

The **ET models** represent technologies converting material and/or energy inputs into material and/or energy products, by-products, waste and services. These models consist of:

- *Units*: elementary elements of the energy system, enabling mass and energy balances and introducing the operating cost and investment details (e.g., a reactor, a distillation column, ...);
- *Streams*: heat, electricity or material flowing into/out of a unit;
- *Layers*: "pipelines" allowing the streams to flow from one unit to another;

- *Parameters*: used in the definitions of the streams or units (e.g., size, temperature, specific cost, ...).

The **pre-compute** consists of all the necessary calculations performed before the problem optimization, e.g., the determination of a boiler's fuel consumption depending on its efficiency and heat production. The use of external software, e.g., Aspen, for the computation of state variables, such as specific consumption, unit cost or efficiency, is also possible.

After the execution of the pre-compute, the **Mixed-Integer Linear Programming (MILP) Optimization** is carried out as shown in Figure S2. The different ET models are gathered into a data structure. The data is then parsed into .MOD files, storing equations, and .DAT files, storing parameters. The .MOD and .DAT files are sent as input to the MILP solver which solves the optimization problem and generates a .OUT file. Finally, the output file is parsed into a data structure, before being sent to the post-compute module. The MILP problem consists of an objective function, mass and energy balances constraints, heat cascade constraints, and unit sizing constraints.

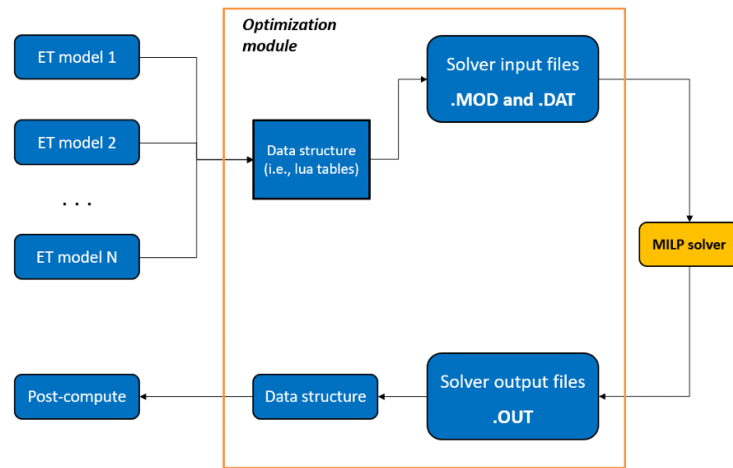


Figure S2: MILP optimization.

The **post-compute** functions allow the computation of various indicators (energy efficiency, environmental impact, cost, ...), as well as the displaying and saving (JSON format) of the obtained results (e.g., composite curves).

S1.2. Modeling and optimization framework¹

The process integration is modeled as a single multi-energy-system optimization problem, representing existing infrastructure, and the energy and material flows exchanged between subunits. On top of the business-as-usual configuration, the superstructure incorporates the potential solutions and associated degrees of freedom considered in the different transition pathways. These include heat-recovery systems, alternative energy vectors, and carbon-capture technologies. The superstructure provides the basis for defining the alternative configurations considered in the study. Based on the combinations of solutions and degrees of freedom represented, a set of configurations is defined for optimization, evaluation, and comparison.

For each configuration, the optimizer determines the installation, sizing, and operation of the technologies (units), subject to the technical and operational constraints of the system. These decisions are determined by minimizing the total annualized cost, which combines the annualized investment cost of the newly installed units with the annual operating cost. The latter accounts for electricity exchanged with the grid, natural gas purchased, the levy applied to fossil CO₂ emissions, etc.

¹ (Flórez-Orrego, Ribeiro Domingos and Maréchal, 2022)

The formulation distinguishes investment decisions from operating decisions. For each candidate technology, the optimizer determines whether the unit is installed and, if so, at what capacity. The optimizer determines how each installed unit operates, including its energy and mass flows. A unit's operating level is bounded by its maximum installed capacity, allowing the optimization to balance investment costs against operating costs while satisfying the system constraints. The total annualized cost minimized by the optimization is formulated as follows:

$$C_{tot} = \sum_{u \in Units} [(C_{1,u}^{op} \cdot Y_u + C_{2,u}^{op} \cdot M_u) \cdot \Delta t + C_{1,u}^{inv} \cdot Y_u + C_{2,u}^{inv} \cdot M_u]$$

where:

- C_{tot} is the total annualized cost of the overall system [€/y],
- $C_{1,u}^{op}$ is the fixed operating cost of unit u [€/h],
- $C_{2,u}^{op}$ is the variable operating cost of unit u [€/kg or €/kWh],
- Δt is the number of operating hours [h/y],
- $C_{1,u}^{inv}$ is the fixed annualized investment cost of unit u [€/y],
- Y_u is a binary variable indicating the presence or absence of unit u [-],
- $C_{2,u}^{inv}$ is the annualized specific investment cost of unit u [€/yr/(kg/h) or €/yr/kW],
- M_u is the installed capacity of the unit u [kg/h or kW].

The optimization is subject to the physical and operational constraints of the system. For each energy or material layer, the flows produced, imported, and consumed must balance:

$$\sum_{u \in Units} F_{u,l}^{out} + F_l^{imp} = \sum_{u \in Units} F_{u,l}^{in} + F_l^{exp}; \quad \forall l \in Layers$$

where:

- $F_{u,l}^{out}$ is the flow of layer l produced by unit u [kg/h or kW],
- $F_{u,l}^{in}$ is the flow of layer l consumed by unit u [kg/h or kW],
- F_l^{imp} is the flow of layer l imported from outside the system boundary [kg/h or kW],
- F_l^{exp} is the flow of layer l exported outside the system boundary [kg/h or kW],
- u denotes a unit, and l a layer.

All import and export flows are non-negative.

Heat is cascaded from higher to lower temperature intervals following the pinch analysis formulation. At each temperature interval r , the heat contributions from the utility units and process streams, together with the residual cascaded from the temperature interval above, must balance the residual passed to the temperature interval below:

$$\sum_{u \in Utilities} M_u \cdot q_{u,r} + \sum_{i=1}^{N_s} Q_{i,r} + R_{r+1} - R_r = 0; \quad \forall r = 1 \dots N$$

The cascade is closed at both ends, and heat can only be cascaded from a higher to a lower temperature interval:

$$R_1 = 0; R_{N+1} = 0; R_r \geq 0 \quad \forall r = 1 \dots N$$

where:

- $q_{u,r}$ is the heating or cooling load of utility unit u in interval r , per unit of installed size [kW],
- $Q_{i,r}$ is the heat load of process stream i in interval r [kW],
- R_r is the heat cascaded from interval r to the interval below [kW],
- N is the number of temperature intervals, defined by the supply and target temperatures of the streams.
- N_s is the number of process streams.

In addition to the general constraints of the optimization formulation, a set of constraints reflects the specific requirements and operating conditions of the system. The optimizer must therefore determine the appropriate installation, sizing, and operating decisions while satisfying all these requirements.

S2. Boiler efficiencies

Depending on the energy resource that is used, the thermal efficiency varies according to the values listed in Table S1 (ElementEnergy, 2018).

Table S1 : Boiler thermal efficiency as a function of the consumed fuel.

Energy source	Efficiency
Natural gas	85%
Biomethane	85%
Solid biomass	80%
Electricity	95%
Hydrogen	80%

S3. CO₂ capture using MEA-based chemical absorption

CO₂ capture with monoethanolamine (MEA) is schematically represented in Figure S3, according to (Kim and Léonard, 2025). Flue gases are first cooled down to 40°C before entering the absorption column. Within this column, CO₂ dissolves selectively in the MEA solution, leaving an almost CO₂-free gas stream at the top of the column. The CO₂-rich MEA is preheated from 51°C to 107°C by the CO₂-lean MEA coming from the bottom of the desorption column. The preheated CO₂-rich MEA stream enters the desorption column in which the MEA solvent is regenerated and leaves at the bottom at 119°C—and the captured CO₂ is retrieved at the top at 101°C. The captured CO₂ undergoes a cooling step—with a temperature decrease down to 40°C—prior a multi-stage compression. After heat exchange with the CO₂-rich MEA, the regenerated MEA at 61°C and make-up solvent are cooled down to 40°C before entering the absorption column.

The CO₂ compression process is depicted in Figure S4. The captured CO₂ enters the compression process at 40°C and 2 bar. Carbon dioxide undergoes a pressure increase in a compressor up to 4.3 bar, is cooled down to 28°C and the condensed water is removed thanks to a flash. These three steps are repeated but with a pressure increase from 4.3 bar to 18.6 bar. Once the CO₂ stream has reached 80 bar after a third compressor, the pressure of the supercritical CO₂ is brought up to 152 bar with a pump. The compressed CO₂ leaves the process at 30°C after passing through a fourth cooler.

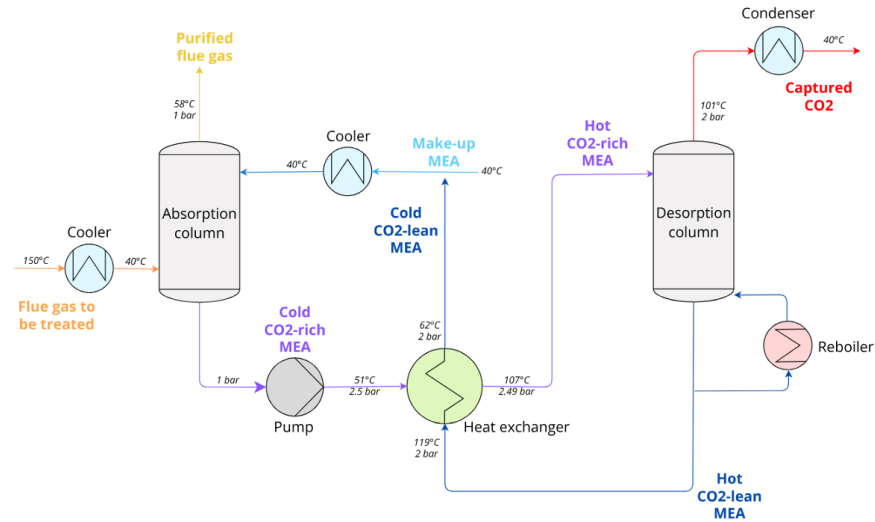


Figure S3: Process flow diagram of MEA-based CO₂ capture.

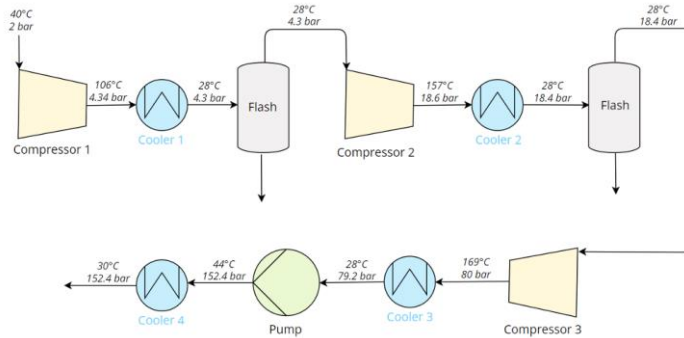


Figure S4: Process flow diagram of the CO₂ compression train.

The capture process requires steam (for the reboiler of the desorption column) produced by a natural gas fired boiler; as well as cooling water (for the coolers), and electricity (for the pump operation). For the CO₂ compression process, electricity (for the compression stages) and cooling water (for the intercooling steps) are necessary. The capture efficiency of the unit is assumed to be 90%. The energy requirements (steam, cooling water and electricity) and the investment costs for the CO₂ capture and compression processes are based on correlations developed by (Kim and Léonard, 2025). These correlations depend on the flue gas flow rate, temperature, and CO₂ concentration. The data used in the model are listed in Table S2.

Table S2: Flue gas flowrate and inlet CO₂ concentration considered for each configuration.

Configuration	Flue gas flowrate (kmol/s)	Inlet CO ₂ concentration (%mol)
NG-CC	0.28	4
BioCH ₄ -CC	0.28	4
BM-CC	0.15	12
BM/NG-CC	0.25	5

S4. Estimation of indirect emissions for electricity in the 2050 scenario

Based on scenarios from the TYNDP report (ENTSOG and ENTSO-E, 2025), the following European electricity mix is considered for 2050.

Table S3: European electricity mix breakdown and corresponding emission factor in the 2050 scenario.

Type	Share	Impact (kgCO ₂ /kWh)	Remarks
Wind onshore	31.7%	0.019	Average of (ecoQuery, 2022k) and (ecoQuery, 2022i)
Wind offshore	24.5%	0.015	From (ecoQuery, 2022j)
Solar	33.1%	0.090	Average of (ecoQuery, 2022f), (ecoQuery, 2022h), and (ecoQuery, 2022g)
Other RES	2.0%	0.063	From (ecoQuery, 2022a)
Hydro and pumped storage	4.6%	0.315	From (ecoQuery, 2022b)
Nuclear	3.6%	0.006	From (ecoQuery, 2022e)
Methane	0.4%	0.501	Average of (ecoQuery, 2022m), (ecoQuery, 2022l), (ecoQuery, 2022d), (ecoQuery, 2022c)

The 2050 global emission factor for electricity can be computed as follows:

$$EmF_e = \sum_{t \in type} s_t \cdot i_t \quad (1)$$

Where s_t and i_t represent, respectively, the share and the specific impact of electricity produced via route t .

S5. Parameters for CAPEX estimation

The parameters used for CAPEX estimation are gathered in Table S4. Since substituting natural gas with biomethane does not pose any technical problems, it is assumed that the same burners can be used. Due to lack of data, only CAPEX values related to the boilers are considered. Auxiliary equipment is assumed identical across all configurations and is thus neglected. Due to lack of data, CAPEX increase to switch from batch to continuous roasting is assumed null.

Table S4: Reference CAPEX, lifetime, and discount rate considered for each unit.

Unit	CAPEX	Lifetime (years)	Discount rate
NG	190 € ₂₀₁₈ /kW (ElementEnergy, 2018)	25	6%
BioCH ₄	190 € ₂₀₁₈ /kW (ElementEnergy, 2018)	25	6%
Electric	137 € ₂₀₁₈ /kW (ElementEnergy, 2018)	25	6%
Biomass	590 € ₂₀₁₈ /kW (ElementEnergy, 2018)	25	6%
Hydrogen	228 € ₂₀₁₈ /kW (ElementEnergy, 2018)	25	6%
CC-MEA	1057–1390 M€ ₂₀₂₃ /Mt/y (Kim and Léonard, 2025)	30	8.5%

S6. Commodities prices and STCs across Europe

In Table S5 are listed the energy commodities prices across Europe, considered for the economic assessment.

Table S5: Electricity, natural gas, biomass, biomethane, and hydrogen prices (in €/MWh) across Europe.

Country	Electricity ^a	Natural gas ^b	Hydrogen ^c	Biomass	Biomethane
Austria	201	69	229	30	95
Belgium	194	50	269	29	85
Bulgaria	143	47	236	24	75
Croatia	228	52	194	25	80
Czechia	183	59	229	26	75
Denmark	123	71	164	26	78
Estonia	142	64	195	21	78
Finland	79	97	191	25	78
France	164	68	221	28	90
Germany	228	72	194	37	98
Greece	195	50	161	32	95
Hungary	211	56	272	24	75
Ireland	270	70	130	29	90
Italy	233	64	194	32	105
Latvia	135	57	218	22	78
Lithuania	158	54	190	22	78
Luxembourg	177	68	283	30	95
Netherlands	202	84	157	29	80
Poland	199	71	193	23	75
Portugal	131	54	171	29	90
Romania	171	56	241	24	75
Slovakia	195	66	254	25	78
Slovenia	154	64	261	25	78
Spain	139	51	171	29	85
Sweden	96	106	179	23	78

a (Eurostat, 2025a)
b (Eurostat, 2025b)
c (European Hydrogen Observatory, 2024)

These commodities costs result in the following specific total costs (STCs) for the different production configurations investigated:

Table S6: Specific total costs (€/t instant coffee) for different configurations across Europe.

Country	NG	NG-CC	BioCH ₄	BioCH ₄ -CC	EL	Green H ₂	BM	BM-CC	BM/NG	BM/NG-CC
Austria	1453	1871	1552	2153	2433	2961	1062	1876	1218	1764
Belgium	1245	1629	1433	2015	2348	3349	1008	1795	1067	1592
Bulgaria	1063	1432	1182	1737	1734	2859	805	1551	894	1388
Croatia	1367	1761	1486	2066	2758	2685	1079	1863	1183	1706
Czechia	1301	1698	1302	1865	2216	2907	933	1691	1096	1599
Denmark	1238	1645	1152	1708	1493	2064	762	1509	998	1495
Estonia	1227	1625	1209	1768	1722	2438	798	1551	1007	1508
Finland	1361	1805	1020	1567	963	2208	626	1360	1044	1532
France	1332	1741	1392	1977	1987	2769	928	1719	1101	1629

Germany	1563	1992	1663	2274	2758	2685	1181	2012	1320	1878
Greece	1248	1633	1534	2134	2360	2250	1052	1865	1070	1615
Hungary	1355	1753	1386	1954	2553	3430	1009	1775	1159	1669
Ireland	1670	2103	1710	2316	3264	2159	1250	2073	1432	1984
Italy	1500	1916	1746	2371	2818	2700	1195	2045	1280	1852
Latvia	1137	1522	1188	1746	1638	2651	781	1532	938	1437
Lithuania	1177	1561	1257	1819	1915	2435	850	1608	987	1490
Luxembourg	1371	1783	1480	2076	2143	3440	990	1797	1140	1680
Netherlands	1603	2047	1408	1983	2445	2230	1017	1794	1324	1842
Poland	1466	1888	1350	1916	2408	2588	969	1731	1226	1733
Portugal	1096	1474	1293	1872	1589	2160	833	1614	906	1427
Romania	1235	1625	1266	1826	2071	2994	889	1643	1039	1540
Slovakia	1405	1817	1368	1938	2360	3198	974	1743	1180	1692
Slovenia	1263	1663	1245	1807	1866	3147	851	1607	1043	1546
Spain	1090	1465	1268	1840	1686	2184	843	1613	909	1422
Sweden	1501	1963	1071	1622	1168	2136	668	1408	1156	1648

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