

DyMod Project description

PROJECT OUTLINE, SCIENTIFIC STRATEGY

The objective of the PEPR Sous-Sol PC2 is to obtain regional estimates of supply/demand of subsoil resources until 2050. For geothermal energy, gas storage and urbanization, it is a matter of "simply" quantifying the subsoil infrastructures to be deployed and converting them into subsoil use volumes. For mineral commodities, the problem is more complex because it is necessary to know in detail the installed infrastructure and products used in France, their material intensity, their lifespan and their recycling potential. This information is necessary to quantify the quantity of primary and secondary (recycling) metals mobilized. Three approaches will be possible to set the dynamics:

- Reading of scenarios produced by other actors than the PEPR community, e.g. IEA, ADEME or others, which list at least the quantities of energy used by sectors (transport, industry, housing) and in the best case the evolution of infrastructures. It is then possible to convert this information into built surfaces, numbers of vehicles, train, boat and planes per type, volume of gas to be stored, etc. using the unit consumption or storage volumes.
- Estimation of existing infrastructures from GDP/capita using logistics functions calibrated on historical data by country (Vidal et al., 2022, Leboulzec et al., 2023). This approach, gives trend evolutions for transport, housing, food, services, etc. It is then possible to modify the energy mix (electric vs. fossil energy), the intensity of use (e.g. average vehicle mileage, use rate or modal shift to other modes of travel). The advantage here is to integrate the scenarization into the model, which avoids using scenarios that were themselves calculated with a model that is not the one used to estimate the impacts, with a risk of inconsistency.
- Addition of a cost minimization function to define the technological mixes, in trend or not. This approach is complementary to point 2 since it gives a unique evolution.

PC2 aims at combining and eventually integrating these three approaches by coupling the existing models. To our knowledge, there is no model (even at the international level) having this flexibility and being able to reproduce past evolutions, which is necessary if we want to have a chance to say sensible things about the future. This objective will be possible thanks to the collaboration between Isterre, Gael, BRGM and IFPEN laboratories. In addition, we will develop approaches to link with the other PEPR PCs, the PC2 being seen as a tool to aggregate very diverse information:

- PC1 to take into account the social aspects, with a decisional aspect: a 50-year scenario is unlikely to be strictly followed, because beyond the resource and technological constraints, there are others that can generate systematic or sporadic opposition from citizens. Legal aspects and regulations (PC8 "Legal regulations") may also change over time and alter the framework of the initial scenario. Finally, trade and especially imports may also change. It is necessary to be able to include them in the model, to be able to modify the initial trajectory and to simulate abrupt changes (e.g. economic crises simulated by an abrupt change of GDP/cap or flow disruption).
- The PC3 ("Technical and economic foresight") for the material intensities of the subsoil technologies that must be integrated in the model (different geothermal and storage technologies, urban structures), and for the estimation of the value of mineral resources (long term price).
- The PC6 ("Environmental assessment and Life cycle thinking") to better integrate the environmental and life cycle dimensions.
- Field studies (PC9 to 13) to go down in scale and test the model at the regional rather than national level.

THE DIFFERENT MODELLING APPROACHES

Dynamic modelling

- A predictive model for the subsurface cannot be restricted to the subsurface. It is necessary to integrate the socio-economic and technological evolutions that will control the level of use. The sectors covered by the model will be at least energy (consumption and production), transportation, industry and construction. The level of industrial detail of subsoil technologies

and resource production (primary and recycled material, fossil and renewable energy) will be specified in consultation with PC3, PC6 and the regional field studies. The social dimension is much more difficult to integrate. The strategy envisaged is to create a variation of the model in the form of a serious role-playing game (WP3); this game will be used to support the societal judgement of the scenarios (multi-actor and multi-criteria evaluation of each scenario to meet the objectives of the actors), leaving the possibility for the players, whose objectives and interests often diverge, to make decisions during the simulation in the game, before the final date of the simulation

- The calibration of infrastructure evolutions and rates of technological progress will be constrained by historical data from different regions. For the future, two types of additional constraints will be introduced: i) thermodynamic limits that limit the incremental improvement capacity of a given technology and operating costs for decreasing qualities of resources (WP1.3), ii) disruptive evolutions that deviate the future trajectories from the trend situation.
- The model must be able to be used with a "What if?" approach. This means co-constructing the scenarios with the stakeholders and then giving the user the possibility to modify the scenario narratives (type of use of the subsoil, the infrastructure, regulatory constraints, etc.). Eventually, the model could be used to simulate trajectories that the user could define in a simple and intuitive way, i.e. by creating his own evolution scenario (WP4.1).
- The model must be understandable, transparent and open (open source and open data), coded in a language commonly used in science and capable of linking to accessible databases. The architecture must allow the addition of modules in an iterative way, especially economic and industrial sectors, without having to recode the core.
- The model must be backed up and linked to a database that is also transparent, referenced, remotely searchable in the form of adapted queries and controlled access rights (WP4.2).

Input/Output (WP2 et WP 3.1)

Flows at national boundaries will be estimated from I/O trade matrices, such as Exiobase. These matrices can be completed by adding specific flow data (MFA) for underground uses. Wherever possible, French regional flows will be compiled.

Aggregated Life Cycle Analyses and environmental impacts (WP1.3)

It is important to be able to follow the evolution of environmental impacts according to the chosen development scenarios in order to limit them. Environmental impacts will be quantified by coupling the biophysical model to LCA data (link with Eco-invent and complemented by PC6 for specific technologies and specific types of use addressed in SousSol). We will develop approaches to adapt the fineness of industrial processes to the less detailed granularity of the model. We will also develop approaches to include technological improvement of industrial processes (dynamic LCA) and regionalization. Finally, the environmental impacts can also be estimated from the Exiobase matrices, which allow regionalization of the impacts.

Energy intensity (WP1.3 et WP2)

The long-term price (value) of mineral and hydrocarbon resources is a function of the evolution of the quality of the exploited resources (ore grade and EROI), which decreases with exploitation. This evolution is a function of the exploitation speed imposed by the country scenarios and resources at the global level. This is why the French model must be coupled with a global model. As for the resources, the embodied energies of goods and infrastructures will be estimated from the prices. This will allow to complete the LCA approaches and to make an empirical link between cost-price and energy.

Agent based modelling (WP3)

In addition to the approaches listed above, we propose the creation of an Agent Based Model (ABM) branch. This is a promising work because it will allow to explore a wider variety of scenarios, including components related to human and social sciences. It will also allow us to adapt the current models to serious games to make them more accessible and to integrate decision mechanisms during the simulations.

SCIENTIFIC AND TECHNICAL DESCRIPTION OF THE PROJECT

WP1 : Estimation of demand in subsurface resources and scenarios of energy

The development of energy infrastructure, transportation, building and underground uses for the urbanized part, geothermal energy and underground storage will be estimated by bottom-up approach, with two evolution drivers:

- the evolution of GDP/capita, which gives an assessment of the evolution of major energy consuming sectors (buildings, transport and industry). Knowing the infrastructure in place, the energy to be produced can be calculated for different assumptions of consumption that depend on the electrification of uses, intensity of use, progress in energy efficiency, and change in consumption patterns. The infrastructure of energy production can then be calculated
- an allocation of technologies by minimizing costs or by minimizing environmental impacts (WP1.3). Other material and energy consumption by chemicals, agriculture, pharmaceuticals, packaging or domestic appliances will be estimated by a top-down (aggregated) approach. The infrastructure will be transformed into material needs by using the material intensities and the anticipated technological progress. Recycling potentials will be estimated for imposed product lifetimes, scrap collection and recycling rates.

The study will focus on France, but the models will integrate other world regions and countries. The approach will allow us to estimate the global footprint of France in Subsoil use and to evaluate the import-export of materials, energy and environmental impacts for scenarios of delocalization or relocation of its activities. We will use the Exiobase input/output matrices that describe bilateral exchanges between countries for 200 consumption and production sectors. A preliminary study conducted at Isterre shows that the approach is possible but it needs further development. These approaches should ultimately allow us to discuss the vulnerability of France to imports in a global context.

Different coupling and benchmarking of available models will be done, to better identify their complementarities, types of input and output data, and underlying assumptions. A general objective of the coupling is to be able to generate scenarios of technology deployment calculated with TIMES or POLES approaches that can be read by MATER to evaluate the needs (and possibly prices) of raw materials.

WP1.1 : Soft coupling of TIMES and MATER models (Isterre-IFPEN)

While issues related to geothermal energy and gas storage can be addressed at the local level, the situation is different for mineral resources. These resources, as well as the associated value chains, are indeed unevenly distributed across the globe. In order to address the issue of supply and demand of mineral resources on a local scale, it is necessary to consider the entire value chain on a global scale.

The MATER model developed by Isterre can be used to model a local scale. It integrates the interdependencies between the different sectors modeled (for example, steel production will evolve with the demand for new vehicles). However, it requires input of deployment curves for each of the technologies modeled. Symmetrically, the TIMES model developed by IFPEN does not integrate a dynamic loop between supply and demand. For example, the demand for steel is an input to the model, and does not depend on the deployment trajectories of the different technologies. On the other hand, the TIMES models propose an optimization of the energy system, and thus of the deployment of technologies. By their very design, the two tools MATER and TIMES present strong synergies since the input data of one is the output of the other. In addition to these conceptual synergies, there are spatial scale synergies. The IFPEN tools represent the global (TIAM-IFPEN) and European (MIRET-EU) scales. MATER, on the other hand, has the global scale, but can go down to the local scale in a simpler way than the TIMES models. The coupling of the two tools can allow to go from the global to the local scale. Finally, complementarities are also to be expected on the side of the modeled value chains. In particular, MATER proposes a recycling value chain that is much more detailed than that modeled in the TIAM-IFPEN or MIRET-EU models. The objective is therefore to use TIAM-IFPEN and/or MIRET-EU to generate technology deployment trajectories, in particular by using the new objective function developed in subtask WP1.3. These scenarios will serve as input data for MATER. It will then be possible to loop back using the outputs of MATER (industrial demand for example) as input to TIAM-IFPEN/MIRET-EU.

The work will consist of adapting the levels of technological and spatial aggregation of the different models, the rates of technological improvement based on historical evolutions, as well as the evolution of the price of technologies and resources according to the learning curves and energy intensity approaches (see 2.1.4).

WP1.2 : Strong coupling of POLES and MATER models (GAEL-Isterre)

As in the case of the TIMES-MATER coupling, the POLES-MATER coupling will allow the endogenization of the allocation dynamics of energy consumption in the different sectors with an

economic minimization constraint. Unlike TIMES, the code of POLES is available and we propose a strong coupling between the POLES and MATER models. The work will consist in translating POLES from Vensim to Python language, and in integrating the cost minimization into the structure of MATER. The coupling will make possible to estimate the dynamics of price, including the raw material long-term prices according to their cumulative consumption with the approach described in 2.1.1.4 and/or by using the results of the PC3 ("economic foresight"). The final modeling structure will allow for the estimation of the national need for primary and secondary material. The project will also allow the modeling of renewable energy production and gas storage technologies as well as evaluation of the net CO2 emission trajectories.

WP1.3 : Environmental impacts and optimization of an energy system on environmental criteria (all PC2 partners, link with PC6)

- Isterre is developing an empirical method for estimating embodied energy from price (Andrieu et al., 2022; Vidal et al., 2022 and submitted). The approach is based on the analysis of the relationship between these quantities (in MJ/euros), for a variety of products in different countries. For mineral commodities, the production energy is calculated as a function of the ore grade of mineral deposits. This approach reproduces both the long-term energy and prices observed from 1900 until today for 15 metals and mineral commodities. For semi-finished and finished products, the embodied energy/price ratio constrained by the Exiobase data is remarkably similar for about 100 consumer sectors. The variation of the ratio over time can be estimated from the historical evolution for ten world regions according to their GDP/capita evolution. Eventually, we hope to be able to estimate embodied energies of goods as a function of prices and GDP/capita. For a given energy mix, it would then be possible to estimate GHG footprints as well as other environmental indicators by producing and consuming sectors and countries.

This approach is less accurate but complementary to the LCAs developed in PC6 to which they will have to be compared. In order to integrate the LCAs in the dynamic models, the different industrial stages of production will be aggregated in 3 stages of production of raw materials, semi-finished products and finished products. These stages will be specified for the particular technologies used for the exploitation of the subsoil.

IFPEN's models optimize the total cost of the energy system under greenhouse gas emission constraints. However, there are several ways to achieve carbon neutrality and the economic criterion is not necessarily the most relevant to discriminate between them. The total consumption of resources (energy, subsoil, materials and other resources) can advantageously replace the economic evaluation. This implies collecting data on resource consumption for all the technologies modeled. It is also necessary to modify the objective function of the models and thus modify the core of the optimization. This will allow us to propose energy transition scenarios optimizing the consumption of one or more resources.

A similar approach will be developed in the POLES model. The objective function will minimize the cost of the global energy system each year under constraints of greenhouse gas emissions reduction implemented by a carbon shadow price. The cost of environmental externalities will be included in the objective function based on the POLES/MATER coupling established in WP1.2 and the environmental constraints (pollution, water...) estimated for the considered trajectories. This approach will allow for the analysis of the combination of public policies.

WP2 : Estimation of local production capacities

WP 2.1. Regionalization (Isterre-BRGM-IRIT)

In contrast to the demand in raw material and energy than can be satisfied by inter-regional flows, the production capacities depend on local parameters. The national demand scenarios (WP1) will have to be compared to local potentials (solar, wind, mineral resources, water, geothermal, type of subsoil and storage, possibility of urban extension, etc). This comparison requires the regionalization of models and the estimation of exchange flows of mineral resources and energy between regions, whether within one nation or between global regions.

The regionalization of models is a real challenge because it must take into account the local specificities such as renewable energy potentials, relief, availability and type of subsoil, socio-economic characteristics (industrial potential, transport and communication routes, current energy production, urban planning, population density, employment basin, etc.) as well as other cultural, regulatory and investment capacity dimensions. Two major difficulties are identified:

1) For the demand side and thus evolution of infrastructures, it is not certain that the GDP/capita-infrastructure-energy relationships used in MATER and validated at the level of nations or large world regions are directly usable at the sub-national level. In addition to the already used variables (population density & urbanization) that control the saturation levels of the infrastructures/cap versus GDP/cap logistic functions, other variables are possibly necessary to reproduce the historical trends observed at the regional scale. Such variables could be the average and extreme temperatures that control the type of construction and degree of isolation, the landform that controls the development of cities and exchange routes, or other parameters that have to be identified.

2) A method must be developed to estimate the future potentials of inter-regional flows. This method must be able to reproduce the magnitude and evolution of historical flows of commodities in ore and in exchanged goods reported in Exiobase for the period 1995-2015. A possible approach would be to describe these flows with Fick's laws, where the gradient is controlled by the difference between local demand and available resources of the exchanging regions, and the diffusion coefficient could be proportional to the transport cost, itself a function of the existing or to be built transport infrastructure, of the distance between production and consumption locations, etc.

To address the two points mentioned above, a great deal of work is needed to collect data and their historical evolution over time. These data are crucial to constrain the regional logistic evolutions and saturation levels (point 1), but also to estimate potentials, production and exchange capacities (point 2). At the subnational level, at least two regions will be studied, including Occitanie, in collaboration with PC13. Another region will be considered, the Paris basin or the Rein Graben being probable targets, to be confirmed according to the available data. If time permits, other sites will be considered.

The ultimate objective of the regionalization work is to eventually couple the dynamics of demand with Geographic Information Systems including transportation infrastructures (material, energy), urban infrastructures, local availability of resources and renewable energy, and subsoil access potentials.

WP2.2. Raw materials supply (BRGM)

For the specific question of raw materials supply at the global scale, an effort will be dedicated to taking into account exploration investments and the life cycle dynamics of local extractive industry projects. This would allow us to consider the possible future unavailability of certain materials due to economic constraints and to create feedback loops to study substitution mechanisms and the transfer of demand to other available materials. These mechanisms are important for establishing development scenarios and trajectories, and for assessing the criticality of mineral feedstocks in a forward-looking approach. A financial support for PhD working on this task will be demanded by the BRGM and CEA through the call to projects organized by the PEPR at the end of 2023 and later.

WP3. Implementation and use of actors' decision models via role-playing, serious and playful game (BRGM-Isterre-Chaire science et jeu vidéo)

The aim is to create a decision component model, driven by the following 5 objectives: (a) to identify the list and respective role and stake of actors influencing – or influenced by - the system (legislator, companies, citizens ...), (b) to represent their features (structural level), (c) to represent the decisions that these respective roles have to take (behavioral level), via two inputs: (d) the interactions between these different roles and (e) the influence of the decisions taken by these roles on, for example, the energy transition and the physical flows that underlie it: flows of goods, of raw materials, of energy, of built-up area estimated in WP2. The first four objectives are fed by PC1 "*Building scenarios for the use of the French subsoil*". The five one could be addressed by the coupling of the decision component with the tools and approaches developed in PC2.

WP3.1. Coupling of existing models with an Agent Based Model (Isterre-BRGM)

The existing models (MATER, TIMES and POLES) do not have the appropriate structure to be used in gaming mode, because gaming requires model able to simulate the actions and interactions of autonomous agents (individual or collective entities). These decisional entities can be individuals or organizations, or even, in some applications, technological units (e.g. cars or a trains, buildings, etc). In order to understand the behavior of a system and what governs its outcomes, agent-based models must be developed with two objectives: 1) integration of the geography and local resources of the regions of interest. This will allow a more precise evaluation of the possible flows of matter and energy between regions, 2) integration of components which are able to make decision.

The expected model developments will open the possibility to go down to the regional scale and offer tools for political and social decision making that are currently missing. The ABM model will also make it possible to explore different energy transition scenarios, taking into account the behavior of the various stakeholders and local environmental constraints. The work will be conducted in close collaboration with WP2 and WP3.2. The creation of an ABM is a central but risky objective of PC2 requiring specific skills and background in modeling and computer coding.

WP3.2 Creation of a role-playing game based on the ABM model (BRGM -Isterre)

The objective is to allow actors to explore and analyze the consequences of the decisions they make during the simulation, which may lead to a deviation of the actual trajectory from the initial scenario trajectory. The game would also make the resulting coupled models of the project accessible to different audiences, including policy makers, scientists, and citizens. The connection between the game and the model (via ABM) will be as follows: (i) each human agent (a player) who wishes to play a given role will choose one of the computer agents that plays that role, and thus will be its representative in the model; this computer agent will be the bi-directional bridge between a player, who will manipulate aggregated indicators, and the model, which can also manipulate complex variables. A detailed reflection will be necessary to define specific indicators intelligible to decision makers and citizens, such as local emissions and consumption of resources and energy, water, land use, visual impact, investments, employment, etc. This requires a detailed study of the positions of the different actors, and a strong link with the PC1. The indicators will be the information the players will use to make their decision to modify the long-term trajectory initially foreseen in the "what if" scenario. The consequence of the decisions will be governed by the model's couplings, so that it will possibly have effects contrary to what was the player was expecting. It will then be possible (at the end of the game) to analyze the mechanics involved and the couplings that were not anticipated by the players. The goal is not to provide an expert and infallible decision support tool, but to make the players/decision-makers perceive the complexity of the couplings and the short-term decisions on the long-term evolution.

WP3.3. Creation of a multiplayer video game based on the dynamic model (Chaire science et jeu vidéo)

The aim here is to turn the scientific model, tested in the form of serious games, into a game accessible to all without any external intervention. The interest is to valorize the scientific work by democratizing the access to the model in a playful way. The creation of an open access version will be entrusted to professionals if they see the interest, but an upstream preparation is necessary. This task will be entrusted to the "science and video game" chair (Ecole Polytechnique-ubisoft) and partly financed in the form of an AAP (internal call to projects of the PEPR "Sous-sol bien commun"). The work will consist in

- 1) establishing the objectives of the game(s) according to the target(s) (Benchmark of comparable games, choice of the target(s), of the scope of the expected learning or awareness topics, of the game model, first estimation of the dimensioning),

- 2) establishing the specifications and the distribution to studios capable of producing the game (Formatting of the specifications, distribution and contribution to the recruitment). This step will require dedicated funding, which will be requested in response to the AAP.

- 3) supervising the work (support in the implementation of the methodology for the realization of the game, monitoring of the realization according to pre-established milestones, participation in intermediate user tests).

- 4) evaluating the results (participation in the final user tests and the diffusion).

WP4 Accessibility to data and models (all partners)

WP4.1. Graphical interfacing

One of the ambitions of PC2 is to develop dynamic models with a robust scientific basis, accessible not only to specialist researchers but also to an audience unfamiliar with modeling. This requires building graphical interfaces to run the models, modify assumptions and scenarios, access input data and results, and visualize them without having to enter lines of code. Building graphical interfaces is not in the realm of research per se, but is absolutely necessary to democratize the use of the models by a non-specialist audience. In addition to the models, we will develop tools to help interpret the results.

WP4.2. Production of a remotely searchable SQL database

A lot of data will be needed for the modeling work. The data will be fed into a database already existing within the framework of an Isterre-Carbone4 collaboration, which currently includes about a hundred technologies, fifty socio-economic indicators and thirty environmental indicators for the years 1930-2020, 15 world regions and different countries like France, the US, Japan and Germany. This database

will be completed during the project and connected to other commercial (Exiobase) or environmental (Ecoinvent) databases. Eventually, we will propose an architecture and a user interface allowing access and sharing of data. Confidentiality and data ownership aspects will of course be handled in a transparent way. The PEPR "*SousSol, bien commun*" would be an opportunity to build a broader base with the contribution of geologists, economists, sociologists and industrial ecologists.