



# TRANSIENCE

**TRANSITIONING TOWARDS AN EFFICIENT,  
CARBON-NEUTRAL CIRCULAR EUROPEAN  
INDUSTRY**

Date: 27/06/2025

## **D4.4 – EU industrial pilot modules**

WP4 – Developing satellite modules



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## EC Summary Requirements

### 1. Changes with respect to the DoA

No changes with respect to the work described in the DoA.

### 2. Dissemination and uptake

This document, Deliverable D4.4 of the TRANSIENCE project, is intended for the broader stakeholder community and the modelling community. It provides an overview of the developed industry pilot module including its planned integration into the Model for European Industry Circularity and Climate Change Mitigation (MIC3). As such, this document and the developed module are a critical element to achieve an integrated modelling framework for the European industry, i.e., MIC3. Energy system modellers may use the models that are part of this module as stand-alone or in combination with the other satellite modules developed within TRANSIENCE to inform decision-makers on diverse pathways toward a material-efficient, circular, climate-neutral, sustainable European industry.

### 3. Short summary of results (<250 words)

This document presents an overview of the developed industry pilot module, which includes two models: FORECAST-Sites and ITOM. It describes the concepts, data inputs and outputs, novelty of the developed models, planned integration into the Model for European Industry Circularity and Climate Change Mitigation (MIC3), as well as exemplary results. FORECAST-Sites assesses industrial transformation pathways with a site-specific resolution based on the structure of the current industrial plant fleet of European energy-intensive sectors (i.e., plant age and lifetime), the techno-economic framework (i.e., energy carrier prices and regulations like price for CO<sub>2</sub> certificates or subsidies) and scenarios for infrastructure connection of sites. It complements this by a top-down approach to cover the complete industry sector. Similarly, ITOM provides a detailed representation of the steel, petrochemicals, and cement sectors, including a highly detailed technology portfolio as well as site- and plant-specific representation of these sectors. ITOM endogenously models the development of production networks across steps in the value chains and sites. Within the MIC3 framework, the industry module gets direct input from the European material flow module (EU-MFA) and the energy system module (OPEN-PROM). The techno-economic industry module itself provides input back to the energy system module, to the LCA module and, if appropriate, to the socio-economic module (OPEN-GEM).

### 4. Evidence of accomplishment

- The [GitHub repository for FORECAST-Sites](#) including an installation guideline, a [journal paper with detailed documentation](#), and a [journal paper with model application, supplementary data and results](#).
- The [GitHub repository for ITOM](#), its documentation (<https://itom.readthedocs.io/en/latest/>), the input and output datasets for ITOM sectoral models for steel, petrochemicals, and cement, and their documentations on Zenodo ([10.5281/zenodo.15772720](https://zenodo.org/record/15772720) for steel, [10.5281/zenodo.15773104](https://zenodo.org/record/15773104) for petrochemicals and [10.5281/zenodo.15773258](https://zenodo.org/record/15773258) for cement).
- This report.

## Preface

The need to approach climate action, resource efficiency, and circularity performance as integrated, economy-wide, cross-cutting issues is growingly gaining attention in the policy world, stimulating the development of new industrial policies in Europe and worldwide. Currently, however, there is little progress in conceptualising the circular economy and understanding its interactions with climate action. State-of-the-art modelling capacity to capture the interplay of the two agendas and their implications for energy-intensive sectors as well as to represent the European industry's transformation in line with the region's vision for climate neutrality is not yet fully developed. TRANSIENCE will undertake a comprehensive characterisation and assessment of circularity principles and measures vis-à-vis decarbonisation, by looking at the twin transition of European industries through the lenses of global competitiveness, innovation, and holistic sustainability. It will then produce MIC3, a consistent, fully open-source model ecosystem to assess industrial circularity, decarbonisation, and sustainability. A series of interoperable modules on the socioeconomic, service and product, material, industrial, energy-system, and environmental perspectives of the transformation of European industry will be developed and integrated, building on and opening the code of leading modelling tools. MIC3 will finally be used in extensive scenario modelling to produce diverse pathways toward a material-efficient, circular, climate-neutral, sustainable European industry. Transparency, openness, and knowledge sharing will be promoted, and technical capacities will be developed in four industrial agglomerations in the EU, moving beyond stakeholder consultation, onto model co-development, continuous validation of assumptions, co-creation of scenario modelling, evaluation of the desirability and usability of the developed model and insights, and eventually co-production of science and action.

<b>ICCS</b> – Institute of Communication and Computer Systems	EL	
<b>CEPS</b> – Centre for European Policy Studies	BE	
<b>E3M</b> – E3-Modelling AE	EL	
<b>Fraunhofer</b> – Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V.	DE	
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<b>PNTEC</b> – Park Naukowo-Technologiczny Euro-Centrum Spolka Z Ograniczona Odpowiedzialnoscia	PL	
<b>TECNALIA</b> – Fundación Tecnalia Research & Innovation	ES	
<b>UU</b> – Universiteit Utrecht	NL	
<b>WI</b> – Wuppertal Institut für Klima, Umwelt, Energie gGmbH	DE	
<b>PSI</b> – Paul Scherrer Institut	CH	
<b>UCL</b> – University College London	UK	

## Executive Summary

This document provides an overview of the industrial techno-economic pilot module of the planned Model for European Industry Circularity and Climate Change Mitigation (MIC3). The module consists of two models: FORECAST-Sites and ITOM. Both models calculate industrial transition scenarios considering macroeconomic trends, effects of circular economy measures, and energy system developments, such as changing energy carrier and CO<sub>2</sub> prices and infrastructure development. While FORECAST-Sites covers the whole industry sector and includes a bottom-up perspective for energy-intensive industries, ITOM offers a very high-resolution representation for the steel, cement, and petrochemicals sectors. Within the MIC3 framework, the developed industry module will receive direct input from the energy system and the European material flow modules. The industry module will in turn provide results to the energy system module and the LCA module. Concluding, the industry module plays a key role within MIC3 for assessing industrial transformation pathways and understanding interdependencies with other parts of the energy system. The module allows the combination of bottom-up and top-down approaches to investigate the entire industry sector while focussing on single important industrial sub-sectors with a high level of spatial and technical detail. Establishing the connection between both models within this module and data harmonisation for linking with other MIC3 modules are major tasks for the second project phase.

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### Code metadata (FORECAST-Sites)

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Current code version	v.1.0
Link to code repository	<a href="https://github.com/fraunhofer-isi/forecast-sites">https://github.com/fraunhofer-isi/forecast-sites</a>
Legal Code License	AGPL 3.0
Code versioning system used	git
Software code language	Python
Particular tools, services, modules used	Mesa <a href="https://mesa.readthedocs.io/">https://mesa.readthedocs.io/</a>
Compilation requirements, operating environments & dependencies	Tested with Python 3.12 and the modules listed in the requirements.txt file
Link to documentation / manual	<a href="https://doi.org/10.1038/s41598-024-78881-7">https://doi.org/10.1038/s41598-024-78881-7</a>

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### Code metadata (ITOM)

---

Current code version	v.0.1
Link to code repository	<a href="https://github.com/wupperinst/itom">https://github.com/wupperinst/itom</a>
Legal Code License	Open-source license (see repository)
Code versioning system used	git
Software code language	Python
Compilation requirements, operating environments & dependencies	Tested with Python 3.9 and the modules listed in the requirements.txt file
Link to documentation / manual	<a href="https://itom.readthedocs.io/en/latest/">https://itom.readthedocs.io/en/latest/</a>
Datasets	
Steel	<a href="https://doi.org/10.5281/zenodo.15772720">https://doi.org/10.5281/zenodo.15772720</a>
Petrochemicals	<a href="https://doi.org/10.5281/zenodo.15773104">https://doi.org/10.5281/zenodo.15773104</a>
Cement	<a href="https://doi.org/10.5281/zenodo.15773258">https://doi.org/10.5281/zenodo.15773258</a>

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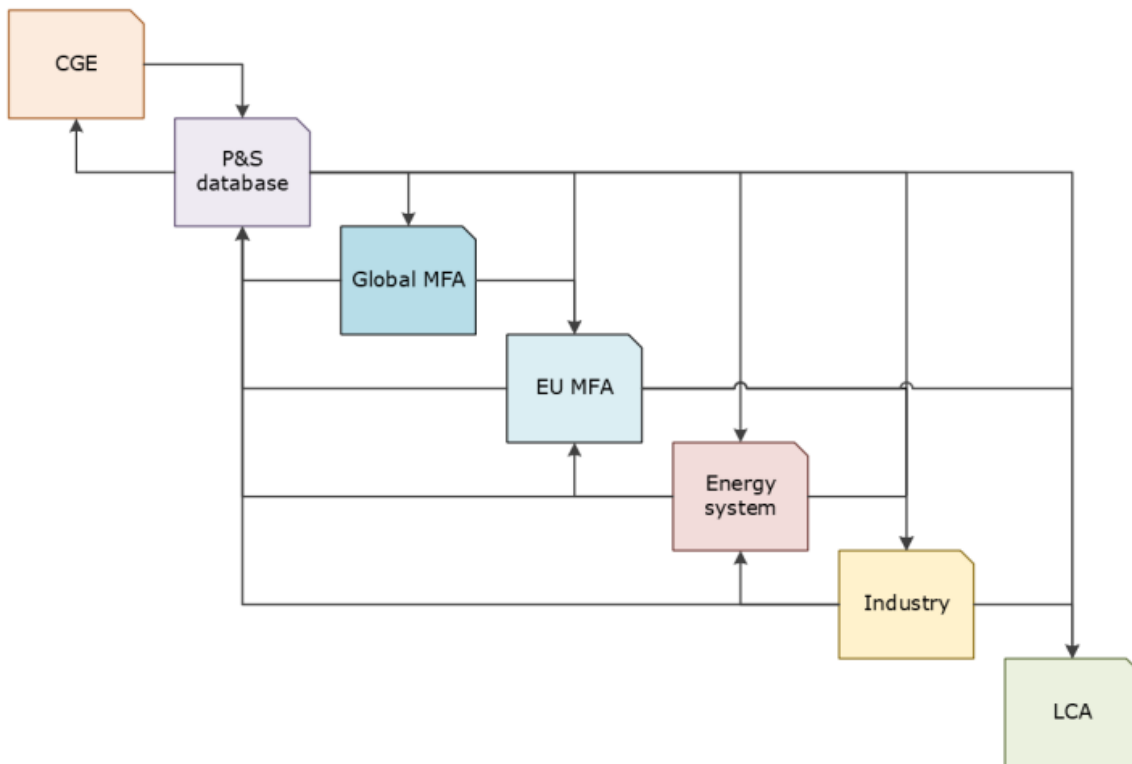
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## 1 Introduction

This document provides an overview of the techno-economic industry models FORECAST-Sites and ITOM for the European Union (EU), each provided as a GitHub repository including a preliminary documentation, which will be further developed and finalised in the second phase of the project<sup>1</sup>.

The industry module is central within the Model for European Industry Circularity and Climate Change Mitigation (MIC3) framework, incorporating circular economy strategies and measures, as well as inputs from socio-economic and energy system perspectives and is linked to nearly all other MIC3 modules, as shown in Figure 1-1. Results from the industry module affect developments in the energy system and vice versa. The energy system module consequently receives iterative inputs from industry modules. Furthermore, the results from industry module will be used by the LCA module.

The following document is separated in two parts. While chapter 2 focuses on the model FORECAST-Sites, ITOM is described in chapter 3.



**Figure 1-1:** Planned interfaces in the MIC3 baseline workflow from D3.4

A comparison of the respective modelling approaches and resulting roles of the two industry models is shown in Table 1-1. While ITOM offers a high-resolution regarding products and processes for the production of steel, cement, and polymers, FORECAST-Sites provides a broader overview across different sectors including other products like lime, glass, and paper. Furthermore, FORECAST-Sites aims to bridge

<sup>1</sup> [www.github.com/fraunhofer-isi/forecast-sites](https://github.com/fraunhofer-isi/forecast-sites); <https://github.com/wupperinst/itom>

the gap between the bottom-up representation of industrial energy demand and the residual energy demand arising from a variety of smaller processes through a simplified top-down approach to reflect the Eurostat Energy Balance.

**Table 1-1:** Comparison of the modelling approaches and resulting roles of the industry models FORECAST-Sites and ITOM

	FC-Sites	ITOM
<b>Sectors</b>	Iron & steel, Chemical & petrochemical, Non-ferrous metals, Non-metallic minerals (including cement), Food, beverages & tobacco, Paper, pulp & printing (Partly Phase 2) considered at once	Cement, Steel and Petrochemicals, each in separate sectoral implementations
<b>Approach</b>	It utilises a bottom-up modelling approach to deduce energy demand from various processes. In Phase 2, it will incorporate a top-down approach to align with the Eurostat energy balance and enable integration of processes within industrial sites, optimising from the perspective of each individual site. It considers infrastructure availability like the hydrogen backbone.	It utilises a bottom-up modelling approach to deduce energy and material demand considering process integration within and between sites through shared infrastructure. It performs model endogenous cost optimisation of production networks across production steps and sites. It finally depicts high granularity regarding processes, products, and intermediate products.
<b>Role</b>	To simulate the future energy demand of the entire European industry at site level.	To identify and analyse (cost-optimal) pathways to climate neutrality for sectoral production networks.

## 2 FORECAST-Sites

### 2.1 Model description

FORECAST-Sites is a site-specific simulation model to assess industrial transformation pathways in scenario studies in dependence on site-specific properties, as well as infrastructure availability and energy prices. FORECAST-Sites investigates investments and resulting transformation pathways, driven by exogenously given projections on economic and regulatory factors, such as energy prices, industrial process costs, CO<sub>2</sub> prices, infrastructure availability, or technology bans. FORECAST-Sites is developed in python using the mesa package. Derived model results are georeferenced energy demands and process diffusion behaviour.

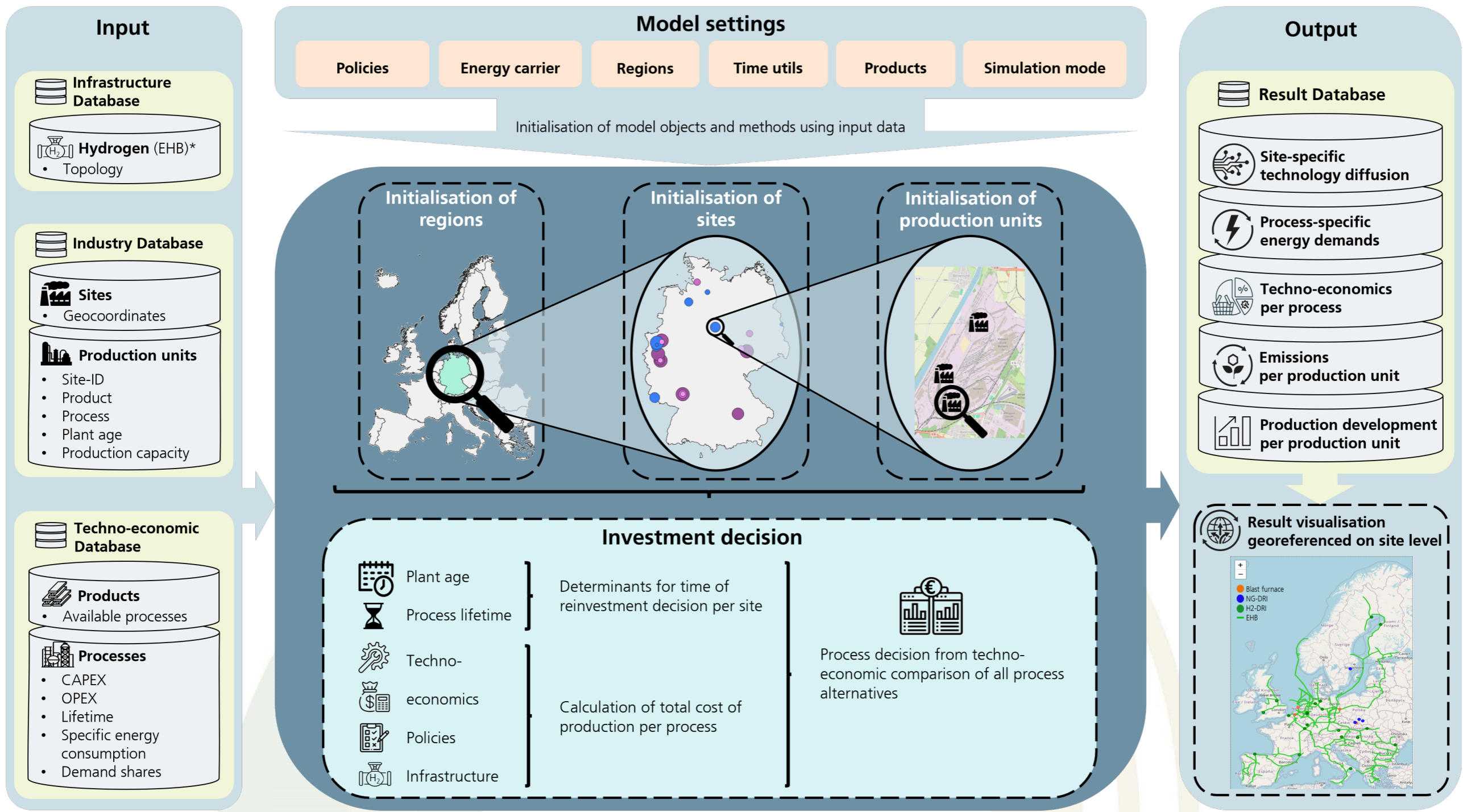
#### 2.1.1 Concept

The method described in [Neuwirth et al. 2024](#) considers existing industry sites and seeks to capture the complexities of process diffusion within the industrial sector. Utilising site-specific industry data allows for consideration of infrastructure and helps bridge the gap in detailed spatial results. The outcomes from the model scenarios facilitate the analysis of investment decisions, using current plant age and typical lifetimes. Currently, the Fraunhofer ISI IndustrialSiteDatabase ([Neuwirth et al. 2022](#)) provides critical inputs for energy-intensive industries. The spatial features and site-specific characteristics are integrated with techno-economic data for fossil and alternative low-carbon industrial processes. In its current state energy-intensive industries can be modelled for the EU. Data for primary steel and basic chemicals, both site-specific information and techno-economic assumption, are already included in the repository of the model while other sectors will be added in the 2<sup>nd</sup> phase of the project.

Three different types of databases provide input to the model. Currently, the model incorporates plans for hydrogen infrastructure development from the European Hydrogen Backbone (EHB) initiative ([EHB 2025](#)). The industry database includes existing sites and their production units, detailing plant age and production capacity. The techno-economic database defines products and parameters for process options. Model settings determine which products are simulated, allowing for scenario variations such as energy price changes and policy implementations like CO<sub>2</sub> prices or process bans. Some of those necessary inputs can be derived from other modules within the MIC3 framework, i.e., energy and CO<sub>2</sub> prices from the energy system module. This framework is available on GitHub, including data for primary steel and basic chemical sites, as published in [Neuwirth et al. 2024a](#). The Fraunhofer ISI IndustrialSiteDatabase is under permanent revision to capture dynamics on plant closures and newly installed plants. However, with more than 5000 industrial sites included it is not realisable to always have the latest information for each individual plant updated. Related to the model development, the methodological advancements focus on two main aspects:

1. Site-specific spatial resolution to evaluate industry transition attributes like hydrogen infrastructure availability and energy demands.
2. Consideration of industrial plants' age and reinvestment cycles to address the timing of hydrogen process diffusion.

Figure 2-1 shows the model overview and corresponding required input data, options for model settings, algorithm for conducting investment decisions and related results as model outputs.



\* hydrogen infrastructure according to plans from European Hydrogen Backbone initiative

Figure 2-1: Graphical overview of the model methodology of FORECAST-Sites (Neuwirth et al. 2024)

## 2.1.2 Data

This modelling approach is highly dependent on detailed and reliable data. Major requirements are the completeness and reliability of industry site data for existing industries as well as well-estimated assumptions on economic data such as energy prices but also process-specific parameters like specific investments in industrial processes or energy consumption.

### 2.1.2.1 Inputs

The FORECAST-Sites model requires a broad range of input data, which are partly derived from other MIC3 modules. The following table presents an aggregated list of exogenous parameters and their source.

**Table 2-1:** Exogenous parameters

Parameter	Description	Type of Sources
<b>Industry site information</b>	Required for initialisation of industrial sites within the model	Industry databases (i.e., IndustrialSiteDatabase)
<b>Techno-economic process data</b>	Determines the calculations for economic competitiveness of various process alternatives and the investment decision algorithm	Literature
<b>Production</b>	Required for calibration of the site-specific production volumes	Literature / Public statistics / MFA Module
<b>Energy price data</b>	Driver for economic calculations	OPEN-PROM
<b>CO<sub>2</sub> price development</b>	CO <sub>2</sub> -Certificate prices until 2050	Scenario data/OPEN-PROM
<b>Infrastructure</b>	Consideration of hydrogen infrastructure as determinant for process switch	European Hydrogen Backbone Initiative ( <a href="#">EHB 2025</a> )

### 2.1.2.2 Outputs

The main results are time series of energy demand, costs of the industry transition (e.g., investment by site, energy costs, costs for EU ETS CO<sub>2</sub> certificates, ...), emission mitigation and respective process diffusion. The table below presents the main output variables, which are used in the energy system module. [Section 4](#) presents some exemplary results.

**Table 2-2:** Outputs to other modules (preliminary)

Parameter	Description	Sink
<b>Energy demand</b>	Energy demand per energy carrier as time series to be covered by the supply sector	OPEN-PROM
<b>Process shares</b>	Shares per process and branch to assess process diffusion patterns in each energy-intensive sector	OPEN=PROM
<b>Emissions</b>	Emissions to estimate total reductions within the energy system	OPEN=PROM

## 2.2 Novelty and next steps

Known existing models to assess industry transition pathways work on national level using public statistics, which are often not available in higher resolution. The core novelty of this approach is the spatially highly resolved detail, which can help for better understanding of the spatial and timely dynamics of process diffusion in the industry sector and to guide effective policies. The developed bottom-up approach helps to understand the systemic challenges with a higher level of detail and enables the integration of necessary data granularity in energy system models to provide an improved understanding of the implications of industry transition pathways on the entire energy system.

Moreover, the following points highlight the contribution to the scientific progress:

- [Neuwirth et al. 2024](#) presents a first first-of-a-kind open-source industry model with a transparent method to assess industry decarbonisation pathways by incorporating site-specific data, which allows to investigate spatial dynamics of industry transition. For the present version, site-specific data and techno-economic parameters for primary steel and basic chemicals for the EU27+3 are already included and available in the models' GitHub repository.
- The bottom-up approach helps to understand the constraints in energy infrastructure and spatially resolved need for action to support industries in their transformation from supply side and regulatory view. The hydrogen infrastructure according to [EHB 2025](#) is included with information on coordinates and commissioning date, which restricts the availability of hydrogen for the individual sites, if no pipeline exists in a proximity of a certain distance in the respective years.
- [Neuwirth et al. 2024a](#) delivers open data for the core sectors of primary steel and basic chemicals production, including the site information (e.g., production and plant age) as well as parameterisation on CAPEX, OPEX, specific energy consumption (SEC), lifetime, and emissions.

Consequently, future work in phase 2 focusses primarily on two aspects:

1. Data curation: Integration of further industry branches and parameterisation of further process options, focussing on the direct electrification of industrial process heat and the implementation of carbon capture and utilisation or storage (CCU/S) processes. Those options should complement the delivered input data to investigate on reliable and credible industry transition scenarios.
2. Model development: Additional functionalities the developing team is currently already working on is the consideration of the entire industry sector by using a top-down approach for all branches, which cannot be assessed site-specifically due to restrictions from data availability. In addition, the current open-source version v1.0 is going to be updated to assess industrial symbiosis and cross-cutting technologies in line with the expansion to further industry branches. An extensive update of the current prototype and pilot model will be uploaded open source as v2.0 during phase 2 of the project.

**Table 2-3:** Exemplary optional topics of planned model implementation during phase 2 of the project

Planned Extension		Planned implementation
<b>Optimised production units</b>	Sub-production units for the implementation of the process fuel switch, steam module and cross-cutting	v2.0 (in testing)

Planned Extension		Planned implementation
	technologies	
<b>Roll out of further processes, sites and subsectors</b>	Roll out of further processes, sites and subsectors	v2.0 (in testing)
<b>Complete coverage of industry sectors</b>	A top-down approach that takes all industry sectors and their transformations into account based on energy balances.	v2.0 (concept developed)
<b>Infrastructure</b>	Power grid and potential CO2 infrastructure availability at the site to determine technology options	v2.1
<b>Trade module</b>	Trade of intermediate products between different sites	v3.0
<b>Energy carrier competition</b>	Endogenous distribution of limited energy carriers such as biomass and plastic waste	v3.0
<b>Visualisation Tool</b>	Dynamic visualisation of model results	v2.0 in development
<b><i>Extended documentation</i></b>	<i>Increased user friendliness and transparency through an extended documentation</i>	

## 2.3 Exemplary results

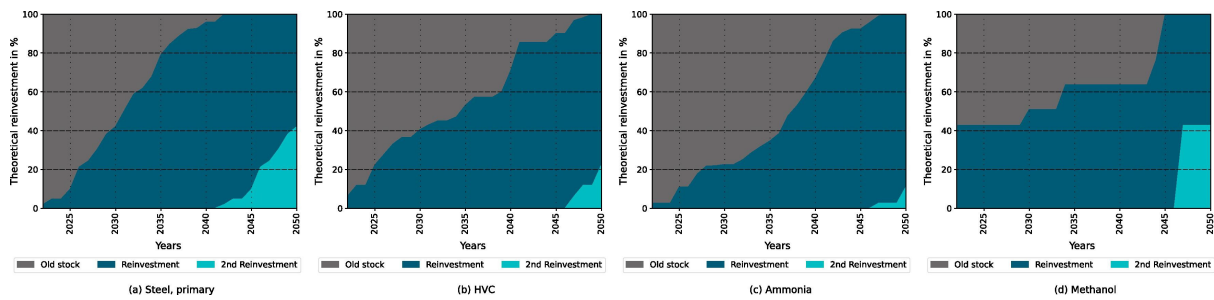
This section presents in the following exemplary results for the transition and diffusion of hydrogen in European primary steel and basic chemicals production. The whole analysis can be accessed in [Neuwirth et al. 2024a](#):

1. Sensitivity analysis of prices for hydrogen and CO<sub>2</sub>-certificates and their effect on a possible diffusion of hydrogen-based process options for steel, ammonia, methanol and high value chemicals (HVC).
2. Results for the respective pathways on investments, energy demand, and emission reduction.

### 2.3.1 Analysis of the age structure for the current plant fleet

The analysis of the European primary steel, ammonia, methanol, and HVC plants in a site- and plant-specific bottom-up manner leads to the theoretical reinvestment cycles presented in Figure 2-2, and thus, to the

possibility to invest into hydrogen-based process alternatives.



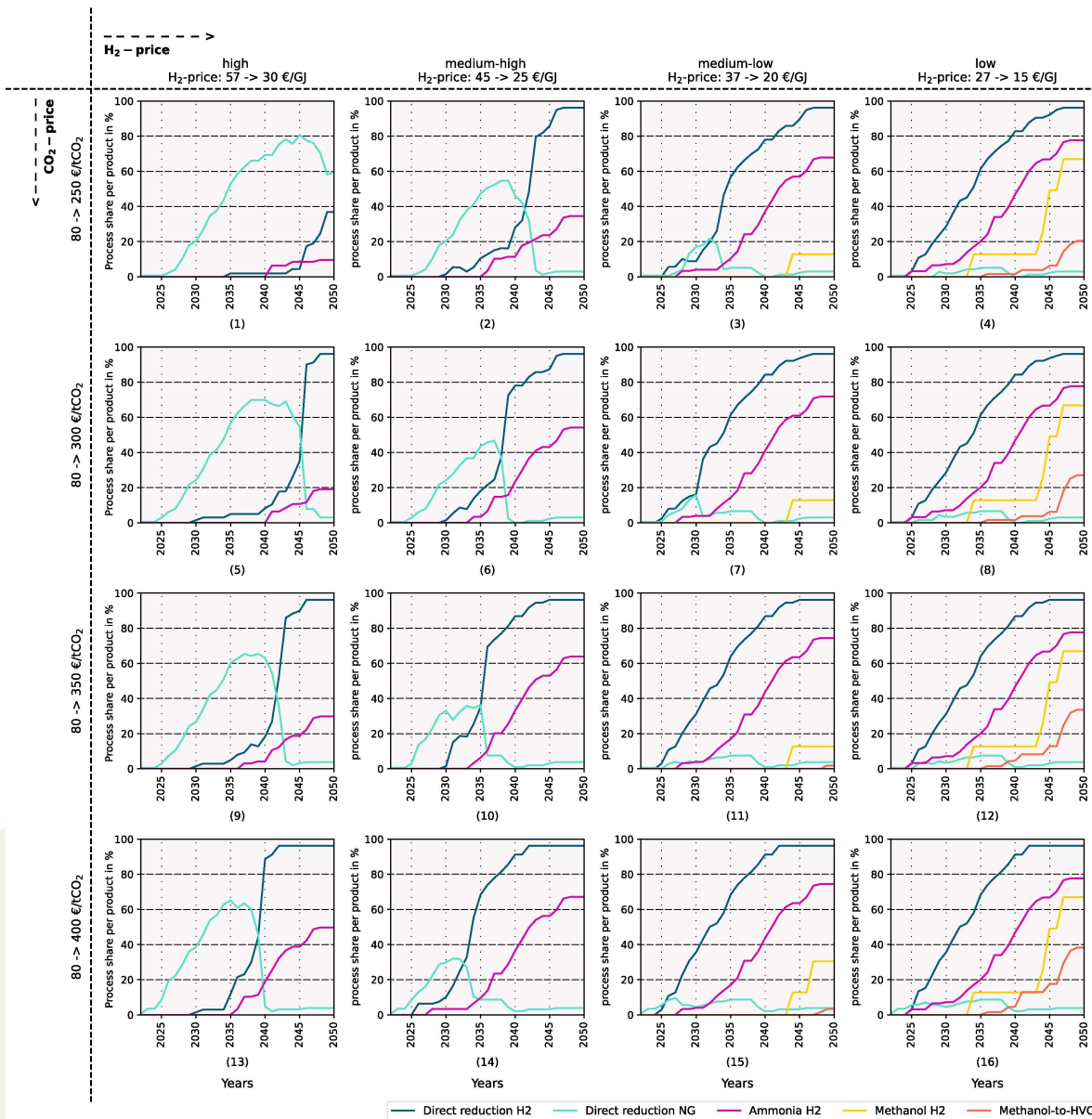
**Figure 2-2:** Theoretical reinvestment options for primary steel, ammonia, methanol and HVC according to the age of the currently existing plants.

As a result, all covered plants require at least one investment decision until 2050. However, around 36% of all plants require reinvestments until 2030, which indicates that often only one window of opportunity is left as lifetimes are at minimum 20 years. Summarised, there is a high risk for carbon lock-in from necessary investments within the upcoming years if no climate-neutral alternative will be available and economically competitive.

### 2.3.2 Development of process diffusion

To assess the investment behaviour of the individual industry sites depending on different economic conditions, a sensitivity analysis was conducted by varying the prices for hydrogen and EU ETS CO<sub>2</sub> certificates (4 variations each, leading to 16 sensitivities). Figure 2-3 shows the possible diffusion based on the investment decisions for the mentioned 16 sensitivities of prices for hydrogen and CO<sub>2</sub>-certificates using a fixed set of fossil energy price projections.

In the vertical axis, the development of prices for CO<sub>2</sub>-certificates increases, while the horizontal axis reflects the cases from high to low hydrogen prices. The results show that low prices for CO<sub>2</sub>-certificates and high hydrogen prices result in late and low diffusion of hydrogen-based processes from around 2040 onwards, with NG-DRI taking early large production shares due to lower emissions compared to blast furnaces. Thus, for the lowest case of CO<sub>2</sub>-certificates and highest hydrogen price sensitivity, the switch from natural gas to green hydrogen remains incomplete until 2050. In contrast, the share of H<sub>2</sub>-DRI increases drastically with increasing prices for CO<sub>2</sub>-certificates and decreasing hydrogen prices. In summary, prices for CO<sub>2</sub>-certificates would have to reach 300 €/tCO<sub>2</sub> for high hydrogen prices above 100 €/MWh to make H<sub>2</sub>-DRI competitive even for high hydrogen prices and achieve 2050 climate targets in steelmaking. For chemicals hydrogen prices below 60 €/MWh would be required to trigger investments into hydrogen-based processes and, related to the reinvestment cycles seen from section 2.3.1, this would have to happen before 2030 to reach climate goals. While reaching prices for CO<sub>2</sub>-certificates up to 300 €/tCO<sub>2</sub> could be a realistic case from today's view, reaching early green hydrogen prices below 60 €/MWh can most likely not be reached according to existing price projections. Therefore, the defossilisation of basic chemicals requires additional regulatory instruments. Further analysis and results are available as open data in [Neuwirth et al. 2024a](#).



**Figure 2-3:** Development of production shares for hydrogen-based processes for the covered products primary steel, ammonia, methanol, and HVCs

Exemplary key conclusions from Figure 2-3 could be that:

1. Natural gas-based direct reduction (DRI) for primary steel could serve as a bridging option towards future use of hydrogen for steelmaking.
2. The price of CO<sub>2</sub>-certificates is no proper instrument to trigger process switch towards hydrogen alternatives for products of the basic chemical industries where the carbon is embedded within the product.

### 2.3.3 Yearly energy demand for steel and basic chemicals in EU27+3

Figure 2-4 shows the resulting yearly energy demand for the above-mentioned sensitivities. Focusing on hydrogen, the projected demand differs from 64 TWh to around 500TWh in 2050, which would have a

significant impact on the design of the energy system and related infrastructure and could be further elaborated with the energy system module OPEN-PROM within the MIC3 framework.

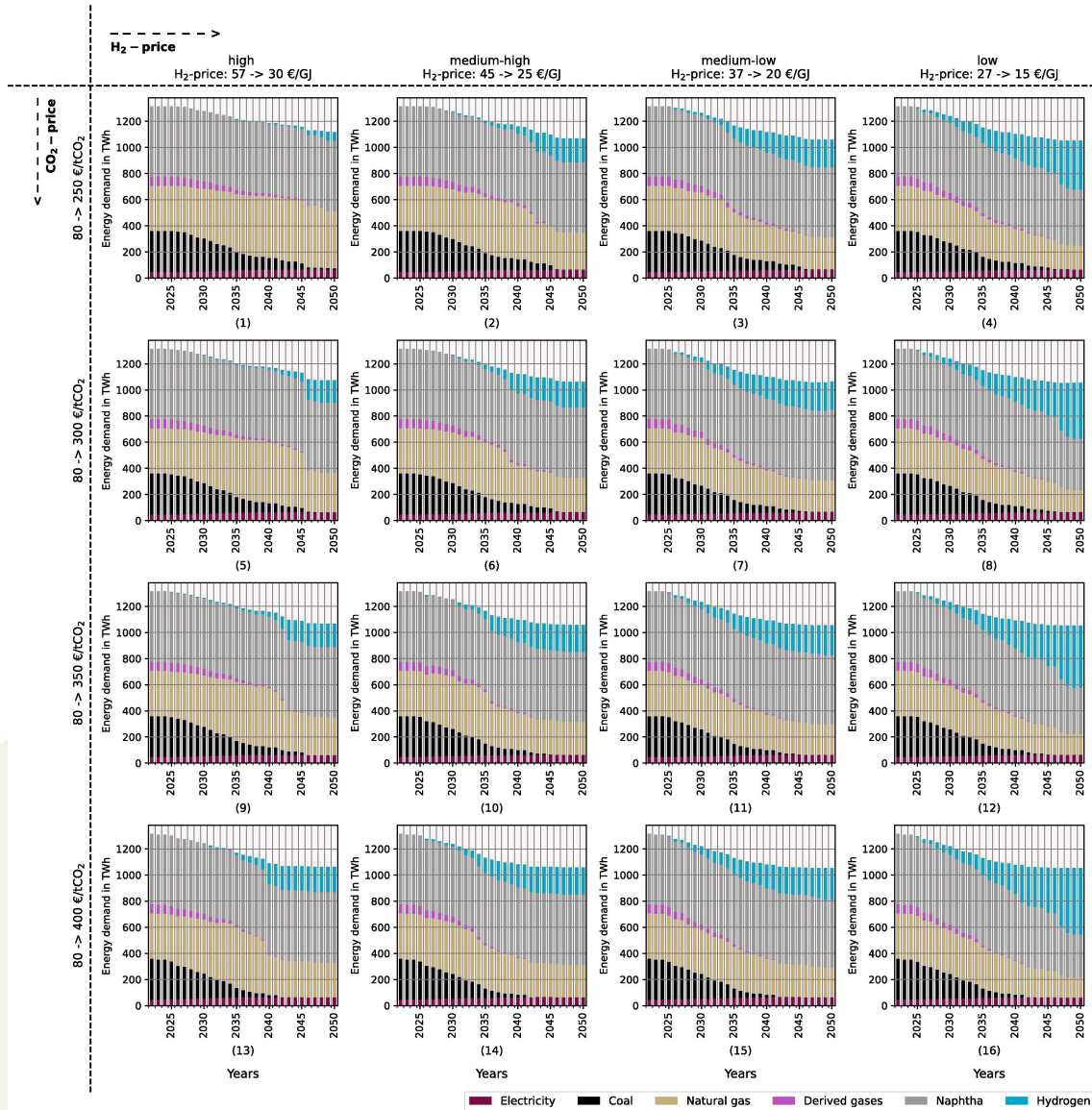


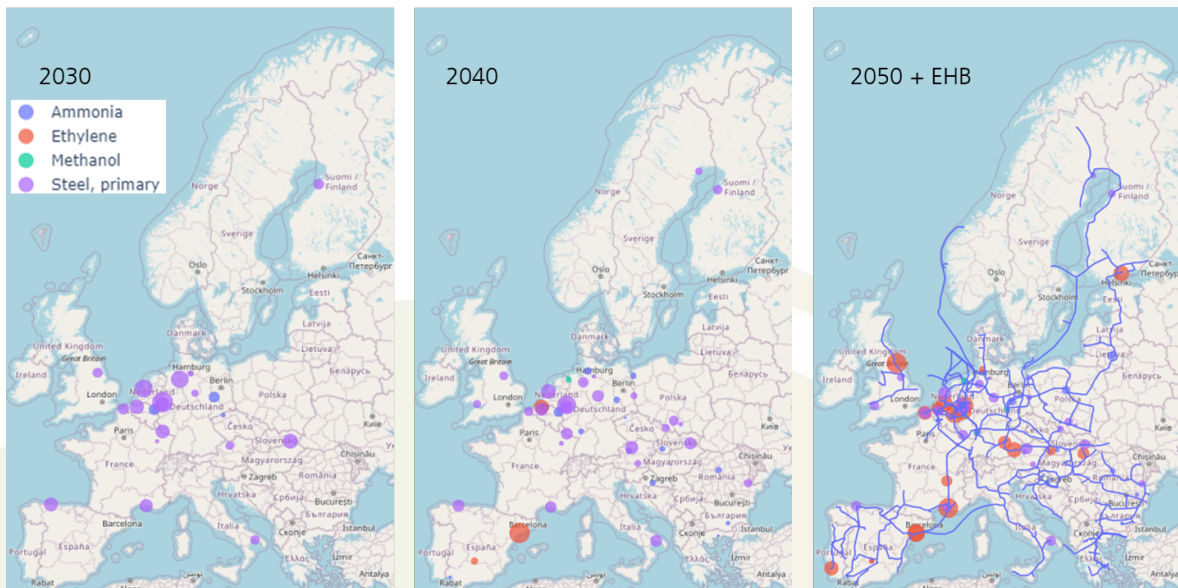
Figure 2-4: Development of the yearly energy demand for considered for primary steel and basic chemicals production

### 2.3.4 Spatial visualisation of model results

As one of the key advantages of the FORECAST-Sites model is the site-specific resolution, spatial visualisation of derived models is of huge interest.

Figure 2-5 shows exemplarily the spatial development for 2030, 2040, and 2050 in dependence of existing hydrogen infrastructure, considering theoretical investment cycles and the economic competitiveness between conventional fossil processes and hydrogen-based alternatives.

Interpreting Figure 2-5, it gets clear that the transition will most likely start using hydrogen in hydrogen-based DRI, while basic chemical plants start switching to hydrogen-based alternative in the late phase towards 2050.

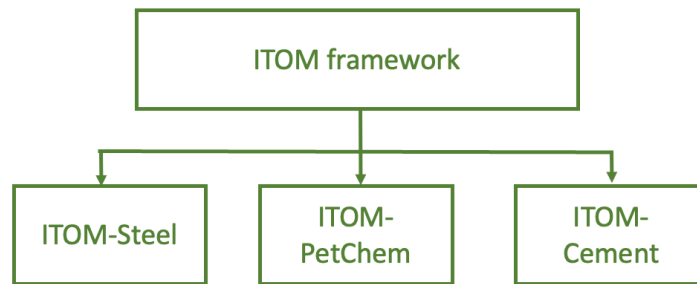


**Figure 2-5:** Spatial development of the diffusion of hydrogen-based processes in an optimistic case for 2030, 2040, and 2050

## 3 ITOM

### 3.1 Introduction

ITOM (Industrial Transformation Optimisation Model)<sup>2</sup> has been continuously developed over the last ~10 years at the Wuppertal Institute—including the targeted developments in the context of TRANSIENCE (see below). ITOM is a framework for the modelling of transformation processes in single basic industry sectors in the middle- to long-term. The framework so far has been implemented for the steel, cement and petrochemicals industries (see Figure 3-1).



**Figure 3-1:** The ITOM framework and implementations

ITOM can be used to derive detailed technological pathways for the production of basic materials, including energy and material demand, CO<sub>2</sub> emissions, investments and production costs. It features high technological detail including:

- differentiation of production by product types
- a differentiation of the production chain into various steps
- an explicit representation of individual sites and plants
- and an endogenous optimisation of the production network across sites and production steps.

Within MIC3, ITOM is closely connected to the EU MFA module (see D4.3) that provides the production volumes (differentiated by products) and available amounts of plastic waste and scrap that are main drivers for ITOM. It is also closely connected to the energy system module (D4.6) which provides energy costs – another important driver for ITOM.

### 3.2 Model description

Technically, ITOM and the data and software for its use consist of:

- The ITOM framework, implemented in Python
- Excel files that specify the input data for a particular industrial sector (“sectoral models” from here on)

Table 3-1 provides an overview of the software, input data and documentation of ITOM and its sectoral models which are part of this Deliverable. In the following, the ITOM framework is briefly introduced before core aspects of the sectoral models are presented.

<sup>2</sup> ITOM was until recently known as WISEE EDM-Invest.

**Table 3-1:** Overview of ITOM components

ITOM component	Type	Link
ITOM Framework code	Python code	<a href="#">GitHub repository</a>
ITOM Framework technical documentation	ReadTheDocs	<a href="https://itom.readthedocs.io/en/latest/">https://itom.readthedocs.io/en/latest/</a>
ITOM-Steel input data	Xls-files	<a href="https://doi.org/10.5281/zenodo.15772720">https://doi.org/10.5281/zenodo.15772720</a>
ITOM-Steel documentation	Document	<a href="https://doi.org/10.5281/zenodo.15772720">https://doi.org/10.5281/zenodo.15772720</a>
ITOM-PetChem input data	Xls-file	<a href="https://doi.org/10.5281/zenodo.15773104">https://doi.org/10.5281/zenodo.15773104</a>
ITOM-PetChem documentation	Document	<a href="https://doi.org/10.5281/zenodo.15773104">https://doi.org/10.5281/zenodo.15773104</a>
ITOM-Cement input data	Xls-files	<a href="https://doi.org/10.5281/zenodo.15773258">https://doi.org/10.5281/zenodo.15773258</a>
ITOM-Cement documentation	Document	<a href="https://doi.org/10.5281/zenodo.15773258">https://doi.org/10.5281/zenodo.15773258</a>

### 3.2.1 The ITOM framework

From a mathematical point of view, the ITOM framework is a linear optimisation model inspired by the OSeMOSYS framework by (Howells et al. 2011). ITOM optimises the total discounted costs of an industrial production system over the whole simulated time period, given a *demand*<sup>3</sup> for basic materials that must be met and (user-defined) constraints that need to be respected. The production chain is mainly represented by *products* and *technologies* and relationships between both, with *technologies* requiring certain *products* as inputs and producing (other) *products* that can be inputs to subsequent *technologies* in the production chain, or be final *products* used to satisfy the pre-defined product *demand*. *Technologies* can operate in various *modes of operation* that allow a flexible shift between inputs while using the same installed *capacity*.<sup>4</sup> Production *capacity* per *technology* is located at specific *locations* within *regions*. *Products* can be transported between *locations* and *regions* with transport costs depending on *transport mode* (e.g., onsite, interregional, pipeline) and *product*. Production *capacity* (per *technology* and *location*) may be exogenously defined but can also be invested in endogenously by the model. The model allocates production of (intermediate) *products* in an optimal way across locations and time. Details are provided in the technical documentation.

With regards to the modelling of possible circular economy measures, ITOM endogenously decides on the use of available input materials and thus has the capability to analyse the potential use of secondary

<sup>3</sup> Intermediate product demand for basic materials from the manufacturing industry (e.g., steel demand of the car industry by type of steel product)

<sup>4</sup> E.g., a cement kiln can be fired with coal or waste-based fuels; a shaft furnace with reformer for DRI production can use natural gas, syngas or hydrogen for iron reduction; a naphtha steam-cracker can use conventional fossil naphtha or renewable Fischer-Tropsch naphtha.

materials such as steel scrap, plastic waste and supplementary cementitious materials based on their availability, quality (e.g., copper contamination of scrap) and costs in relation to primary production. The details are specified in the sectoral models.

Within TRANSIENCE, we developed the tinyomo<sup>5</sup> ("tiny Pyomo") module, a light-weight clone of the python library Pyomo (Bynum et al. 2021). It defines classes replacing Pyomo objects and includes necessary methods to build an LP problem. Tinyomo is less user-friendly than Pyomo but requires significantly less memory to build and store a LP problem. It is critical with large problems (large number of equations) such as those resulting from the sectoral ITOM models that would otherwise require much more memory if built with Pyomo.

### 3.2.2 ITOM Steel

From a geographic perspective, ITOM-Steel covers the primary and secondary steel production sites in the EU27+3<sup>6</sup>. The production chain includes technologies for the production of (various forms of) iron from iron ore and iron pellets, the production of steel from iron and scrap and the finishing of steel in (a sequence of) rolling mills and by casting processes (see Figure 3-2). The technical basis features a highly detailed representation of production technologies as well as material, energy, carbon and CO<sub>2</sub> flows, including for example energetic use of off-gases in heat furnaces for steel finishing (see Figure 3-3). The main driver is an externally given production volume of finished steel, differentiated by 13 different products and four quality levels (copper tolerance).

In the scope of the TRANSIENCE project, the technology basis of the model has been further developed, allowing the model to mix direct reduced iron (DRI), hot briquetted iron (HBI) and scrap in electric arc furnaces (EAFs). This enables the flexible operation of EAFs for various steel quality requirements and the analysis of the impacts of such flexibility on circularity and recycling in the steel production system.

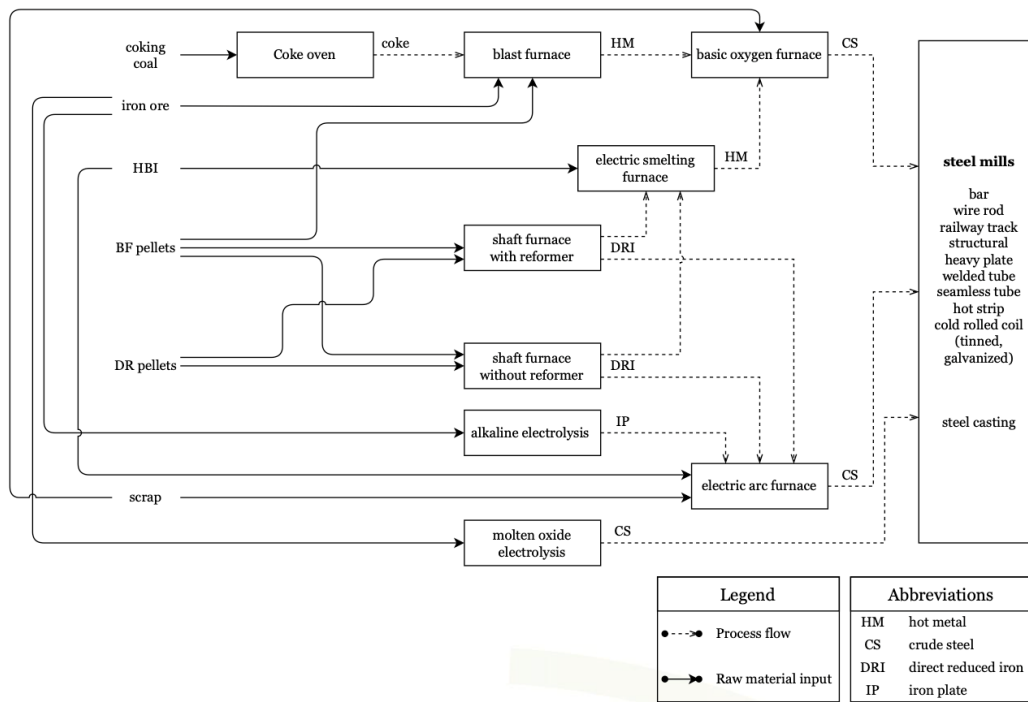
Key features of ITOM-Steel are:

- Consideration of copper tolerance of final steel products to endogenously model (limits to) scrap use in steel production
- Country specific costs for green electricity, hydrogen, as well as natural gas
- Green iron imports from non-EU countries whose costs are externally defined and on whose use ITOM decides endogenously
- Endogenous modelling of an intra-EU iron trade

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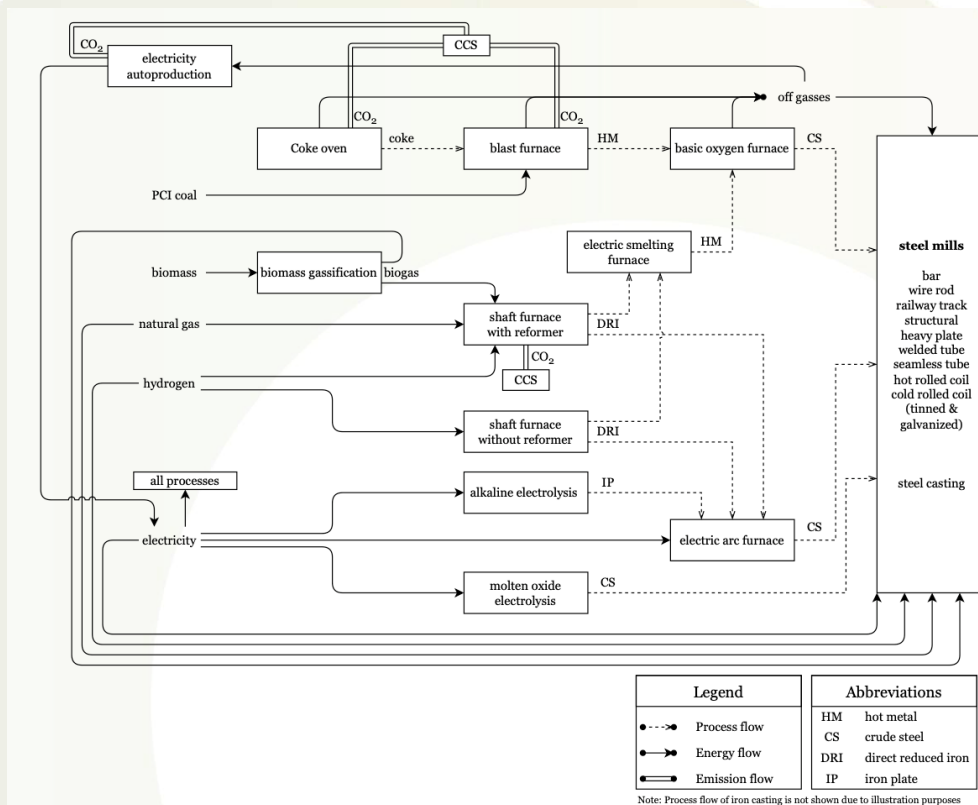
<sup>5</sup> <https://github.com/wupperinst/tinyomo>

<sup>6</sup> +3 refers to UK, CH, and NO



Note: Process flow of iron casting is not shown due to illustration purposes

Figure 3-2: Material flows in ITOM-Steel



Note: Process flow of iron casting is not shown due to illustration purposes

Figure 3-3: Schematic overview of energy and carbon flows in ITOM-Steel

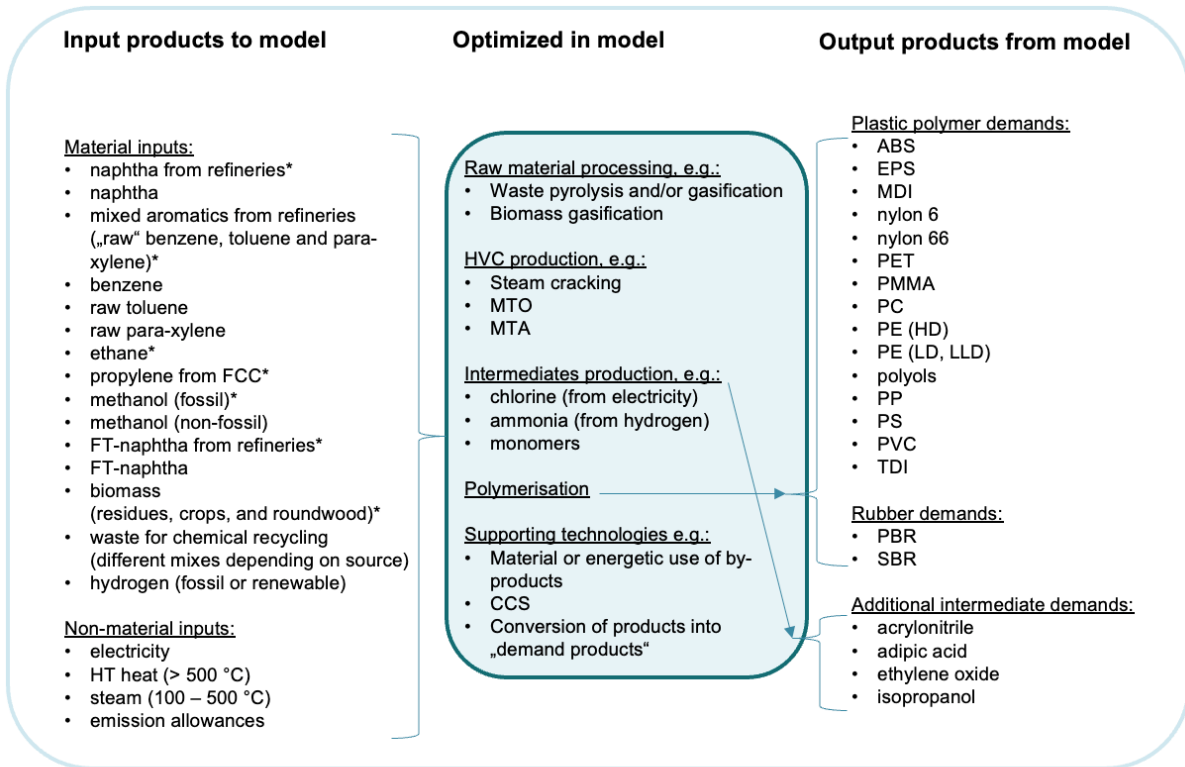
### 3.2.3 ITOM-PetChem

ITOM-PetChem covers the value chain of the petrochemical sector, including the production of polymers from a range of raw materials, feedstocks and energetic inputs. The driving requirement of the model thus is to produce an externally defined amount of final products (polymers). Polymers are produced from intermediate products (High-value chemicals (HVC), chlorine, ammonia). HVC in turn can be produced from various types of processed feedstocks and secondary materials (see Figure 3-4). The technical basis of the model includes various technologies for each of these steps in the production value chain. Geographically, ITOM-PetChem covers the locations in the EU27+3, while the EU27+3 are divided into five regions.

Note that the ITOM-PetChem does not cover the whole chemicals industry. Parts such as ammonia production for fertilisers, chlorine production for sanitation and specialty chemicals are not included. The production of process heat in CHP plants and boilers is also not part of the model. The demand for heat is instead expressed as fixed specific demand of processes for high-temperature heat (> 500°C) and Steam (100-500 °C) while the energy supply costs that arise from total heat demand and externally defined costs for heat supply are considered as part of the cost optimisation.

Key features of ITOM-PetChem are:

- Spatially explicit representation of existing base chemicals sites and capacities in EU 27+3, as well as transport routes between them (product pipelines, shipping routes)
- Model endogenous optimisation of production networks across sites and steps in the value chain (feedstock, HVC, polymers)
- Includes chemical recycling technologies and biomass-based production, as well as use of imported synthetic feedstocks
- Includes modelled regionalised polymer demand and plastic waste for chemical recycling in different sectors over time (mechanical recycling is not part of the optimisation, it is modelled in the MFA module, see D.4.3)
- Explicit consideration and endogenously optimised usage of by-products of various production processes



\*The input into the model is limited via ActivityLimit or capacities

Figure 3-4: System boundary of ITOM-PetChem

### 3.2.4 ITOM-Cement

The production chain of ITOM-Cement includes production of clinker from limestone and the production of cement from clinker and supplementary cementitious materials (SCMs) such as ground blast furnace slag and calcined clays (see Figure 3-5 for a schematic overview of the production chain). The model covers the cement demand and the cement clinker kilns in the EU27 and cement mills aggregated on a regional level. ITOM-Cement features a rich representation of clinker production technologies and of cement types. Demand is specified by cement application areas<sup>7</sup> (called “ConcreteX” in Figure 3-5) that may be restricted to certain cement types due to requirements with regards to compressive strength, durability and other cement properties in that application area. The driving requirement of the model is to satisfy an externally defined amount of cement demand from concrete applications per region while externally defined parameters such as energy costs, availability of SCMs and CO<sub>2</sub> prices change over time.

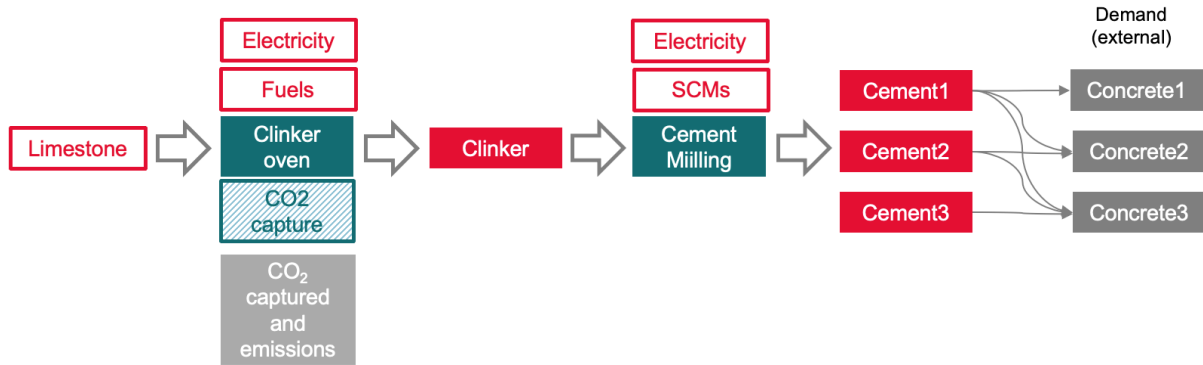
Key features of ITOM-Cement are:

- Differentiation of cement demand by country and application types with specific requirements
- Differentiated representation of cements (6 different types of cement)<sup>8</sup>
- Spatially differentiated availability of SCMs and alternative fuels

<sup>7</sup> Application areas are currently differentiated by a) in-situ concrete for interior components, b) in-situ concrete for exterior components, c) precast concrete, and d) miscellaneous. This may be subject to amendments during integration of the model into MIC 3 in the second phase of TRANSIENCE.

<sup>8</sup> The number of cement types included in the model will be increased during the second phase of the TRANSIENCE project.

- Flexible switch between and blending of fuels (such as coal, waste-based fuels, pet coke and biomass) for clinker production
- Spatially differentiated representation of transport and storage costs for captured CO<sub>2</sub>



**Figure 3-5:** Schematic overview of the production chain of ITOM-Cement

ITOM-Cement has been newly developed in TRANSIENCE from scratch and at the time of writing this deliverable partly uses place-holder data based on expert knowledge, for example for the age of kilns, regional availability of SCMs and alternative fuels as well as regional demand for cement. This will be reviewed and updated during the second phase of TRANSIENCE, for example based on data from the (announced) global cement and concrete tracker.<sup>9</sup>

### 3.2.5 Data (inputs and outputs)

#### 3.2.5.1 Model inputs

The ITOM framework uses input data that must be provided as an xls-file following a prescribed structure (see technical documentation<sup>10</sup>) that contains data on products, technologies, the relationships of technologies and products, transport routes and modes, cost parameters (capital, variable OPEX, fixed OPEX), demand for final basic materials, emission costs and limits, material resource potentials, and other constraints. These input-files reflect the “sectoral models” described above and the sectoral model documentations explain the “translation” of content-related concepts into the framework’s data structure. Model application and scenario analysis is then typically done by varying the input data of the sectoral models.

The content data is sector-specific but in general includes technologies and their parameters (energy and material use and production, CO<sub>2</sub> emissions, CAPEX, fixed OPEX, variable OPEX), CO<sub>2</sub> costs, energy costs, import options for materials and intermediate products (costs, limits), existing and announced capacities and user-defined constraints. The most relevant parameters for scenario design are listed in Table 3-2,

<sup>9</sup> <https://globalenergymonitor.org/projects/global-cement-and-concrete-tracker/>

<sup>10</sup> <https://itom.readthedocs.io/en/latest/>

including (potential) sources from within MIC3.

**Table 3-2:** Overview of main input parameters of ITOM

Parameter	Description	(Potential) source within MIC3
Demand for basic materials	Differentiated by products, years and regions	EU-MFA module
Energy costs	Differentiated by year; for some energy carriers furthermore differentiated by country	OPEN-PROM
CO <sub>2</sub> certificate costs	Differentiated by year. Can be differentiated by region	Energy system module
Material costs	Typically differentiated by year. May include different sub-categories (e.g., different scrap qualities in ITOM-Steel)	ITOM database; scenario assumptions
CO <sub>2</sub> transport and storage costs	Differentiated by year. Moreover, differentiated by spatial zones in ITOM-Cement	Scenario assumptions
Installed plants	Capacity and age of plants at the beginning of the simulation period and announced (or expected) projects	ITOM database; scenario assumptions
Other constraints	For example: limits to use of resources (e.g., biomass, waste), limits to installed capacity per year (e.g., to limit upscaling speed)	Scenario assumptions

### 3.2.5.2 Model outputs

Output of the ITOM framework consists of 53 csv files that cover capacity development, production by technology, costs, material and energy use, imports and exports, transport and emissions in various degrees of detail and using various perspectives, including location specific data for most outputs. Analysis of the outputs typically requires loading selected csv-files into additional tools (such as spreadsheet applications).

From a content perspective, typical core outputs of ITOM are listed in Table 3-3, including their potential uptake within MIC3.

**Table 3-3:** Main outputs of ITOM

Output	Description	Potential uptake in MIC3
Production volume by technology / mode of operation	Per product (final or intermediate), and per region / location and year.	Energy system module; LCA module
Material use, including use of	Per region and year	CGE module

secondary materials		
Installed capacity by technology	Per region / location and year. Can e.g., be used to examine intra-EU relocation.	CGE module
Energy use	Per technology, and per region / location and year	Energy system module
CO <sub>2</sub> emissions	Per technology, and per region / location and year	Energy system module
CO <sub>2</sub> captured and stored	Per region and year	

### 3.3 Novelty of the model, integration in MIC3 and next steps

A key innovative feature of the ITOM framework is its ability to model the transformation of production networks across sites and production steps endogenously through breaking up production routes into a chain of interconnected processes and through inclusion of various transport options for (intermediate) goods. In particular in combination with the EU-MFA module it provides an integrated perspective on core aspects of the twin transition to a Circular Economy and a decarbonised industrial production:

- Changing demand patterns and product design (translated into demand for basic materials by the EU-MFA module)
- Changing availability of secondary materials and other alternative feedstocks, and their use in production depending on competitiveness with primary production
- Changing energy costs
- Increasing CO<sub>2</sub> certificate costs

ITOM enables the integrated analysis of the effects of these aspects on industrial production and the associated energy and material demand and CO<sub>2</sub> emissions.

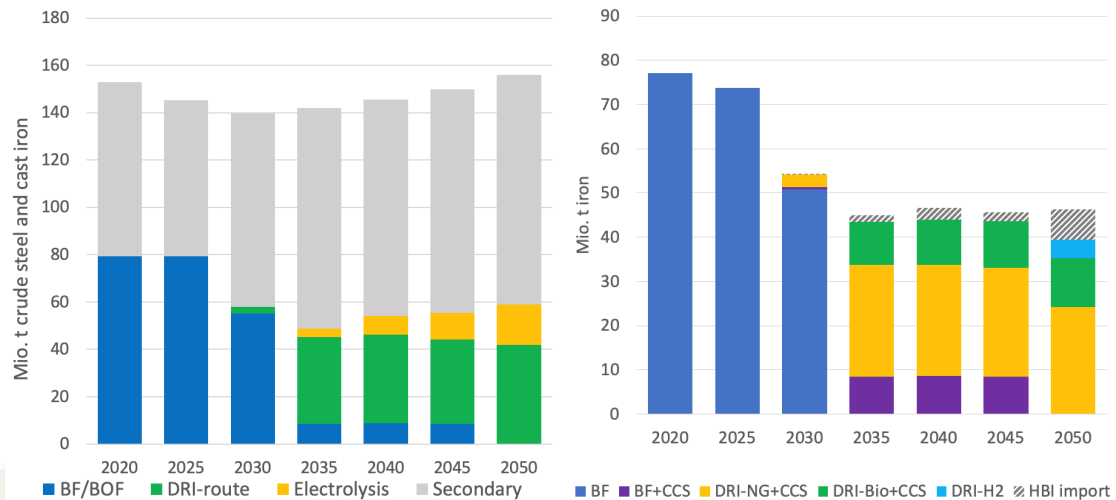
The integration of ITOM into MIC3 – in particular, its link with the EU MFA module that in turn is driven by the CGE and energy system modules – provides the opportunity to feed ITOM with well-founded scenarios for production volumes. Moreover, if the energy system module is also harmonised with the same set of drivers it can provide energy and CO<sub>2</sub> prices as inputs into ITOM that are consistent with the scenario for production volumes, leading to an overall consistent input data set for ITOM.

In order to realise this potential, interfaces between all ITOM sectoral models and other modules in MIC3 need to be implemented (or – where they already exist – be checked and improved). This will be the focus of the 2<sup>nd</sup> project phase.

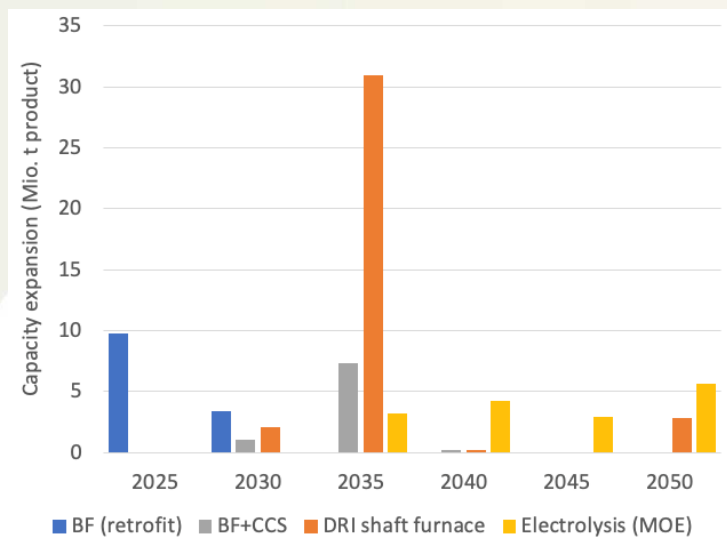
### 3.4 Exemplary results

In this section some exemplary results obtained with ITOM-Steel are provided in order to show the capabilities of the model and typical key result elements. Figure 3-6 shows the crude steel and iron production of the EU27 per plant type. While Figure 3-6 (left) shows the crude steel (and cast-iron) production per steel production route Figure 3-6 (right) focusses on the iron provision step at greater detail.

In sum, Figure 3-6 shows how the blast furnace route (BF-BOF) is equipped with CO<sub>2</sub> capture or replaced over time by electrolysis or direct reduced iron (DRI), which is processed in electric arc furnaces (EAF) or in smelters and the existing basic oxygen furnaces (BOF). DRI is produced with various fuels. In this scenario, imports of HBI<sup>11</sup> become relevant from 2035 onwards. Figure 3-7 focusses on the capacity expansion associated with the changes in production. Figure 3-8 traces the relocation of crude steel and iron production across EU regions over the simulation period. Figure 3-9 exemplifies a closer view on resource use by showing the use of scrap for various steel types in the model regions in the year 2050. The CO<sub>2</sub> emissions are shown and disaggregated by source in Figure 3-10, including negative emissions from the use of biomass-based syngas as reduction gas for DRI in combination with CCS.



**Figure 3-6:** EU crude steel production by plant type (left) and iron provision by source (right)



**Figure 3-7:** Newly built capacity of iron production plants (including molten oxide electrolysis)

<sup>11</sup> Hot briquetted iron – a transportable form of DRI

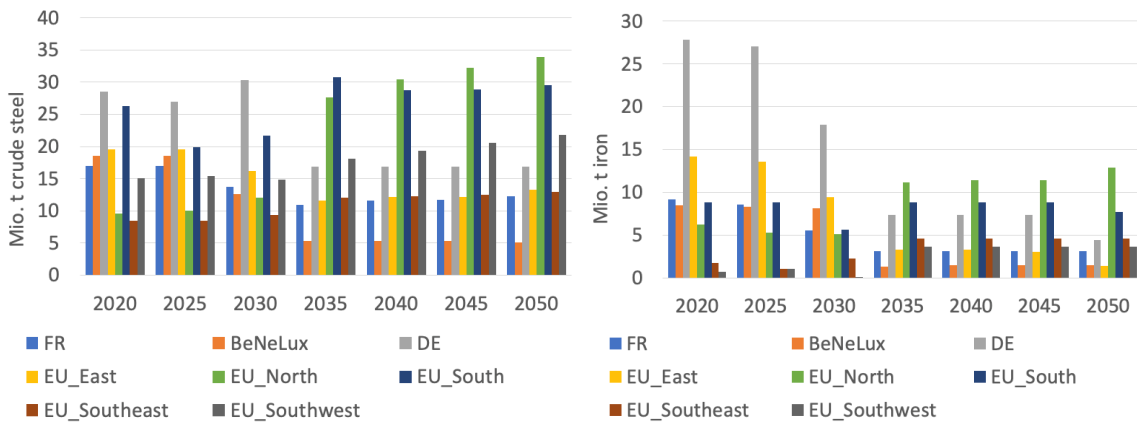


Figure 3-8: Crude steel (left) and iron (right) production by EU region

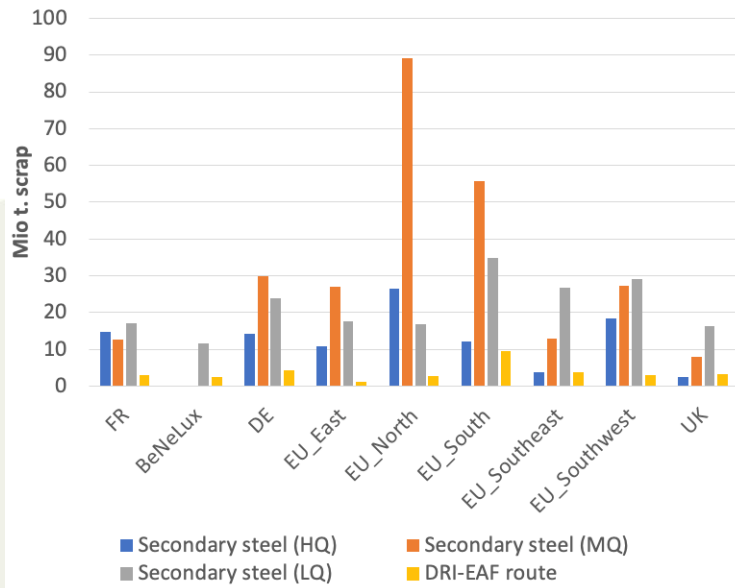


Figure 3-9: Scrap use in model regions in the year 2050 for different types of steel, considering steel quality of secondary steel (HQ = high quality, MQ = medium quality, LQ = low quality)

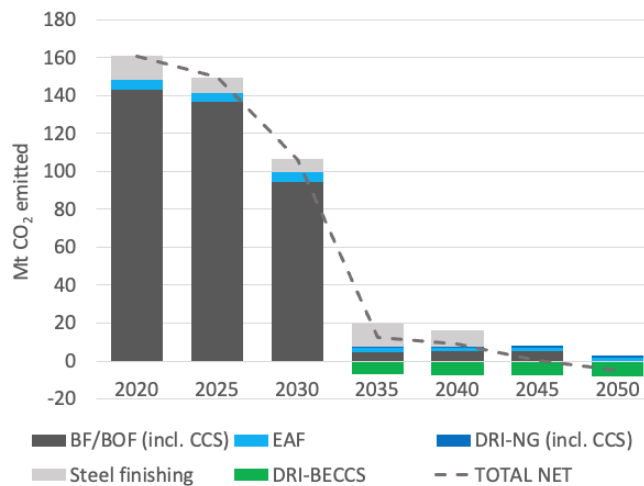


Figure 3-10: CO<sub>2</sub> emissions of the steel industry by source

## 4 Outlook

The present deliverable D4.4 consists of two separate models representing the techno-economic industry module within TRANSIENCE. Both presented models, ITOM and FORECAST-Sites, are planned to cooperate with their respective strengths in Phases two and three of the TRANSIENCE project.

FORECAST-Sites provides a more generic method to cover the entire industry and to model consistent industrial transformation pathways with various decarbonisation options, while the ITOM framework allows analysing in detail industrial production networks for particular sectors, such as steel, petrochemicals, and cement. Depending on the research question, either or both models may be used.

Both models use different approaches to project investment decisions and plant utilisation. While in FORECAST-Sites decisions are made from the perspective of individual sites, ITOM optimises investments and plant utilisation from the perspective of the whole production network. Scenario analyses can take advantage of these differences and conduct model comparisons to explore a robust space of plausible system development.

## Bibliography

European Hydrogen Backbone Initiative (EHB) (2025): Hydrogen Infrastructure Map - Showcasing concrete European hydrogen infrastructure projects and possibilities for transport routes and corridors, URL: <https://www.h2inframap.eu/>

Neuwirth, M.; Fleiter, T.; Hofmann, R. (2022): The future potential hydrogen demand in energy-intensive industries - a site-specific approach applied to Germany, Energy Conversion and Management 252, 115052, DOI: <https://doi.org/10.1016/j.enconman.2021.115052>

Neuwirth, M.; Fleiter, T.; Hofmann, R. (2024): Modelling the transformation of energy-intensive industries based on site-specific investment decisions. Sci Rep 14, 30552 (2024). DOI: <https://doi.org/10.1038/s41598-024-78881-7>

Neuwirth, M.; Fleiter, T.; Hofmann, R. (2024a): Modelling the market diffusion of hydrogen-based steel and basic chemical production in Europe – A site-specific approach. In: Energy Conversion and Management 322, 119117. DOI: <https://doi.org/10.1016/j.enconman.2024.119117>

Bynum, Michael L.; Hackebeil, Gabriel A.; Hart, William E.; Laird, Carl D.; Nicholson, Bethany L.; Sirola, John D. et al. (2021): Pyomo - optimization modeling in Python. Third edition. Cham, Switzerland: Springer (Springer Optimization and it's applications, volume 67).

Howells, Mark; Rogner, Holger; Strachan, Neil; Heaps, Charles; Huntington, Hillard; Kypreos, Socrates et al. (2011): OSeMOSYS: The Open Source Energy Modeling System. In: Energy Policy 39 (10), S. 5850–5870. DOI: 10.1016/j.enpol.2011.06.033