

Enabling an open database of ex-ante models and a process integration framework for supporting industry decarbonization

Daniel Florez-Orrego, Oktay Boztas, Meire Ribeiro Domingos, Pullah Bhatnagar, João Ferreira, Joseph Losteau, Luc Girardin, Bastian Bonard, Vibhu Baibhav, Dareen Dardor, Shubhangi Mishra, François Maréchal*

Industrial Process and Energy Systems Engineering (IPESE), École Polytechnique Fédérale de Lausanne (EPFL), Sion, Switzerland

* Corresponding author: daniel.florezorrego@epfl.ch

Abstract

Research outputs about industrial process decarbonization are frequently disseminated as insufficiently documented, static datasets behind access barriers. Thus, modelling efforts across institutions are usually duplicated rather than built upon prior validated work, limiting comparability, reproducibility, and validation by a broader community. Persistent knowledge-sharing deficiencies slows down the implementation of decarbonization pathways, as many industrial partners lacks resources, time or expertise to conduct comprehensive energy audits, remaining unaware of untapped efficiency gains. At the same time, the process integration methods have expanded their classical heat recovery approach into a systemic dimension encompassing other aspects of energy efficiency and conversion; carbon capture, use, and sequestration; industrial symbiosis and urban systems integration; waste management; electrification, power-to-X, and grid systems, demanding powerful modelling and decision-support tools that are seldom accessible to practitioners. To address these challenges, the IETS Task XXIV "Process Integration for Industry Decarbonization" enables an open-source, software-agnostic database of ex-ante models that captures model interfaces (energy, mass, emissions, and information connectors) exchanged with infrastructure grids, storage systems, or other models. Rather than enforcing complex ontological representations or exchange protocols, the template defines how a model connects to the external world through quality-attributed flows (e.g. composition, temperature, pressure, phase), and documents heating and cooling demands for heat cascade representation and process integration analysis. Structured metadata, referenced assumptions for engineering variables, and a class hierarchy model representation facilitates findability, validation, and versioning. A seven-tier sharing framework with data access, updating and maintenance protocols addresses intellectual property and confidentiality concerns across various academic and industrial stakeholders. An open-source computational framework leverages the models database to formulate a mixed-integer linear programming (MILP) problem that identifies the combination of models operating conditions, background ambient conditions, energy prices, infrastructure and regulatory constraints that minimize total cost and environmental impact. In this way, the generation, comparison, and selection of decarbonization scenarios can be automated, ranking them through sustainability metrics that can be visually reported to inform fast and accurate decision-making and support recommendations for the most suitable industry transition roadmaps.

Keywords: process integration, industrial decarbonization, open-source database, ex-ante models, pinch analysis, MILP, heat cascade, IETS Task XXIV.

1. Introduction

The transition toward carbon-neutral industrial systems requires comprehensive knowledge of process energy demands, waste heat availability, and performance characteristics of the decarbonization technologies. However, data underpinning industrial decarbonization studies is frequently scarce, paywalled, poorly documented, or unreliable. On the one hand, research outputs are often presented as static datasets that are difficult to compare, reproduce, or validate across institutions and software environments [1]. Researchers routinely duplicate modelling efforts rather than building upon validated, peer-reviewed contributions, resulting in an inefficient allocation of resources and inconsistent technology assessments. On the other hand, industries, mainly small and medium enterprises, often lack resources or expertise to conduct thorough energy audits, leaving substantial improvement potential unidentified within their own facilities [2]. These knowledge-sharing deficiencies create a fragmented landscape in which promising decarbonization configurations remain confined to individual research groups, while industrial partners lack actionable benchmarks for investment decisions, and policymakers rely on disparate datasets for energy transition planning. The absence of standardized, transparent, and accessible model repositories constitutes a significant barrier to the acceleration of industrial decarbonization at the pace required by international climate targets.

Meanwhile, process integration (or pinch analysis) has evolved from its classical heat recovery approach to include other decarbonization strategies, such as industrial heat electrification; fuel switching; carbon capture, use and sequestration; biomass conversion; and power-to-gas systems. More recent dimensions include seasonal storage, renewable energy management, and industrial-urban symbiosis for waste heat valorization and circular production strategies. This expanded scope demands a new generation of modelling and decision-support tools capable of handling multi-scale, multi-objective problems, while remaining accessible to academic researchers and industrial practitioners. To address these knowledge-sharing and dissemination gaps, Industrial Energy-Related Technologies and Systems (IETS) Technology Collaboration Programme (TCP) of the International Energy Agency (IEA) established Task XXIV “Process Integration for Industry Decarbonization” in early 2025. The Task gathers academic and industry participants across 13 countries (Belgium, Canada, Chile, Colombia, Denmark, France, Germany, Italy, Netherlands, Norway, Portugal, Sweden, and Switzerland) with a common interest in sharing models, methods, tools and experiences on industrial decarbonization through process integration [3]. Around 50+ participants from 25 institutions contribute to the Task under the coordination of the Swiss Federal Institute of Technology in Lausanne (EPFL).

The objective of Task XXIV is to enable international collaboration to create, document, and maintain an open-source database of ex-ante models covering industrial processes, energy technologies, and energy systems. Subtask 1 is organized into six main activities (Table 1): (1) standardizing ontologies and procedures for metadata, variables and models structure definition; (2-3) documenting model interfaces between processes, energy technologies, and energy systems; (4) comparing process integration techniques and tools; (5) recommending sustainability metrics for consistent performance benchmarking; and (6) disseminating results via meetings, annual reports, workshops, conferences, and engagement with professional societies. This paper presents the advances in two developments addressing the identified gaps: (i) the open-source IETS Task XXIV database of ex-ante models with its ontological framework, software-agnostic template, and tiered sharing protocols; and (ii) PinchSM, a

computational framework for process integration and optimization designed to interface with the database, and mandated by the Swiss Federal Office of Energy. The following sections describe the methodology, present the results of the frameworks development, and discuss implications for international collaboration on industry decarbonization.

Table 1. Overview of IEA IETS Task XXIV activities and their primary deliverables.

Activity	Description	Primary deliverables
1. Ontologies and procedures	Standardize ontologies and procedures for metadata, variables and models structure definition, and models sharing.	Software-agnostic template, metadata structures, confidentiality protocols, seven-tier sharing framework, class hierarchy tree
2-3. Model interfaces	Document interfaces between industrial processes (2), decarbonization technologies (3.1), energy systems (3.2).	Documented models and visualization tools for connectors, collaborative population of the open-access database
4. Process integration	Share experiences and compare process integration techniques and tools.	Repository of documented methods and optimization frameworks (MILP, metaheuristics)
5. Sustainability metrics	Compare results consistency across case studies and roadmaps through agreed performance metrics.	Benchmarking of decarbonization configurations, uncertainty ranges for technology performance
6. Dissemination and reporting	Disseminate via reports, workshops, conferences, and continuing education.	Annual reports, workshops, conferences, collaborative publications and industry engagement.

2. Methods

In this collaborative effort, intra- and inter-Task participants meetings and workshops helped define the models metadata and data essential for process integration, complying with FAIR (Findability, Accessibility, Interoperability, Reusability) principles for scientific and industrial database management [4–7]. Plenum meetings aligned the model representation concepts, addressed concerns on data disclosure levels, and outlined protocols for models validation and maintenance. Bilateral meetings served to express expectations, discuss specific issues, and build understanding within participant countries. Dissemination outside Task community (including a keynote lecture at ESCAPE 2025 conference and joint session at EUBCE 2025 conference) introduced perspectives on the complexity of existing ontological model standards and representations, and its pertinence for the scope of the Task XXIV. A comprehensive survey and bilateral engagement campaign (September to November 2025) gathered insights from all participating countries about other intellectual property concern and implications for leveraging industrial data to develop open models. Finally, the preliminary “rules of the game” were endorsed in the first in-person meeting at IBBCE 2025 conference in December 2025, where participants elaborated on the protocols for sharing, validating, and documenting a set of starting-point models. Next, the methods to define the minimum model content deemed necessary to achieve process integration and decarbonization analyses are presented. The tiered sharing protocol that handles data disclosure levels is described, and the proposed procedure for documenting ex-ante models is summarized.

2.1. Software-agnostic model concept definition

Formal ontologies and heavyweight standards offer comprehensive coverage but impose significant adoption costs, requiring extensive training and infrastructure that may not be

justified for process integration applications. Although lightweight ontologies may lack the precision needed for complex modelling scenarios, such as dynamic simulation or control-based modelling, a pragmatic approach can draw on existing ontological and standardization work, adapting it to specific requirements of process integration and industrial decarbonization assessments. Task XXIV adopts a simplified model structure designed to capture essential information for process integration analyses, while remaining accessible to partners with different modelling backgrounds and tools. This approach favors clarity and implementability over ontological completeness, while maintaining rigor for meaningful inter-institutional model exchange.

A process plant within an industrial cluster can be represented by an ex-ante model comprising process units operating under either continuous or batch regimes, each responsible for processing, treating, storing, or supplying process utilities. Each plant item (filters, columns, rotating equipment, vessels, reactors, heat exchangers, and pipelines) is associated with a specific unit operation within process units (separation, mechanical, storage, conversion, heat and mass transport). These items contribute to the mass, heat, power, and equipment-related flows that define interfaces through which the industrial process interacts with its surroundings: ecosphere, technosphere, infrastructure grids, and other process models. These interfaces ultimately define the integration opportunities available when the plant is embedded within a broader industrial or energy system. Figure 1 illustrates the structure of an ex-ante model that contains a process unit U with a nominal size S^*_u . The unit has associated a binary variable y_u (unit activation) and a continuous load factor f_u (capacity utilization factor). Depending on the modelling detail (white, grey, or black box), more than one representation (interface i) may exist with corresponding binary variables $y_{u,i}$ and load factors $f_{u,i}$. For instance, a white box model of a unit U involving detailed flow compositions and heating/cooling demands declares a different interface than a black box model that only provides knowledge about overall fuel and power consumption at the plant boundaries.

Internal transformations are governed by thermo-physical models and constitutive equations, which determine the mass flows $\dot{M}^-_{m,u,i} = F_{m,u,i}[\pi_{u,i}, S^*_u, (x \cdot \dot{M})^+_{m,u,i}]$, thermal demands $\dot{Q}_{T,u,i} = F_{Q,u,i}[\pi_{u,i}, S^*_u, (x \cdot \dot{M})^+_{m,u,i}]$, electricity demands $\dot{E}E_{u,i} = \Gamma_{EE,u,i}[\pi_{u,i}, S^*_u, (x \cdot \dot{M})^+_{m,u,i}]$, and equipment-related correlations $S_{Eq,u,i} = F_{Eq,u,i}[\pi_{u,i}, S^*_u, (x \cdot \dot{M})^+_{m,u,i}]$, where S^*_u is the process reference size. These equations are parametrized by physical constants and operating conditions ($\pi_{u,i}$) and inlet flows compositions $(x \cdot \dot{M})_{m,u,i}$. The impact accounting for equipment encompasses the construction ($S_{Eq,u,i} \cdot \dot{m}^{-C}_{Eq,e,i}$), lifetime auxiliary flows ($S_{Eq,u,i} \cdot \dot{m}^{-U}_{Eq,e,i}$), and end of life ($S_{Eq,u,i} \cdot \dot{m}^{-EoL}_{Eq,e,i}$). These relationships describe the ex-ante model as a bounded entity with clear-cut connections with the industrial infrastructure and other ex-ante models. Those connections include inlet material flows of feedstock ($\dot{M}^+_{F,i}$) and support material, energy, and waste streams ($\dot{M}^-_{r,i}$); outlet material flows as products ($\dot{M}^-_{P,i}$) and elementary flows to environment ($\dot{M}^-_{e,i}$); as well as interfaces for electricity input/output ($\dot{E}E^{\pm}_{u,i}$) and heat cascade contributions (heating or cooling demands $\dot{Q}^{\pm}_{T,u,i}$). In this way, the model supports process integration analysis by characterizing heat cascades and mass balances with quality attributes, while capturing lifecycle impacts from equipment construction through end of life.

Once the mathematical formulation of the ex-ante model is established, a class-attribute tree can provide a formal representation of the information architecture (metadata, data, and specifications) underlying the ex-ante model exchange template.

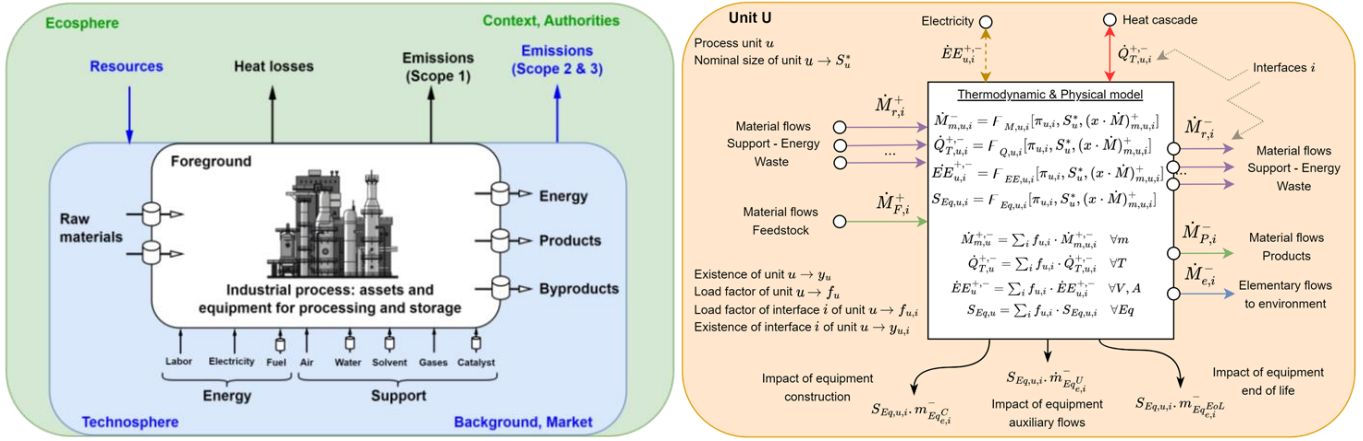


Figure 1. Mass, heat, power, and equipment-related interfaces for a process unit (foreground) embedded in a technosphere and ecosphere (background) [8].

2.2. Seven-tier models sharing framework

A central challenge identified through bilateral discussions with participating countries is the tension between transparency and confidentiality. Industrial partners require proprietary data to be protected, while research community benefits from maximum open-access. To address this issue, a seven-tier layered sharing framework was proposed, enabling model contributors to select the appropriate level of disclosure (Table 2). Survey results indicated strong support for layers L0-L2 (70–90% unconditional support), with progressively conditional support for layers L3-L5 and more restrictive positions for L6. Confidential industrial data and unpublished research were identified as the factors with the highest impact on sharing willingness.

Table 2. Seven-tier layered sharing framework for ex-ante models database.

Layer	Content	Access level
L0: Public metadata	Author, sector, technology, reference capacity, keywords, TRL	Completely open
L1: Structure and topology	Block flow diagrams, unit connections, process architecture	Completely open
L2: Mass and energy balances	Stream flows, temperatures, pressures (anonymized)	Verified users with data use agreement
L3: Thermodynamic and validation data	Literature benchmarks, performance metrics, sensitivity analyses	Verified users with data use agreement
L4: Detailed parameters	Thermodynamic correlations, reaction data, kinetic parameters	On-demand with data use agreement
L5: Economic and proprietary data	Cost functions, full software files, proprietary kinetics	Approval required, possibly NDA
L6: Combined innovations	Novel process integrations, optimization strategies, patentable combinations	Restricted, NDA required

2.3. Model sharing, validating and maintenance procedure

A standardized procedure handles the lifecycle of models within the database, from initial submission through long-term maintenance (Fig. 2):

Phase 1: Submission. The model contributor proposes a model, selects the model type, checks template compatibility, and assesses data sensitivity. The model is adapted to the

template by completing metadata fields, defining connectors and variables, preparing documentation, and checking flow diagrams. If the template structure is incompatible, an alternative structure may be proposed and discussed with sub-teams. A completeness check validates required fields, documentation, and supplementary files.

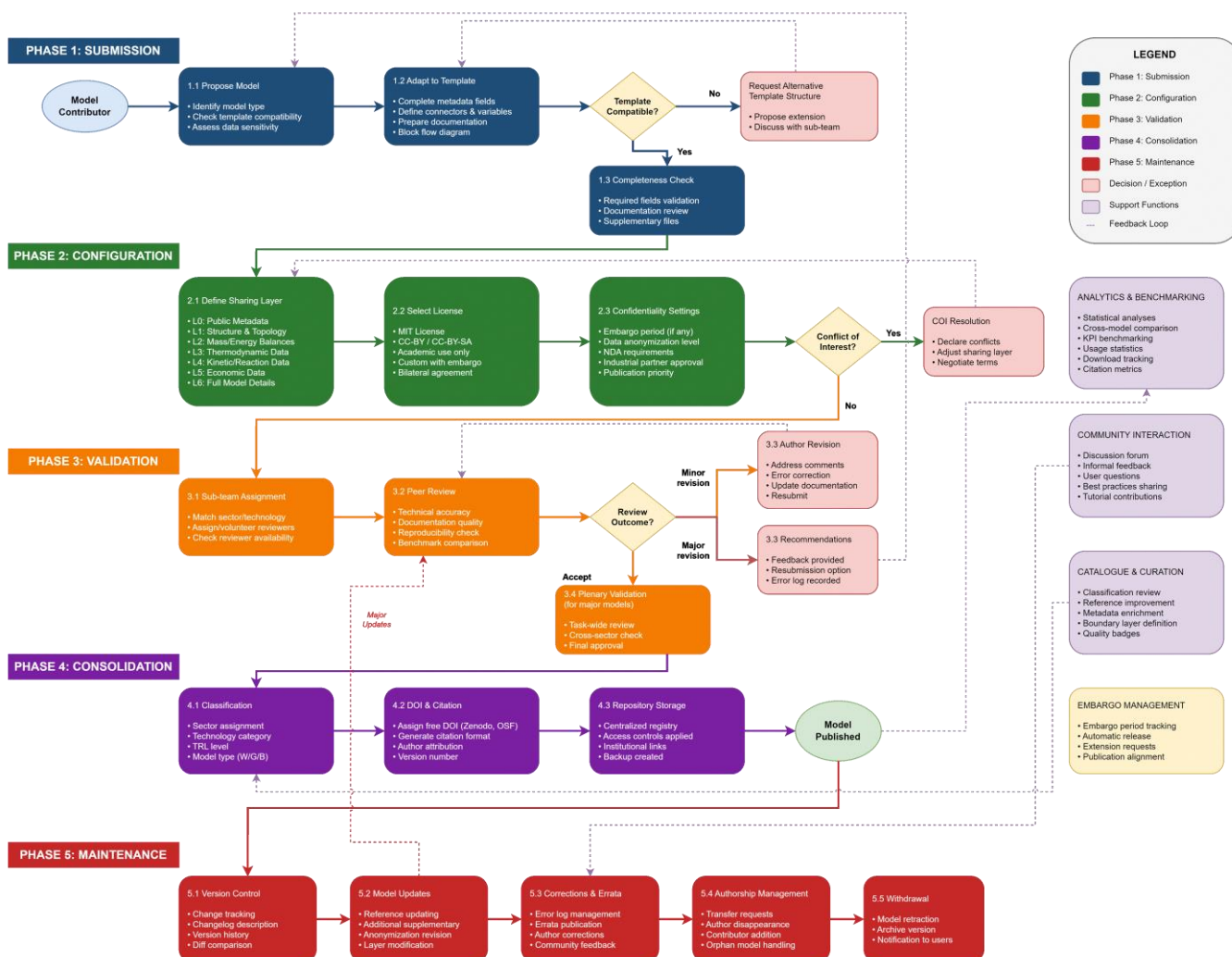


Figure 2. Ex-ante model sharing procedure: submission, configuration, validation, consolidation, and maintenance. Supporting functions include analytics and benchmarking, community interaction, catalogue and curation, and embargo management.

Phase 2: Configuration. The sharing layer (L0-L6) is defined, a license is selected, and confidentiality settings are configured (embargo periods, data anonymization levels, NDAs, and industrial partner approval). Conflicts of interest are assessed; if identified, the model enters a resolution process involving disclosure certificates and alternative sharing layer agreements.

Phase 3: Validation. Sub-teams are assigned based on sector expertise, and review criteria (technical accuracy, documentation quality, benchmark comparison) are applied. Minor issues entail author revision; major issues trigger a review loop. Upon acceptance, recommendations and an error log are recorded. Both validated and non-validated models are nevertheless maintained.

Phase 4: Consolidation. The validated model is classified by sector, technology category, and TRL, a free DOI is assigned (Zenodo, OSF), and the model is stored in the repository with

centralized registry, access controls, metadata indexing, and backup systems, thus attaining a published status.

Phase 5: Maintenance. Version control, change tracking, and citation history are maintained. Model updates follow a streamlined process with contributors, accomplished revision, author corrections, and layer modifications records. Corrections and errata are managed through error log management system. Authorship management handles transfer requests, contributor additions, and tiered access updates.

2.4. Computational framework for process integration: PinchSM

PinchSM is an open-source computational framework designed to interface with the ex-ante model database and provide a complete environment for process integration optimization, scenario generation, and reporting. The framework architecture is organized around four principal components: context definition, infrastructure specification, optimization engine, and reporting module (Fig. 3).

Context definition. PinchSM defines the background environmental conditions in which models operate, including weather parameters, as well as energy and material prices (electricity, fuel, raw materials, heating tariffs, etc.) and regulatory constraints (carbon taxes, emission caps, renewable portfolio standards). These contextual parameters govern the economic and environmental performance of all models loaded into a given scenario.

Infrastructure and clustering. The framework specifies the infrastructure to which models can connect, including electricity, heat, fuel and material distribution grids, as well as thermal and electrical storage systems. Models are organized into clusters that restrict heat exchange across boundaries for techno-economic reasons (e.g., geographic distance, incompatible temperature levels, or regulatory constraints), reflecting real-world site limitations. This clustering mechanism prevents unrealistic cross-site heat integration while preserving intra-cluster optimization opportunities.

MILP optimization engine. The process integration problem is formulated as a mixed-integer linear programming (MILP) model [9]. Binary decision variables (y) determine the existence (activation) of each unit, while continuous variables (f) determine the load at which each activated unit operates. The heat cascade constraint from higher to lower temperature levels enforces thermodynamic feasibility. Mass, energy, and emission balances are satisfied across all activated units and infrastructure connections. The objective function is configurable to minimize total annual cost, CO₂ emissions, or multi-objective formulations. The separation between data (fetched from the database) and systemic process integration equations (handled in PinchSM) ensures that different model versions can coexist, compete and be compared within the same superstructure based on sustainability metrics.

Scenario generation and reporting. PinchSM supports the generation and comparison of multiple scenarios by activating or deactivating certain models, varying contextual parameters, or modifying infrastructure configurations. Users can select key performance indicators (KPIs energy efficiency, exergy efficiency, carbon intensity, specific energy consumption, levelized cost of energy or product, water consumption, waste generation, payback period, among others) and the framework populates structured markdown reports. These reports include an executive summary for decision-makers and a detailed engineering summary with composite curves, grand composite curves, heat cascade tables, cost breakdowns, and sensitivity analyses. In this way, any compatible optimization environment (e.g., Pyomo, AMPL, GAMS,

or custom solvers) can leverage the database, although PinchSM provides a readily available, community-driven implementation.

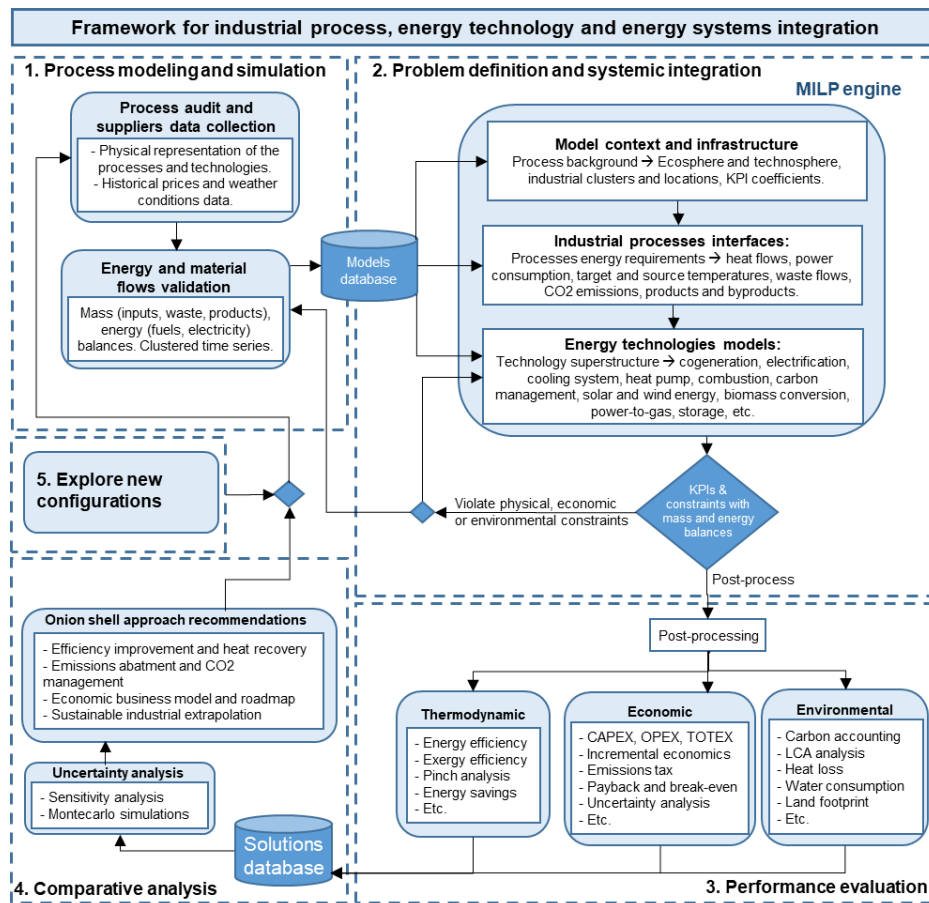


Figure 3. Schematic of the PinchSM framework architecture and its interaction with the ex-ante model database [10].

Table 3. Summary of the MILP formulation for process integration in PinchSM.

Component	Description
Decision variables	Binary: y (unit existence); Continuous: f (unit load, bounded by capacity multipliers)
Objective function	Minimize total annual cost (CAPEX annualized + OPEX) or CO ₂ emissions; multi-objective via ϵ -constraint or weighted average.
Heat cascade	Temperature interval decomposition; heat residuals $R_k \geq 0$ at each interval k ; feasibility condition ΔT_{\min} defined per heat per stream
Mass balance	Conservation across all connectors of type 'mass' for each species
Energy balance	Electricity and fuel balances across grids, storage, and process demands
Emission balance	Scope 1 (direct), Scope 2 (electricity), Scope 3 (upstream) accounting
Infrastructure	Grid import/export limits, storage charge/discharge rates, seasonal profiles
Clustering	Heat exchange restricted within defined clusters; mass and electricity flows can be also restricted (if required).

Regarding software environments, participating institutions employ a diverse range of tools, including Aspen® Plus, Python-based frameworks (e.g. Pyomo, equation-oriented solvers), MATLAB®, Excel®, and other tailored platforms. This heterogeneity reinforces the necessity of a software-agnostic schema that documents model interfaces. The proposed model structure, discussed in the next section, ensures that different modeling paradigms across diverse industrial sectors and energy technologies can be meaningfully integrated within the same database, in which metadata, engineering variables (incl. physical units and source) and connectors attributes are consistently specified.

Table 4. Task XXIV participating countries, institutions, and indicative model contributions.

Country	Institutions	Indicative model domains
Belgium (BE)	University of Liège, University of Ghent	Chemical processes, stakeholder analysis
Canada (CA)	NRC/CanmetENERGY, Polytechnique Montréal, CIRAIQ/UQAM	Biorefineries, pulp and paper, LCA
Chile (CL)	Fraunhofer Chile	Solar thermal integration, industrial decarbonization
Colombia (CO)	UIS	Process simulation, educational models
Denmark (DK)	Danish Technological Institute, DTU, SDU	Heat pumps, refrigeration, industrial cooling
France (FR)	Mines Paris, CEA	Energy systems, nuclear-industrial coupling
Germany (DE)	U. Paderborn	Process synthesis, mathematical optimization
Italy (IT)	Politecnico di Milano	Chemical engineering, process simulation
Netherlands (NL)	TU Delft	Carbon capture, Power-to-X, techno-economics
Norway (NO)	NTNU	Process systems engineering, modular design
Portugal (PT)	IST Lisbon, ISEC, FEUP, GML	Pinch analysis, industrial audits, SME engagement
Sweden (SE)	Chalmers University	Biomass gasification, industrial symbiosis
Switzerland (CH)	EPFL, HES-SO Valais	Process integration, MILP optimization, LCA

3.2. Model schema and class hierarchy

For the sake of process integration analysis, industrial processes (e.g., food and beverage, pulp and paper, chemicals, metals and minerals, cement, and glass), energy conversion technologies (e.g., heat pumps, boilers, furnaces, turbines, engines, fuel cells, electrolyzers, gasifiers), and energy system components (e.g., grids, storage, renewable energy sources, district heating networks) can be represented in a simple and standardized way, facilitating data indexation, validation, and maintenance to ensure accessibility, integrity and continuity of the shared model. To this end, a model schema is implemented as a class hierarchy tree, in which each class inherits common attributes from its parent class, while defining the specific attributes of its own type (Figure 5). At the root level, a MODEL branches into METADATA (status, attribution, references, and documentation), CHANGELOG (version control and change tracking), SUPPL MATERIAL (auxiliary flowsheets, portable text documents, spreadsheets, bibliographic files, figures, etc.), VARIABLES (specification of engineering parameters and model variables), UNIT (definition of mass and energy streams, as well as equipment, to account for investment flows associated with process units), and CALCULATIONS (additional derived quantities). The tree structure ensures that each information element has a defined position, type, and relationship to other elements in the model schema, enabling consistent interpretation and operationalization across Task XXIV participants. This serves as a primary communication tool between model developers and

users, allowing non-specialists to understand what a model offers to and requires from the surrounding energy systems.

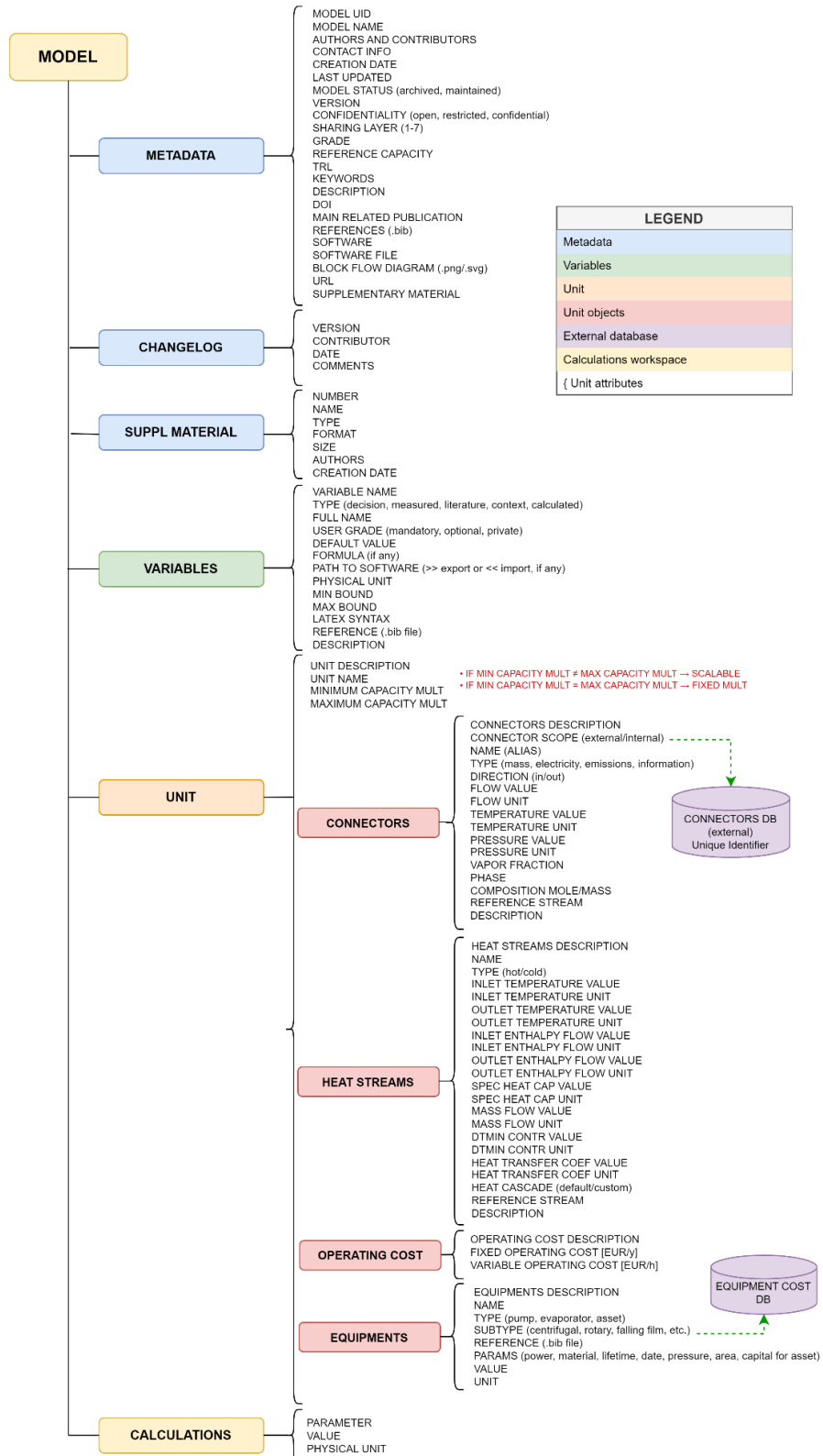


Figure 5. Class hierarchy tree of the software-agnostic ex-ante model structure, incl. metadata, engineering, variables, unit objects and streams, external databases (connectors properties, equipment costs), supplementary calculations, and units attributes.

Metadata encompasses model identification (unique identifier, name, authors, contact information), version control (creation date, last update, status), confidentiality settings (open, restricted, or confidential), the sharing layer (L0–L6), technology readiness level (TRL), keywords, description, digital object identifier (DOI), main related publication(s), references, software environment, block flow diagram, and supplementary material and URLs. **Variables** define the model's parametric space with attributes including variable name, type (decision, measured, literature, context, or calculated), user grade (mandatory, optional, or private), default value, formula (if any), path to software object (for import/export interoperability), physical unit, bounds (min. and max.), markup syntax (LaTeX), bibliographic reference, and description. Figure 6 shows a mapping process of a flowsheet model into unit operations, and the respective streams and equipment lists. This approach enables visualization of model interfaces with associated quality attributes (e.g. mass, energy, emission, and information flows) across the model boundary, independently of the internal model complexity.

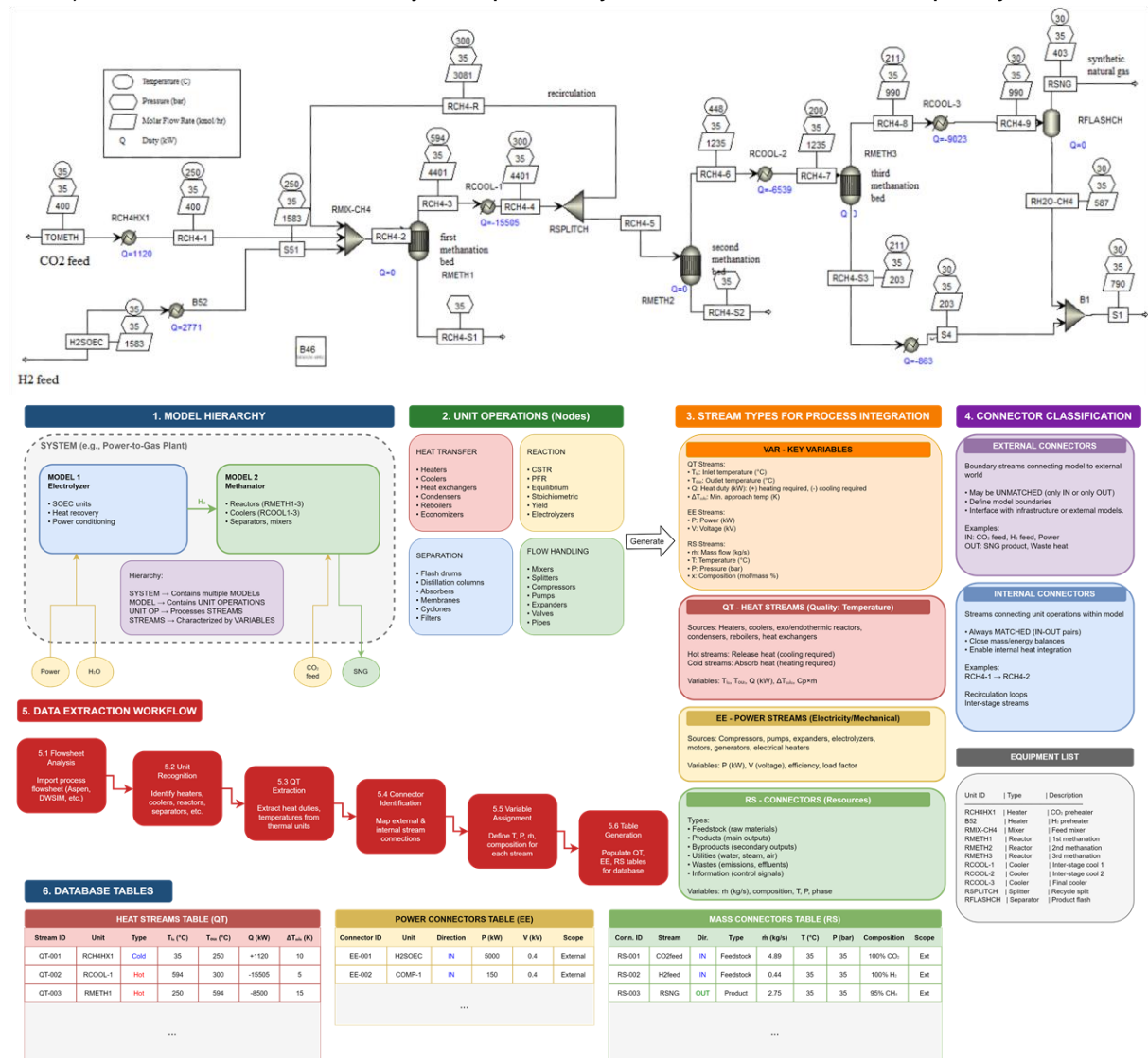


Figure 6. Model data mapping and objects representation applied to a methanation model developed in a sequential modular simulator (Aspen® Plus).

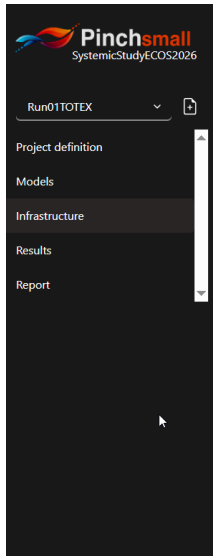
The **Unit** further specifies minimum and maximum capacity multipliers, as it models units' load can be ranged or operate at fixed capacity. Unit objects represent the core subprocesses or energy technology models, and divide into three sub-sections. **Connectors** define the model's

interfaces with the external world, characterized by scope (external or internal), name and alias, type (mass, electricity, emissions, or information), direction (input or output), flow value and unit, temperature, pressure, vapor fraction, phase, and composition. External connectors should link to an external connectors database with unique identifiers, enabling standardized interconnection between ex-ante models. Moreover, **Heat streams** document the thermal demands enabling heat cascade analysis, with attributes including type (hot or cold), inlet and outlet temperatures, enthalpy flows, specific heat capacity, mass flow, minimum temperature difference contribution (ΔT_{\min}), heat transfer coefficient, and assignment to default or custom heat cascades. Any of the connectors or heat streams can be assigned as sizing or reference stream, depending on the application. Meanwhile, **Operating cost** captures fixed (EUR/y) and variable (EUR/h) components associated to operation and maintenance (O&M). **Equipments** field documents the process units with type, subtype, and techno-economic parameters (power, material, lifetime, pressure, area, capital cost) linked to an equipment cost database. Finally, **Calculations** provide an auxiliary workspace for derived parameters with their values and physical units; **Changelog** tracks version history with the contributor attribution, whereas **Supplementary material** allows attachment of additional files with their metadata (ID, name, format, size, authors, creation date, etc.).

3.3. PinchSM process and technology database integration framework

PinchSM has been developed as a Python framework (FastAPI) interfacing the OSMOSE Lua engine [11] with the model database through standardized file formats (JSON, CSV). The modular architecture comprises (Figure 7):

- *Context manager* configures background ambient conditions (e.g. weather data), energy prices, infrastructure and regulatory constraints (e.g. carbon taxes) which are location-specific parameters and exhibit temporal profiles (hourly, seasonal, or annual resolution). It enables to evaluate the same set of models under different geographic and regulatory conditions.
- *Model loader* reads model entries from the database, and instantiates unit objects with their connectors, heat streams, variables, and cost parameters. Multiple versions of the same technology (e.g., alkaline vs. PEM vs. solid oxide electrolyzers) can be loaded simultaneously into the superstructure as redundant, complementary or competing alternatives.
- *Project settings* generates the optimization problem from the selected objective function, loaded models and infrastructure specifications. The heat cascade constraints are constructed from heat stream data in each model, with minimum temperature difference contributions (ΔT_{\min}) ensuring thermodynamically feasible heat exchange. Clustering constraints partition the models and units into defined locations, each corresponding to physical or technological boundaries within which direct heat, mass or electricity exchange is technically possible.
- *Report generator* produces structured markdown documents with configurable content. The executive summary presents key findings for decision-makers (technologies selection and activation load, economic and investment indicators, emissions reduction, and other relevant results). The engineering summary includes composite curves, grand composite curves, Sankey diagrams for energy and mass flows, detailed cost breakdowns, and sensitivity analyses. Reports can be generated for individual scenarios or as comparative analyses across scenario portfolios (Figure 8).



Infrastructural Flows

NATURALGAS Type: ENERGY Temperature: 5 °C	Direction: OUT Pressure: 30 bar	→
ELECTRICITY Type: ENERGY Temperature:	Direction: OUT Pressure:	
WATER Type: MASS Temperature: 12 °C	Direction: OUT Pressure: 1 bar	
WATER Type: MASS Temperature: 12 °C	Direction: IN Pressure: 1 bar	
EnvCO2Em Type: EMISSIONS Temperature: 25 °C	Direction: IN Pressure: 1 bar	

Connector configuration

MASSFRAC:CH4[1]

Min Bound (Value): 0 Min Bound (Formula): Optional formula

Max Bound (Value): 10000 Max Bound (Formula): Optional formula

KPI Energy Coefficient: 1 KPI Energy Unit: Enter unit

KPIs

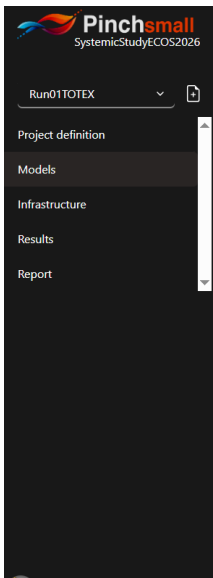
KPI name: Add KPI

default

Cost Coefficient: 0.04 Cost Unit: EUR/kWh

CO2 Coefficient: 0.0018 CO2 Unit: kgCO2e/kWh

Cancel Save

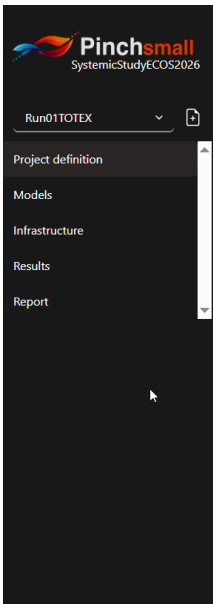


Models

Superstructure + Add model

- CheeseUnit location1
- CIPDairy location1
- CoolingTower location1
- EvaporationUnit location1
- NGFurnace location1
- PasteurizationUnit location1
- Refrigerator location1
- WasteWaterTreatment location1
- HeatPump location1
- BiodigesterUnit location1

Previous Next



Project settings

Project name: SystemicStudyECOS2026

Project Description: This Systemic Study of an Industrial Plant is

Objective: TotalCost

Capex weight factor: 0	impact_weight_factor: 0	storage_enabled: 0	integer_constraint_cuts: 0	remove_binaries: 0
doRound T: 3	doRound H: 2	doRound M: 2	doRound Spaghetti: 3	Interest rate (%): 2

operational_costs_file: op_hours.csv Change Download

coordinates
 heat_load_distribution
 area_estimation
 graph_real_temperature
 infrastructure

Clusters

Location ID	Clusters	X	Y	Z
location1	1 selected	0	10	0

Figure 7. PinchSM interface of the context manager, model loader, project setter for the mixed integer linear programming (MILP) problem configuration.

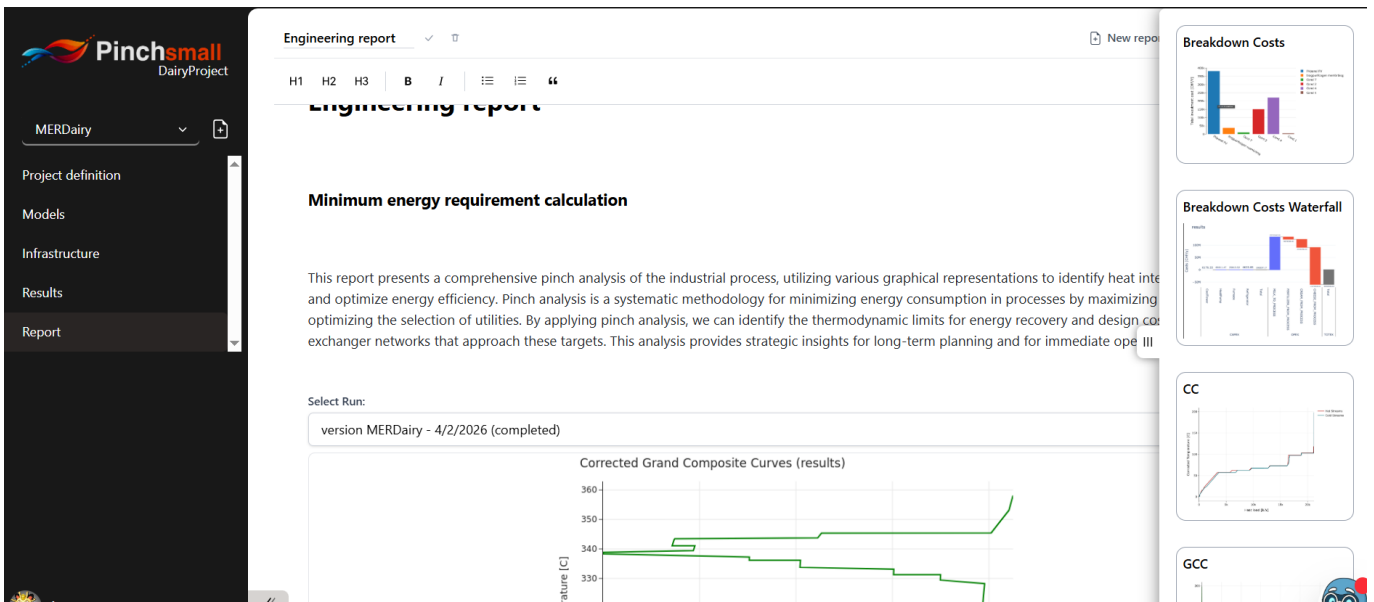
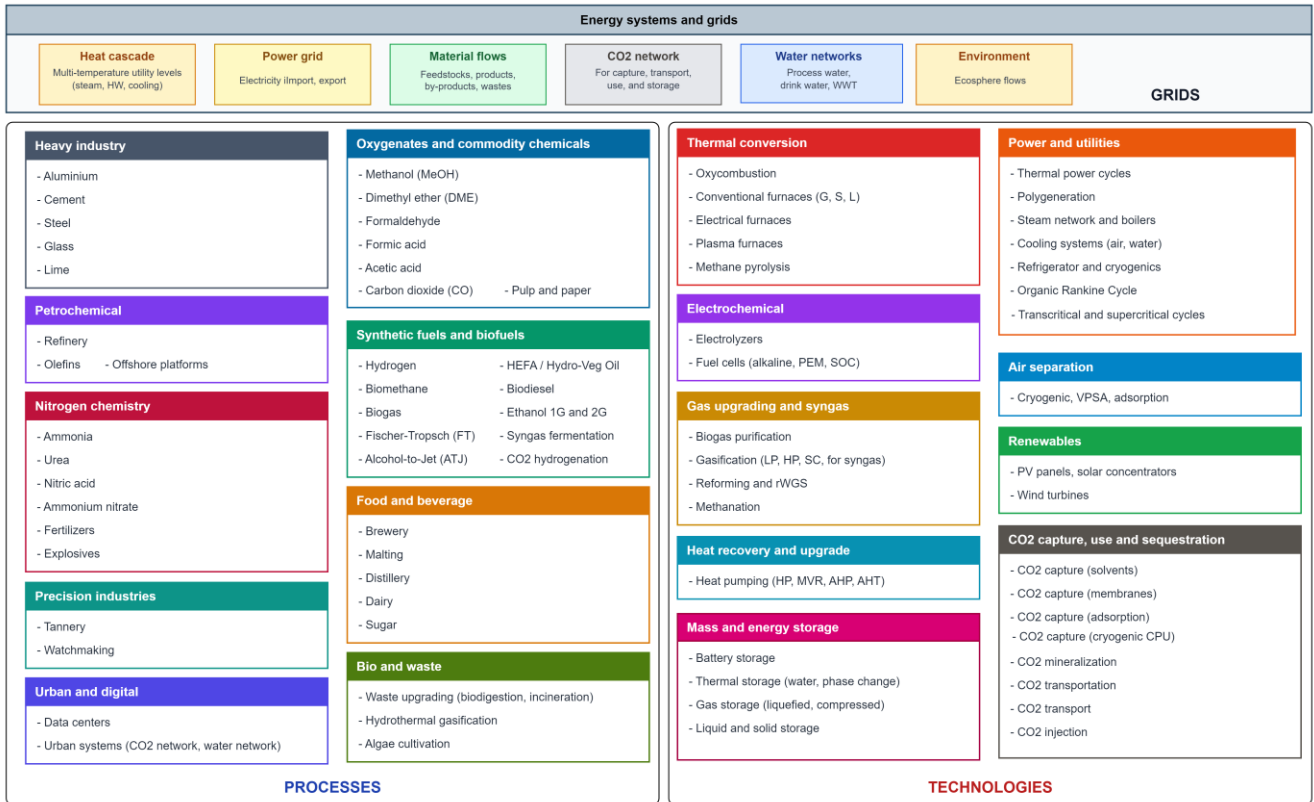


Figure 8. PinchSM output: report manager and plotting configuration interface.

An architectural choice in the design of the database and the process integration framework is the separation between data (i.e. model parameters and variables stored in the database), model equations (i.e. constitutive relations for each technology model), and framework logic (i.e. optimization formulation, scenario management, reporting). This separation offers several advantages. First, the database can be leveraged by any compatible optimization framework. Although PinchSM provides a readily available implementation, researchers using AMPL, GAMS, Pyomo, Julia/JuMP, or custom solvers can import the same model data and formulate their own optimization problems. This avoids vendor lock-in and encourages methodological pluralism within the community. Second, model updates (e.g., revised cost data, updated performance parameters) propagate immediately to all frameworks consuming the database without requiring framework-level code changes. A model contributor correcting a heat transfer coefficient or updating an equipment cost function need only to modify the database entry; and all downstream analyses automatically reflect the update. Third, the separation facilitates the documentation and reproduction of case studies. A complete case study specification comprises a reference to specific model versions in the database, a context definition file, an infrastructure configuration file, and a scenario specification. This package is sufficient for any researcher with access to the database and a compatible framework to reproduce the analysis. A preliminary version of the models database is under construction and includes a set of industrial processes and energy technologies (Figure 9). The database framework has the possibility of uploading model templates, such as Excel, and also supports loading supplementary material and figures (svg) (Figure 9).



IDP Industrial Data Platform

Models Database **Connectors Database**

DualBedGasifFT

Biomass gasification is a thermochemical conversion that decomposes biomass at elevated temperatures (>700°C) in presence of a gasification agent such as H_2 , CO_2 , steam, CO_2 or combination thereof. The gasification process is typically modeled as a series of interrelated drying, pyrolysis, reduction and combustion processes. The actual mass yields of volatiles, condensables, and solids in the pyrolysis reaction step, as well as the gaseous volumetric fractions of the hydrogen, carbon monoxide, carbon dioxide, methane produced in the reduction step strongly depend on the gasifier operating parameters, such as temperature, pressure, feed moisture and chemical composition, gasification agent, energy supply among other hydraulic and structural characteristics. In particular, a dual bed gasifier consists of two interconnected fluidized beds. The first bed is a bubbling fluidized bed, in which biomass is converted into syngas. The second bed is a fast fluidized combustion bed, which oxidizes the residual char with air or oxygen, thus providing the heating requirements of the highly endothermic gasification reactions occurring in the first bed. The bed of biomass or other gasifying materials is supplied to the first gasifier bed with the help of a screw conveyor. The two fluidized beds are controlled separately, but they are interconnected via a non-mechanical valve, such as a loop seal valve, to ensure the circulation of the bed particles. A cyclone separator is employed to separate the heat-carrying material (e.g. sand with fines) and the fine gases in the top of the combustion bed. The heat-carrying material is returned to the first gasifier, while the fine gases are sent to the heat recovery system. The product gas obtained from the gasifier is primarily composed of H_2 , CO , CO_2 , CH_4 , and small amounts of tar and other undesired components. The gaseous mixture continues to the purification units (e.g. water scrubber and 2nd guard bed) in order to remove the impurities and to upgrade the syngas quality via water gas shift reactions with interesting.

Max Multiplier: 0 Max Multiplier: 0.1

Block Flow Diagram

Click to enlarge

Show Details

Add Model From Excel

Convert an Excel template and publish it directly into the models database

Excel File

Choose File: no file selected

No file selected

Supported formats: xlsx, xlsm, xls

Store In

Process Models Energy Technology Models

Import Model Clear

Models Database

Browse and explore process engineering models

Rebuild Database

Industrial Process Models

Search by name, description, or keywords...

- BeerProcessing**
 - Food: Milk
 - Units: 3 Variables: 37
 - Reference Capacity: 103877 high Beer
- Dairy Process**
 - Food
 - Units: 7 Variables: 476
 - Reference Capacity: 2024.9 high cheese
- Dual Bed Gasifier**
 - Dual Bed Gasifier
 - Units: 2 Variables: 203
 - Reference Capacity: Kerosene

Energy Technology Models

Search by name, description, or keywords...

- CoolingTower**
 - Cooling
 - Units: 1 Variables: 12
 - Reference Capacity: 1000 kW
- HeaterEE**
 - Heat Supply: Electrified
 - Units: 1 Variables: 15
 - Reference Capacity: 1000 kW
- NGFurnace**
 - Heat Supply: Natural Gas Fossil Combustion
 - Units: 1 Variables: 27
 - Reference Capacity: 1000 kW

Figure 9. Model database framework separated from the process integration framework.

3.4. Ongoing case studies and shared experiences

Several illustrative applications are under development within the Task XXIV framework to gather valuable information on the models and tools sharing. These case studies span sectors including food and beverage processing (waste heat recovery and heat pump integration, Figure 10), aluminum recycling (high-temperature electrification and oxy-fuel combustion), pulp and paper (biomass gasification and CHP optimization), and fuels & chemical production

(combining power-to-x and carbon utilization). Each case study helps demonstrate specific aspects of the role of the process integration in the industry decarbonization, such as the efficiency intensification, electrification and cross-site industrial symbiosis. The generation of scenario-based techno-economic assessments under uncertain energy prices and regulations will be accelerated by leveraging not one but a collection of models, allowing to perform statistical analysis of the performance ranges and improving the accuracy of the assumptions.

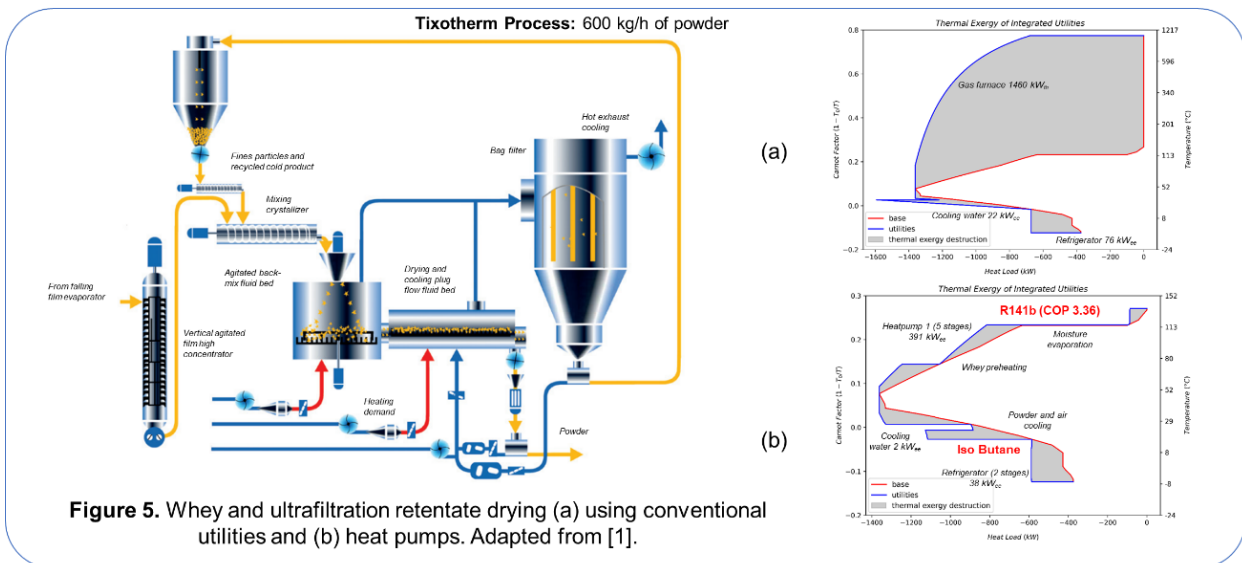
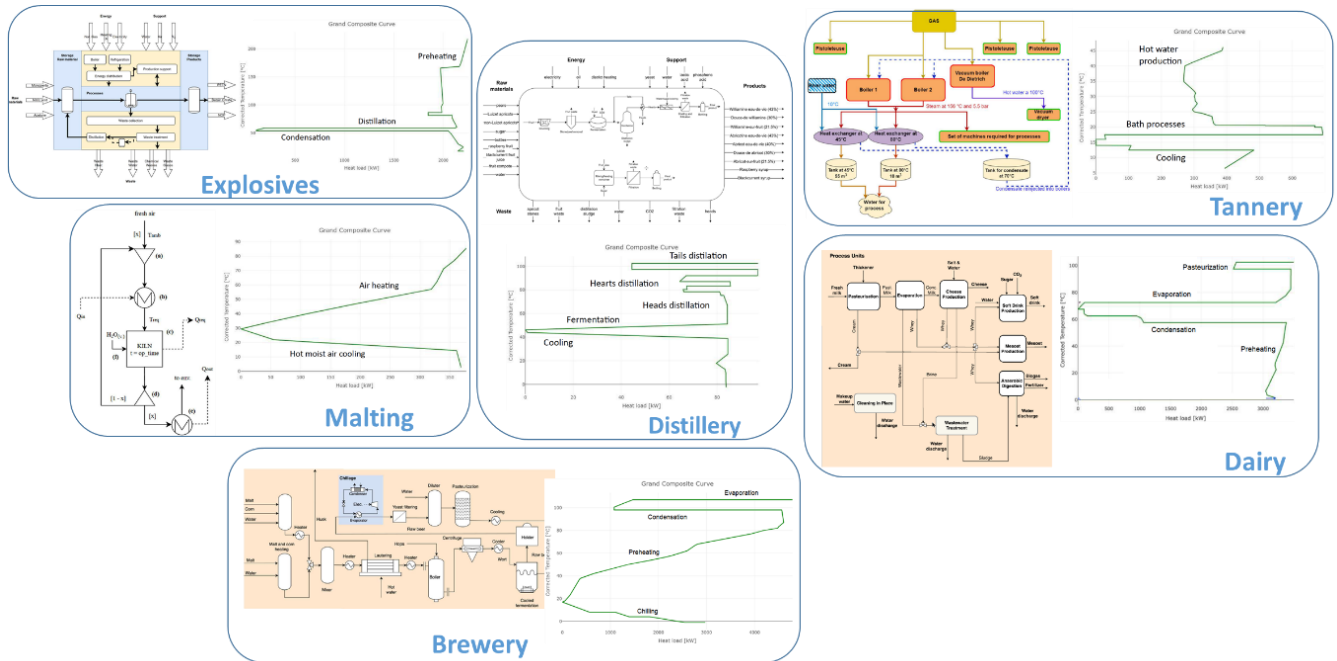


Figure 5. Whey and ultrafiltration retentate drying (a) using conventional utilities and (b) heat pumps. Adapted from [1].

Figure 10. Reporting process integration visualizations: (above) GCCs of selected industrial processes; (below) integrated heat pump technologies for supplying heat demand to a whey ultrafiltration retentate drying.

4. Conclusions

In this work, the learnings of the ongoing Industrial-related Energy Technology Systems (IETS) Task XXIV of the Technology Collaboration Programme (TCP) by International Energy Agency (IEA) are summarized. This Task aims to addressing a persistent knowledge-sharing gap in

industrial decarbonization by developing an open-source database of ex-ante models that can be leveraged by a process integration framework. The database builds on a software-agnostic template that captures model's interfaces (i.e. connectors through which models exchange energy, mass, and emissions with surroundings) in a documented, validated and shareable format. This design enables meaningful comparison and integration of models originating from different simulation paradigms (sequential modular or equation-oriented simulators) within a common superstructure. A seven-tier sharing framework, developed through extensive bilateral consultation with participant countries, successfully reconciles the competing demands of transparency and confidentiality, enabling participation from open-access academic institutions and industry-partnered consortia. Meanwhile, the integration tool provides a computational environment for loading models from the database, defining operational contexts (environmental conditions, energy prices, regulations), specifying infrastructure and clustering constraints, formulating and solving MILP optimization problems, generating comparative scenarios, and producing structured reports with executive and engineering summaries. Distinction between the data, the models, and the framework ensures interoperability with alternative optimization environments and facilitates reproducibility of case studies. A five-phase model sharing procedure (submission, configuration, validation, consolidation, maintenance) establishes governance mechanisms for quality assurance, version control, and proper attribution. Together, these developments aim to provide first-hand validated models to the community, encourage transparent and reproducible modelling practices, promote international networking across disciplines and sectors, avoid duplication of effort, to ultimately accelerate the transition from energy audit to actionable decarbonization strategies. Future work within Task XXIV will focus on the collaborative population and validation of the database during 2026-2027, with planned contributions from all participating countries. Illustrative case studies spanning multiple industrial sectors will demonstrate the framework's capabilities for cross-site optimization, technology benchmarking, and scenario-based decision support. Integration with life cycle assessment (LCA) tools and alignment with emerging interoperability standards (FMI, CAPE-Open, DEXPI) are planned to enhance the relevance for the international process systems engineering community.

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