1. Supplementary materials

Appendix A : Model documentation

A.1 MIRET-EU model

A complete description of the TIMES model equations appears in the ETSAP[1] documentation. The model estimates the energy dynamics by minimizing the total discounted cost of the system over the selected multi-period time horizon through powerful linear programming optimizers. The components of the system cost are expressed on an annual basis while the constraints and investment variables are linked to a period. The total cost is an aggregation of the total net present value of the stream of annual costs for each of the countries modelled. It constitutes the objective function (Eq. 1) to be minimized by the model in its equilibrium computation. A detailed description of the objective function equation is provided in Part II of the TIMES documentation (Loulou et al., 2016). We limit our description to giving general indications on the annual cost elements contained in the objective function:

- investment costs incurred for processes,
- fixed and variable annual costs,
- costs incurred for exogenous imports and revenues from exogenous exports,
- delivery costs for required commodities consumed by processes, and
- taxes and subsidies associated with commodity flows and process activities or investments.

$$NPV = \sum_{r=1}^{R} \sum_{y \in YEARS} (1 + d_{r,y})^{REFYR-y} * ANNCOST(r, y) \qquad (A.1)$$

NPV is the net present value of the total cost for all regions (the objective function);

ANNCOST(r,y) is the total annual cost in region *r* and year *y* (more details in section 6.2 of PART II (Loulou et al., 2016)

$\boldsymbol{d_{r,y}}$ is the general discount rate;

REFYR is the reference year for discounting

YEARS is the set of years for which there are costs, including all years in the horizon, plus past years (before the initial period) if costs have been defined for past investments, plus a number of years after end of horizon (EOH) where some investment and dismantling costs are still being incurred, as well as Salvage Value; and

R is the set of regions/countries in the area of study.

The MIRET-EU model is data driven[2], its parameterization refers to technology characteristics, resource data, projections of demand for energy services, policy measures, among other. This means that the model varies according to the data inputs while providing results such as technology pathways or changes in trade flows for policy recommendations. For each country, the model includes detailed descriptions of numerous

[1] https://iea-etsap.org/index.php/documentation

[2] Data in this context refers to parameter assumptions, technology characteristics, projections of energy service demands, etc. It does not refer to historical data series

technologies, logically interrelated in a Reference Energy System – the chain of processes that transform, transport, distribute and convert energy into services from primary resources and raw materials to the energy services needed by end-use sectors.

A.2 Integrate Europe

Integrate is a software for planning of complex and geographically confined energy systems.[3] The model can optimize investments in infrastructure for the most relevant energy carriers, including electricity, heating, cooling, natural gas, hydrogen, waste, and biomass, including conversions between these. Each technology is represented by a separate module in the model. The main energy component types are sources, conversion, storage, transport/distribution, end-use and markets.

The model combines linear programming (LP) for the calculation of operating costs with dynamic programming (DP) for the calculation of optimal investments. As shown in **Erreur ! Source du renvoi introuvable.** b), the model first calculates operating costs for all states and years, and then the optimal investment path is calculated.

The objective of the investment optimization is to find the investment pathway that minimize the net present value of all costs in the planning period, cf. Eq. (A.2).

$$\min_{I_{t\in T, d\in D}} \left\{ \sum_{t\in T} \delta^{t-T_{start}} \left(c_t^{inv} + c_t^{ope} \sum_{\tau\in\{1,\dots,T_{step}\}} \delta^{\tau-1} \right) - \delta^{T_{end}+T_{step}-T_{start}} \Phi \right\} \tag{A.2}$$

The Boolean investment variable I_{td} is one if investment *d* is carried out in year *t* and zero otherwise. See **Erreur ! Source du renvoi introuvable.** for a further elaboration of the Integrate model.

<u>Symbols</u>

c_t^{inv}	Investment costs in investment period *t*
c_t^{ope}	Annual operating costs for years in investment period *t*
D	Set of investment options
I_{td}	Binary investment variable, for investment period t and investment option *d*
T_{end}	First year of final investment period
T_{start}	First year of first investment period
T_{step}	Number of years for each investment period
δ	Discount rate for one year
Φ	Residual value of investments at the planning horizon

Integrate Europe is based upon the Integrate model methodology. For the representation of the European energy supply system as an aggregated single geographical node, a new set of components were developed

[3] https://www.sintef.no/en/software/integrate/

to represent 12 European energy resource types, 6 markets trade to/from the European energy system, 24 conversion technologies, 3 storage types, 10 end-use energy carrier types, and 7 energy need types. For each component type, a subset of technologies can be specified to represents the variation in characteristics for existing capacity or new investment options. Feasible energy flows between components are specified by connecting them, as shown for hydrogen components in **Erreur ! Source du renvoi introuvable.** a).

For each coupling between an end-use energy carrier and energy need there is a subset of corresponding end-use technologies. Among other things, those technologies are represented by existing capacities at the start of the planning period, levelized investment costs, and a maximum relevant utilization. The latter is included because the energy needs are aggregated categories. Existing capacities are depreciated linearly, whereas new capacity is optimized as a part of the operational optimization, typically once per decade.

A.3 HyPE model

HyPE is a delivery chain optimization model aiming at minimizing the total cost of hydrogen supply for a given set of production locations, exporting points, importing points and demand clusters. Choosing the most cost-efficient way to supply hydrogen to Europe requires considering different production technology options in the upstream (e.g. renewable energy, natural gas), transport modalities (e.g. trucks, pipeline and cargoes) and transport molecule (i.e. ammonia, liquified hydrogen, gasified hydrogen) in the midstram. The importing points and demand clusters are defined in the downstream. The resulting cost structure for supplying hydrogen from point-to-point is therefore driven by each of the steps of the delivery chai, ie. production costs, conversion and reconversion costs, terminal loading and unloading for the case of maritime routes and transport cost, which depends on the transport technologies and routes considered.

$$\begin{aligned} min_{(tech,xp,t,xe,xi,tmol,tm,trans)} \{ & \sum_{(\boldsymbol{tech},\boldsymbol{xp},\boldsymbol{t}) \in (\boldsymbol{TECH},\boldsymbol{XP},\boldsymbol{T})} \boldsymbol{PC}_{\boldsymbol{tech},\boldsymbol{xp},\boldsymbol{t}} + && \textit{(Production costs)} \quad \text{(A.3)} \\ & \sum_{(\boldsymbol{xe},\boldsymbol{xi},\boldsymbol{tmol},\boldsymbol{t}) \in (\boldsymbol{XE},\boldsymbol{XI},\boldsymbol{TMOL},\boldsymbol{T})} (\boldsymbol{CC}_{\boldsymbol{xe},\boldsymbol{tmol},\boldsymbol{t}} + \boldsymbol{RC}_{\boldsymbol{xi},\boldsymbol{tmol},\boldsymbol{t}}) + && \textit{(Conversion and reconversion costs)} \\ & \sum_{(\boldsymbol{xe},\boldsymbol{xi},\boldsymbol{t}) \in (\boldsymbol{XE},\boldsymbol{XI},\boldsymbol{T})} (\boldsymbol{LC}_{\boldsymbol{xe},\boldsymbol{t}} + \boldsymbol{UC}_{\boldsymbol{xi},\boldsymbol{t}}) + && \textit{(Terminal loading and unloading costs)} \\ & \sum_{(\boldsymbol{trans},\boldsymbol{ts},\boldsymbol{tm},\boldsymbol{t}) \in (\boldsymbol{TRANS},\boldsymbol{TS},\boldsymbol{T})} \boldsymbol{TC}_{\boldsymbol{trans},\boldsymbol{ts},\boldsymbol{tm},\boldsymbol{t}} + && \textit{(Transport costs)} \\ & \sum_{\boldsymbol{xi},\boldsymbol{t} \in (\boldsymbol{XI},\boldsymbol{T})} \boldsymbol{NSDP}_{\boldsymbol{xi},\boldsymbol{t}} \} && \textit{(Non-served demand penalty)} \end{aligned}$$

Symbols

$tech$	Set of production technologies
$trans$	Set of transport alternatives
xp	Set of production locations
t	Set of time steps
xe	Set of export points

xi	Set of import points
$tmod$	Set of transport modalities
$tmol$	Set of transport molecule
ts	Set of transport segments

The cost-minimization is performed in a country-neutral and technology neutral way. hydrogen production costs are calculated based on the time and location specific considerations (i.e. renewable potential, natural gas prices, land availability, WACC, etc) to compute the LCOH for the different production technologies considered. The countries under the scope are covered with a grid of 2.5 degrees from which centroids are defined to calculate the location specific LCOH of renewable hydrogen. Low-carbon hydrogen from natural gas and biomass are assumed to be produced nearby consumption and/or export sites within the exporting countries. The time availability of infrastructure for handling hydrogen (i.e., new hydrogen pipelines, natural gas pipelines reconverted to hydrogen and hydrogen terminals) are assumptions to the model which costs are integrated in the optimization. Further details are available in ref. **Erreur ! Source du renvoi introuvable.**.

A.4 Technical assumptions

Technological data regarding hydrogen production technologies used in the model are described and detailed in the table below.

Table 1 : Hydrogen production technologies – Technological Data

Technology	Size [MW]	Fuel Efficiency [PJ/PJ$_{H2}$] (LHV)				Life			Source
		Fuel	2020	2030	2050	2020	2030	2050	
Coal gasification, large size, centralized	1667	Coal	1.67	1.67	1.67	25	25	25	6, 9, 10
Coal gasification, medium size, centralized	434	Coal	1.67	1.67	1.67	25	25	25	6, 9, 10
Coal gasification + CO_2 capture, large size, centralized	1667	Coal	1.72	1.72	1.72	25	25	25	6, 9, 10
Coal gasification + CO_2 capture, medium size, centralized	442	Coal	1.72	1.72	1.72	25	25	25	6, 9, 10
Biomass gasification, small size, decentralized	0.7	Biomass	2.10	2.10	2.10	25	25	25	6, 8, 9, 10
		Grid electricity	0.03	0.03	0.03				
Biomass gasification, medium size, centralized	33	Biomass	2.10	2.10	2.10	25	25	25	6, 8, 9, 10
		Grid electricity	0.03	0.03	0.03				
Biomass gasification + CO_2 capture, medium size, centralized	33	Biomass	2.10	2.10	2.10	25	25	25	6, 8, 9
		Grid electricity	0.03	0.03	0.03				
SMR, large size, centralized	1530	Natural gas	1.32	1.32	1.32	25	25	25	1, 9
		Grid electricity	-0.02	-0.02	-0.02				

SMR, medium size, decentralized	2	Natural gas	1.36	1.27	1.27	25	25	25	6, 8, 10
		Grid electricity	0.25	0.07	0.07				
SMR + CO_2 capture, large size, centralized	1502	Natural gas	1.385	1.385	1.385	25	25	25	1, 8, 9
		Grid electricity	0.015	0.015	0.015				
ATR + CO_2 capture, large size, centralized	1260	Natural gas	1.36	1.36	1.36	25	25	25	8, 9
		Grid electricity	0.04	0.04	0.04				
GHR + ATR + CO_2 capture, large size, centralized	1260	Natural gas	1.28	1.20	1.20	25	25	25	8, 9
		Grid electricity	0.06	0.05	0.05				
Ethanol steam reforming, decentralized	0.01	Ethanol	1.47	1.47	1.47	10	10	10	6
		Grid electricity	0.08	0.08	0.08				
PEM electrolyzer	NA[4]	Grid electricity	1.60	1.55		6[5]	7	9	2, 3, 7, 9, 10
Alkaline electrolyzer, large size, centralized	72	Grid electricity	1.55	1.45		20	20	20	2, 3, 7, 9, 10
Alkaline electrolyzer, wind off grid, centralized	NA[4]	Wind off grid	1.55	1.45		30	30	30	2, 3, 7, 9, 10
Alkaline electrolyzer, PV off grid, centralized	NA[4]	PV off grid	1.55	1.45		30	30	30	2, 3, 7, 9, 10
PEM electrolyzer, offshore, centralized	NA[4]	Wind offshore	1.5			20	20	20	2, 3, 7, 9, 10
Alkaline electrolyzer, small size, decentralized	0,6	Grid electricity	1.55	1.45		20	20	20	2, 3, 7, 9, 10
Very High Temperature Reactor CHP, centralized	600	Uranium		1.5			60	60	6, 10
Kvaerner process, centralized	19	Natural gas	1.75	1.75	1.75	25	25	25	6
		Grid electricity	0.35	0.35	0.35				
Molten media methane pyrolysis, large size	420	Natural gas	2.05	2.05	2.05	20	20	20	11
Non-catalytic methane pyrolysis, small size	2.8	Natural gas	2.50	2.50	2.50	20	20	20	12

Source :

1. IEA 2019: The Future of Hydrogen
2. Blanco H., Nijs W., Ruf J., Faaij A., 2018a, Potential for hydrogen and Power-to-Liquid in a low-carbon EU energy system using cost optimization, Applied Energy 232, pp. 617-639
3. Blanco H., Nijs W., Ruf J., Faaij A., 2018b, Potential of Power-to-Methane in the EU energy transition to a low carbon system using cost optimization, Applied Energy 232, pp. 323-340
4. Sgobbi A., Nijs W., De Miglio R., Chiodi A., Gargiulo M., Thiel C., 2016, How far away is hydrogen? Its role in the medium and long-term decarbonisation of

[4] No reference size for costs provided. However, it is expected that the sizes are in the range between *Alkaline electrolyzer large size* and *Alkaline electrolyzer small size*, that is between 0.6 MW and 72 MW.

[5] The lifetime in *PEM electrolyser* are increasing due to R&D. Direct application in offshore parks has a higher lifetime due to the lower capacity factor and may be limited by the lifetime of the offshore wind turbines.

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5. Bolat P., Thiel C., 2014a, Hydrogen supply chain architecture for bottom-up energy systems models. Part 1: developing pathways, International Journal Hydrogen Energy 39, pp. 8881-8897
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10. NREL Technical Report NREL/TP-560-46267 September 2009 and NREL Technical Report NREL/TP-6A10-60528
11. Parkinson, B.; Tabatabaei, M.; Upham, D. C.; Ballinger, B.; Greig, C.; Smart, S.; McFarland, E., 2018, Hydrogen production using methane: Techno-economics of decarbonizing fuels and chemicals, International Journal of Hydrogen Energy 43, pp. 2540-2555
12. Keipi, T.; Tolvanen, H.; Konttinen, J., 2018, Economic analysis of hydrogen production by methane thermal decomposition: Comparison to competing technologies, Energy Conversion and Management 159, pp. 264-273