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A framework for global sensitivity analysis in long-term energy systems planning using optimal transport

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ABSTRACT

This paper introduces a framework for applying global parametric sensitivity analyses to energy system optimization models. The methodology presented is based on the optimal transport theory, enabling the identification of the most influential model inputs in shaping key outputs, such as energy mix composition, technology deployment, and system costs. The technique is applied to an instance for Italy within the Tools for Energy Model Optimization and Analysis energy planning tool. Algorithms devoted to managing inputs samplings, model runs and outputs postprocessing are developed and presented. Results are derived by exploring their dependency on the assumed energy scenarios and inputs variability. The findings of the paper show that demand levels and costs are the most influential inputs in business-as-usual scenarios, while techno-environmental constraints and efficiencies represent the most important inputs in decarbonization scenarios. Expanding input sampling ranges leads to the emergence of additional clusters of solutions, revealing alternative cost-optimal technology configurations and energy mixes that may not appear under narrower input variations. The proposed methodology helps in identifying parametrically the most impacting sources of uncertainty in energy planning and is openly available for future applications.

Abbreviations

ENSPRESO	Energy System Potentials for Renewable Energy Sources
ESOM	Energy System Optimization Model
GHG	Greenhouse Gas
GSA	Global Sensitivity Analysis
IV	Importance Value
LSA	Local Sensitivity Analysis
MCA	Monte Carlo Analysis
O&M	Operation and Maintenance
OAT	One-at A Time
OT	Optimal Transport
RFR	Random Forest Regressor
SA	Sensitivity Analysis
SALib	Sensitivity Analysis Library in Python
TEMOA	Tools for Energy Model Optimization and Analysis
XAI	Explainable Artificial Intelligence

1. Introduction

The ongoing global energy transition, driven by the urgency to mitigate climate change and ensure sustainable energy access, is fundamentally transforming energy systems worldwide. The integration of renewable energy sources is rapidly increasing, as highlighted in Ref. [1]. At the same time, there is a growing trend towards the electrification of energy demand across sectors [2]. Additionally, widespread adoption of energy efficiency measures is reshaping the supply and demand landscape. However, these shifts bring significant uncertainties, ranging from technological advancements to socio-economic and geopolitical dynamics, which require robust planning tools to

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ensure resilient and adaptive energy system designs [3].

Energy system optimization models (ESOMs) have emerged as indispensable tools for analyzing and guiding long-term energy planning. ESOMs represent the intricate and dynamic interactions of the energy system with a technology-based (bottom-up) approach [4]. These complex models enable researchers and policymakers to evaluate cost-optimal pathways under various scenarios, accounting for technological, economic, and environmental constraints [5]. By representing energy systems as interconnected networks of supply, conversion, and demand sectors, ESOMs provide valuable insights into resource allocation, technology deployment, and policy impacts [6]. Their versatility has made them central to scenario analysis in both global and regional contexts, including the modeling of energy transitions under ambitious decarbonization goals.

Recent advances in ESOMs have expanded their scope to incorporate climate-related risks. The inclusion of these risks is a key development, as highlighted in Ref. [7]. Furthermore, the models now account for critical raw material constraints, as discussed in Ref. [8]. Another significant advancement is the integration of multiple sectors, as demonstrated in Ref. [9]. At the same time, the impact of climate change on energy systems has been investigated in Ref. [10]. The urgency of net-zero emissions targets and the increasing complexity of decarbonization pathways demand the inclusion of not only economic and technological considerations but also supply chain disruptions, extreme weather events [11], and regulatory uncertainties. However, the reliability of ESOM-driven insights relies on their ability to capture and quantify the uncertainties inherent in long-term energy planning [12]. Addressing these uncertainties is crucial to enhancing the credibility of model-based decision-making, particularly in the context of national and regional energy transition roadmaps and potential use of such models for policy design [13].

As the energy transition is characterized by significant uncertainties, including technology costs and performance, resource availability, and demand evolution, sensitivity analysis plays a critical role in evaluating how and how much variations in input assumptions impact model outputs. By systematically exploring uncertainties, sensitivity analysis enhances model transparency and provides decision-makers with insights into the robustness of policy recommendations. Furthermore, it identifies the assumptions that warrant the most attention, ensuring a more informed approach to addressing the challenges of long-term energy planning. At the same time, identifying the most impactful uncertainties concerning the technology performance calls for more technical development to narrow them.

Historically, most studies on sensitivity analysis in ESOMs have relied on one-factor-at-a-time methods, where a single input variable is perturbed while all others remain fixed [12]. While these methods provide a straightforward way to assess the marginal effect of the variation of individual parameters, they intrinsically overlook interactions between correlated uncertain variables, which are particularly relevant in complex, multi-sectoral energy models. For instance, the one-at-a-time (OAT) input perturbation sensitivity analysis using an ESOM carried out in Ref. [14] has demonstrated that variations in fuel prices and technology capital costs can lead to significant divergences in long-term greenhouse gas emissions projections. However, such localized analyses can misrepresent the true range of uncertainty propagation, especially when nonlinear dependencies and cross-sectoral interactions and correlations play a crucial role in shaping energy system outcomes.

As a matter of fact, traditional sensitivity analysis methods in ESOMs often fail to capture the multivariate and interdependent nature of energy system outputs, which span multiple sectors and metrics [15]. As a result, they provide only partial insights into model behavior, limiting their effectiveness for robust decision-making. A more systematic and computationally efficient approach is required to quantify and understand the impact of uncertainties not only on aggregated system outcomes but also on sectoral and technology-specific metrics, ensuring that ESOMs provide reliable, policy-relevant insights for long-term energy transition planning.

More advanced sensitivity analysis techniques provide a systematic way to assess how uncertainties in various inputs influence model outcomes. Variance-based methods, as described in Ref. [16], are one such approach providing a direct measure of each input's effect on the output's uncertainty. Sobol' indices are another method used to quantify the relative importance of each input [17]. Finally, Optimal Transport (OT)-based sensitivity metrics measure the distance between output distributions under different input assumptions [18]. Recent literature shows an increasing interest in global sensitivity analysis (GSA) techniques that can address these gaps by evaluating the relative influence of multiple uncertain inputs simultaneously, rather than isolating their effects. GSA applications in the energy field have so far focused mainly on specific technologies. For instance, Sobol' indices have been used to assess the design of a hydrogen regasification process [19]. On the other hand, the study in Ref. [20] applies GSA to nuclear district heating. Machine learning techniques have been adopted to investigate a range of topics. For example, their role in examining the effects of fuel properties on the combustion process and emissions is assessed in Ref. [21]. Their application has also extended to the energy planning context, particularly those related to thermal networks [22].

However, the application of GSA in ESOMs remains limited. This is largely due to the high dimensionality of these models and the significant computational effort required for large-scale scenario analysis. Although ESOMs are typically based on linear programming, their structure gives rise to quasi-nonlinear behaviors due to features such as piecewise-linear representations (e.g., for learning curves or price elasticities), sequential decision-making across time periods, and discrete capacity investments that introduce non-convexities in the solution space. These characteristics call for advanced sensitivity analysis methods that can capture complex input-output relationships.

This paper makes four main contributions to address these gaps. First, it introduces a novel framework for applying Global Sensitivity Analysis (GSA) to ESOMs using Optimal Transport (OT)-based sensitivity metrics [18], enabling the systematic quantification of how multiple uncertain inputs simultaneously influence model outputs. Second, it demonstrates the feasibility of applying this GSA approach to a full-scale, multi-sectoral ESOM, overcoming computational and methodological barriers that have so far limited GSA applications in energy system planning. Third, the proposed methodology provides a targeted and interpretable assessment of uncertainty by identifying the most influential uncertain inputs at system-wide, sectoral, and output-specific levels, rather than merely characterizing overall uncertainty propagation. Finally, the framework offers concrete engineering value by highlighting which technology and resource assumptions have the greatest impact on energy transition pathways, thereby supporting prioritization in data collection, model refinement, and technology development to enhance the robustness and reliability of energy system planning under uncertainty.

To demonstrate the utility of the proposed framework, the TEMOA (Tools for Energy Model Optimization and Analysis) modeling framework is employed, with a specific focus on the TEMOA-Italy model instance [23]. The TEMOA open-source, modular structure and multi-sectoral representation make it a suitable case study for this analysis. The inclusion of sectoral couplings and the explicit representation of interdependencies between inputs and outputs provide an ideal platform for exploring the multivariate nature of uncertainty impacts. TEMOA-Italy, with its detailed characterization of the Italian energy system, offers a realistic context for assessing the framework's applicability and relevance to real-world energy planning challenges [24].

Section 2 discusses the GSA methodology with OT and how it has been integrated within the ESOM. Section 3 presents TEMOA-Italy as the specific model instance used to test the methodology, the inputs and outputs that are the object of the analysis and the investigated model configurations. Section 4 reports the outcomes of the analysis at system-wide and sectoral level and for specific outputs, alongside with their implications for energy planning and the main sources of uncertainties. Conclusions, limitations of the study and perspective work are presented in Section 5.

2. Methodology

As presented in Fig. 1, this section presents the main features of ESOMs and the most relevant uncertainty-affected parameters (Section 2.1). Subsequently, Section 2.2 introduces sensitivity analysis techniques typically applied to ESOMs and Section 2.3 discusses the GSA with OT methodology used in this paper to evaluate the importance ranking of inputs for the selected outputs. Eventually, Section 2.4 presents how the GSA with OT technique has been applied to the selected case study, and the related computational dataflow.

2.1. *Energy system optimization models*

ESOMs are essential tools for energy system planning and for supporting the energy policymaking process. Among them, capacity expansion ESOMs have a specific focus on investment over the long run, producing the optimal evolution of technological capacity according to a set of scenarios. Such scenarios may be used to investigate the implications of alternative socio-economic developments or policy targets, the effectiveness of possible energy policies on the system behavior, and the competitiveness of both traditional and innovative technologies under different assumptions. ESOMs typically assume perfect foresight, meaning that the future evolution of techno-economic performance of available technologies, demands and in general any boundary condition is known from the beginning of the considered time horizon with no uncertainties. Such a time horizon is typically structured on a set of several milestone years, while ESOMs also consider operational details by adopting time-slices to represent infra-annual variability of renewable energy sources, demand profiles, and maintenance costs.

Widely used long-term optimization frameworks include TIMES/MARKAL [25], MESSAGE [26], OSeMOSYS [27] and TEMOA [6]. These models are typically formulated as linear optimization problems that minimize the discounted total cost of the energy system over the modelling horizon. The optimization process is driven by the competition among different technologies in all sectors and produces their optimal capacity and activity level. While the capacity represents the maximum annual production or nominal power of technology, the activity represents its actual production level in the different time periods. The typical formulation of the ESOMs objective function is reported in Equation (1), where $Cap_{t,p}$ and $Act_{t,p}$ represent the installed capacity and activity of technology t in period p, $C^{inv}_{t,p}$ denotes the annualized investment cost, $C^{fix}_{t,p}$ fixed O&M costs, and $C^{var}_{t,p}$ variable O&M costs.

$$\min \sum_{p \in P} \frac{1}{(1+r)^p} \left(\sum_{t \in T} C^{inv}_{t,p} \cdot Cap_{t,p} + \sum_{t \in T} C^{fix}_{t,p} \cdot Cap_{t,p} + \sum_{t \in T} C^{var}_{t,p} \cdot Act_{t,p} \right) \qquad 1$$

The optimization is subject to technical and environmental constraints such as capacity limits, activity bounds (which account for capacity factors and efficiency coefficients), service demand balancing and emissions ceilings. The input parameters (e.g., costs, efficiencies, capacity factors, emission factors, and demand profiles) define the feasible space, and the solution identifies the optimal evolution of technology capacity and activity. Conceptually similar formulations are used in a number of existing model instances, including the JRC-EU-TIMES model [28] (representing the evolution of the EU energy system based on TIMES), the Open Energy Outlook [29] (built on TEMOA and focused on the U.S. energy transition), and OSeMOSYS Global [30], which provides a global representation of the energy system using the open-source OSeMOSYS framework. Model instances for smaller regions have been proposed as well, e.g., TEMOA-Piedmont [31] and TEMOA-Pantelleria [32]. These examples illustrate the flexibility of the underlying optimization structure in capturing regional, national and global long-term energy planning problems.

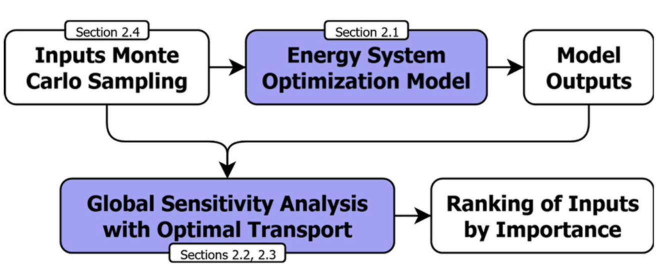

Fig. 1. Flowchart to represent the flow of information for ESOMs inputs and outputs and the application of the GSA with OT.

As illustrated in Fig. 2, ESOMs typically rely on lumped parameters to represent the aggregated techno-economic and environmental performance of technologies, simplifying complex system behaviors into values suitable for tractable optimization. Investment costs refer to the upfront capital expenditure needed to install additional capacity (e.g., €/kW), including equipment, installation, and other capital costs, which are annualized using the global discount rate and considering the expected technology lifetime. This discount rate reflects the social time preference for money, influencing optimal investment timing and the attractiveness of capital-intensive technologies. Some models apply technology-specific hurdle rates instead or in addition, reflecting financing conditions, risks, and investor expectations, which increase the effective annualized cost of high-risk technologies and affect deployment choices. Fixed O&M costs are annual expenses for operating and maintaining installed capacity, independent of utilization, while variable O&M costs are incurred per unit of activity, covering consumables and minor use-related maintenance. These inputs are often interdependent. For example, market prices of energy commodities and investment costs of related technologies tend to be correlated to some extent. Efficiency defines the output per unit of input, capturing conversion losses, whereas capacity factor indicates the fraction of time a technology is available for production, considering maintenance and resource availability, often defined seasonally or diurnally. Capacity credit represents the share of installed capacity considered reliable during peak demand, relevant to system adequacy planning. Lastly, emission factors quantify GHGs and pollutants emitted per unit of activity or input physical commodity consumed, enabling calculation of total system emissions and evaluation of environmental impacts or decarbonization policies.

Given the necessity of modeling future available technologies and to include in the technology inventory also innovative options to explore their potential role in the future energy system, the adopted parameters are typically affected by significant uncertainties, which propagate to the model outcomes.

Together with techno-economic data for the technology portfolio, also constraints are key inputs for ESOMs. Indeed, they may be used to model maximum future potential for the deployment of specific technologies and technology groups and, in general, to exclude from the possible solution space any system configuration which is not feasible, for reasons not directly considered by the model items. For instance, maximum capacity constraints are typically used to account for the limited number of sites suitable for power systems deployment (in case of land-intensive facilities), which is often taken from external literature (and affected by uncertainties).

Among the available ESOMs, TEMOA allows building complex model instances modeling both sectors devoted to energy primary supply, transformation processes, and end-use sectors. The representation of the modeled energy system is based on the construction of a network of technologies and commodities, representing existing and future processes and material, energy, and greenhouse gas emissions flows, respectively [33]. TEMOA is mainly oriented to capacity expansion and

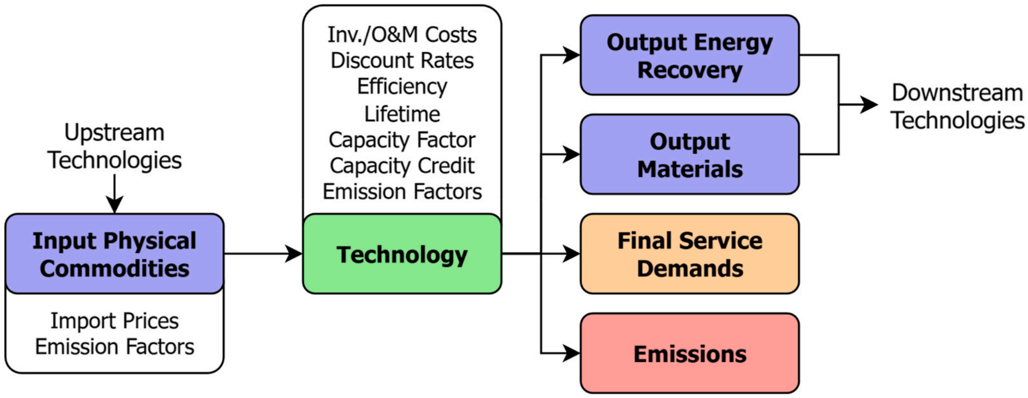

Fig. 2. Illustration of the most important techno-economic parameters used to describe a technology in ESOMs and the connection with the different commodity categories: energy flows, material flows, final service demands and emissions.

investments, although it also includes items to model the operation of technologies over shorter time steps than the annual one [34].

Given the structural features of ESOMs and TEMOA, the use of rigorous sensitivity analysis techniques may significantly enhance the quality of energy system planning, providing policymakers with a clear understanding of the probability distribution of the various model outputs, rather than with single deterministic solutions.

2.2. Overview of sensitivity analysis techniques

In a decision-making context, sensitivity analysis (SA) is a critical tool for understanding how variations in input parameters affect the outputs of complex models. Local sensitivity analysis (LSA) evaluates the effects of small, incremental changes in a single parameter, typically around a baseline value. Commonly implemented using finite difference methods or partial derivatives, LSA is computationally efficient and straightforward. However, it assumes linearity and independence of parameters, which limits its applicability for highly non-linear models or when parameter interactions are significant [35]. LSA is commonly used in ESOMs due to its simplicity and ease of interpretation. Techniques such as shadow price analysis or dual-variable sensitivity are employed to measure how incremental changes in costs, resource availability, or demand profiles affect the model's optimal solution. For instance, an LSA might explore how the marginal cost of carbon emissions influences the deployment of renewable energy technologies [36]. One widely used approach is Monte Carlo Analysis (MCA), which systematically propagates uncertainties by perturbing input parameters based on probability distributions, allowing for statistical evaluation of the resulting model outputs [37]. For instance, the work of [38] applied MCA to the UK's ESME model to assess the likelihood of achieving an 80 % carbon reduction target by 2050 under uncertain carbon price levels. However, the complexity and uncertainty of modern energy systems necessitate a broader perspective. For example, the work of [39] highlights the need for methods that can handle the high-dimensional and nonlinear characteristics of energy related models.

In contrast, global sensitivity analysis (GSA) investigates the influence of parameters across their entire range of variability, accounting for interactions and non-linear dependencies. GSA provides a more holistic understanding of parameter effects by using techniques such as variance decomposition (e.g., Sobol indices), screening methods (e.g., Morris's method), or entropy-based metrics [40]. For instance, Sobol sensitivity analysis quantifies the contribution of both individual parameters and their interactions to the variance in model outputs [17]. While GSA is computationally more demanding than LSA, its ability to capture complex behaviors makes it indispensable for high-dimensional models used in fields like climate science and energy systems analysis [41]. GSA methods are increasingly used in ESOMs to assess the impact of uncertain parameters such as renewable resource availability, demand variability, and technology costs (see the work of [42] for an example of global sensitivity analysis for the optimal design of distributed energy systems). Sobol sensitivity analysis is particularly effective for high-dimensional energy models where interactions among parameters play a critical role [17].

Another widely used technique for sensitivity analysis is the Method of Morris screening, which identifies key parameters through computationally efficient elementary effects, focusing subsequent analyses on influential variables [15]. Tools like Sensitivity Analysis Library in Python (SALib) have further streamlined the implementation of GSA in optimization workflows (including Method of Morris), making them more accessible to practitioners [43]. The Method of Morris assesses multiple input factors simultaneously by applying OAT perturbations; however, due to its sequential perturbation approach, it does not fully capture higher-order interactions between input variables [44]. To address these limitations, Optimal Transport (OT)-based sensitivity analysis provides a more comprehensive framework by quantifying the full distributional impact of uncertain inputs on model outputs, rather than relying solely on local perturbations. Unlike Morris screening, OT methods capture nonlinear dependencies and interactions between multiple parameters, offering a richer characterization of uncertainty propagation. Additionally, OT-based metrics enable robust comparisons of sensitivity across different output distributions, making them particularly well-suited for energy system optimization models where sectoral interdependencies play a critical role.

2.3. Dealing with multivariate problems: optimal transport

Optimal transport (OT) has found its way from pure mathematics [45] into applications in statistics, machine learning, and image processing [46]. It provides distance measures between probabilities, which also work in a multivariate output setting. Such a method is used in the general framework for global sensitivity indices introduced in Ref. [47]. This approach quantifies how much knowing the value of a specific input X_i impacts our beliefs about the possible outputs, by measuring the difference between the marginal probability distribution of the output and the conditional probability distribution of the output when X_i is fixed at a specific value x_i, as described in Equation (2) and graphically represented in Fig. 3.

$$\xi^d(Y,X_i) = \mathbb{E}\left[\mathrm{d}\left(\mathbb{P}_Y, \mathbb{P}_{Y|X_i}\right)\right] = \int \mathrm{d}\left(\mathbb{P}_Y, \mathbb{P}_{Y|X_i=x_i}\right)\mathrm{d}\mathbb{P}_{X_i}(x_i) \quad 2$$

Several works have discussed the choice of the distance $\mathrm{d}(\cdot,\cdot)$ [48]. In this context, the distance represents the minimum total cost required to transform one probability distribution into another by shifting probability mass (i.e., the weight assigned to different possible outcomes in a distribution). In particular, the Wasserstein-2 distance [18,49] is

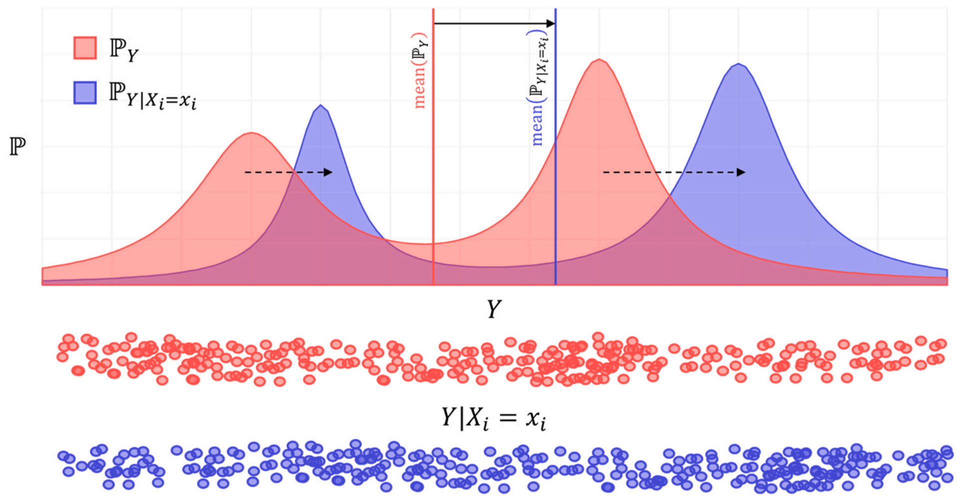

Fig. 3. Schematic representation of the optimal transport methodology concept for evaluating the influence of a single input in determining the probability distribution of a single output.

considered, as defined in Equation (3), where $\|y-y'\|^2$ is the squared Euclidean distance, y is a realization of Y under the marginal probability distribution ($\mathbb{P}_Y$) and y' a realization under the conditional probability distribution ($\mathbb{P}_{Y|X_i}$).

$$d\left(\mathbb{P}_Y, \mathbb{P}_{Y|X_i}\right) = W_2^2(y, y') = \left[\min_{\pi\in\Pi\left(\mathbb{P}_Y,\mathbb{P}_{Y|X_i}\right)} \int \|y-y'\|^2 d\pi(y,y')\right] \quad 3$$

By substituting $W_2^2(y,y')$ into Equation (2), the (unnormalized) sensitivity index is obtained.

$$\xi^{W_2^2}(Y,X_i) = \mathbb{E}\left[\min_{\pi\in\Pi\left(\mathbb{P}_Y,\mathbb{P}_{Y|X_i}\right)} \int \|y-y'\|^2 d\pi(y,y')\right] \quad 4$$

This sensitivity measure can be normalized using twice the (sum of) variance(s) of Y, which is the maximum value that $\xi^{W_2^2}(Y,X_i)$ can attain, as presented in Equation (5), where $\iota(Y,X_i)$ ranges between 0 and 1.

$$\iota(Y,X_i) = \frac{\xi^{W_2^2}(Y,X_i)}{2\text{trace}\text{Cov}Y} \in [0,1] \quad 5$$

Moreover, the index $\iota(Y,X_i)$ has several desirable properties [18]:

- Zero-independence: $\iota(Y,X_i)$ is equal to 0 if and only if Y and X_i are independent.
- Max-functionality: $\iota(Y,X_i)$ is equal to 1 if and only if there is a functional dependence in form of a measurable function g such that $Y = g(X_i)$.
- Monotonicity: $\iota(Y,X_i)$ increases if more refined information on X_i is received.
- Compatibility with Gaussian distributions.

Under multivariate Gaussian assumption on the output $Y \sim \mathcal{N}(\mu_Y, \Sigma_Y)$ and all conditional outputs, the formula for the sensitivity measure is reported in Equation (6) and Equation (7) (explicit), where $\iota^{\text{LG}}(Y,X_i)$ represents the impact of learning X_i on the multivariate output means (see Fig. 3), $\iota^{\Sigma}(Y,X_i)$ accounts for the impact of learning X_i on the variance-covariance matrix and $\iota^{\Gamma}(Y,X_i)$ accounts for the impact on the additional moments. This is graphically represented in Fig. 3, where two means of the probability distributions $\mathbb{P}_Y$ and $\mathbb{P}_{Y|X_i=x_i}$ are represented and determine $\iota^{\text{LG}}(Y,X_i)$, while additional moments are visualized as the differences in the covered areas.

$$\iota(Y,X_i) = \iota^{\text{LG}}(Y,X_i) + \iota^{\Sigma}(Y,X_i) + \iota^{\Gamma}(Y,X_i) \quad 6$$

$$\begin{aligned}\iota(Y,X_i) = & \frac{1}{2\text{trace}\Sigma_Y}\mathbb{E}\left[\left\|\mu_Y - \mu_{Y|X_i}\right\|^2\right. \\ & \left. + \text{trace}\left(\Sigma_Y + \Sigma_{Y|X_i} - 2\left(\Sigma_Y^{1/2}\Sigma_{Y|X_i}\Sigma_Y^{1/2}\right)^{1/2}\right)\right]\end{aligned} \quad 7$$

Note that $\mathbb{E}\left[\left\|\mu_Y - \mu_{Y|X_i}\right\|^2\right]$ is the variance of the conditional expectation and $\mathbb{E}\left[\text{trace}\left(\Sigma_{Y|X_i}\right)\right]$ is the expectation of the conditional variance. Under non-Gaussian assumptions, the study in Ref. [50] shows that this value provides a lower bound to the Wasserstein metric. Equation (7) is named Wasserstein-Bures (WB) distance in the general (not necessarily normal) context. Notably the first item $\frac{1}{\text{trace}\Sigma_Y}\mathbb{E}\left[\left\|\mu_Y - \mu_{Y|X_i}\right\|^2\right]$ is suggested as a multivariate extension to first order effects [51,52]. The first part of Equation (7) can be interpreted as the cost of moving the center of gravity, which so-to-speak is an advective transport property. The second component may be labeled the vortical part and includes diffusive and rotational components of the mass movement. For non-Gaussian, or more generally, for non-elliptically generated distributions, additional nonlinear terms resulting from higher moments may be encountered. Hence, the decomposition into non-negative terms is shown in Equation (8) and Equation (9). Especially the gap between ι^{WB} and ι gives a hint on the nonnormality of the output distributions.

$$\iota(Y,X_i) = \iota^{WB}(Y,X_i) + \iota^{NonElliptical}(Y,X_i) \quad 8$$

$$\iota^{WB}(Y,X_i) = \iota^{Advection}(Y,X_i) + \iota^{Vortex}(Y,X_i) \quad 9$$

For computations, one may be tempted to use a two-stage process, first sampling from X_i and then performing simulations conditional to $X_i = x_i$ to obtain the differences of the empirical output distributions. However, this approach becomes prohibitive for complex simulation models with non-negligible execution times. As an alternative, a data-driven estimation procedure can be adopted, as shown in Refs. [18, 53], where an available Monte Carlo sample can be re-analyzed for obtaining estimates of sensitivity indices, thus drastically cutting simulation costs.

2.4. Application of the optimal transport methodology to energy planning tools

The GSA proposed in this paper is applied to a case study including efficiencies, costs, capacity factors, and capacity credits of a group of future technologies belonging to different sectors of the system, demand levels within the same sectors and constraints representing maximum potentials of specific technology groups. On the output side, the GSA will firstly investigate the importance of inputs for the objective function (i.e., the minimum cost of the system) as a single output representing the overall behavior of the model. Then, the analysis is applied to the outcomes of single sectors to investigate the effects of input variations on sectoral results. Eventually, the outcomes of the GSA application to the whole set of outputs are compared with those associated with the objective function alone to investigate the representativeness of the selected outputs. The precise list of inputs and outputs is presented in detail in Section 3.1.

To apply the OT methodology, a dataset of input-output observations is required. This dataset consists of n realizations of the input vectors (typically obtained via Monte Carlo simulation, or through data collection) and corresponding realizations of the output. The output realizations are obtained by running the model in correspondence of the input realizations. Another ingredient of the method is a measure of the association between the output and the inputs to be computed from the available data. The theoretical foundations of the measure used in this work are discussed in Section 2.3.

The adopted GSA with OT requires a series of n values of the selected model outputs associated with a series of n samplings of the selected model inputs. To produce the necessary set of outputs, specific algorithms have been developed for inputs samplings, management of model runs and results postprocessing, as represented in Fig. 4. Such algorithms are implemented in Python scripts available in the supplementary material. Specifically, an algorithm has been developed to manage multiple TEMOA runs in multiprocessing to efficiently allocate the available computational resources to several series of runs executed in parallel.

Model inputs were sampled independently of each other, as the primary focus of this study is to test the applicability of the optimal transport methodology in long-term energy system planning rather than to provide a precise probabilistic assessment. To partially address correlations where most relevant, input parameters with high structural correlation – such as natural gas and LNG prices – were grouped and sampled jointly. However, for other parameters, explicit correlation measures were not introduced due to limited data availability and the consideration that many correlations in energy systems are partial or scenario-dependent rather than strictly structural.

The sampled realizations of ESOMs input data typically originate from different sources depending on their nature: techno-economic parameters such as efficiencies, investment costs and O&M costs are usually based on central estimates and uncertainty ranges reported in recognized databases, demand projections are often derived from scenario studies and statistical forecasts, and maximum potentials are typically obtained from literature-based techno-economic assessments and regional resource availability studies. In all cases, central values constitute the reference values used in the baseline input vector, and the standard deviations used for the sampling are defined through the reported uncertainty ranges or expert judgement when no quantitative range is available. Details on the specific inputs sampled in this study and assumptions for their probability distributions are provided in Section 3.1.

Given the perfect foresight approach and the long-term perspective adopted by ESOMs, based on a time horizon composed of milestone years, the analysis has been focused on the parametric uncertainties over the long run. Consequently, the sampling algorithm is structured to produce alternative long-term pathways for the considered inputs, excluding any short-term (year by year) volatility. This choice is expected to have a minor effect on deterministic results assuming perfect foresight, as in this study, but it could have significant implications in contexts such as myopic optimization or multi-stage stochastic optimization, where short-term uncertainty realizations influence sequential decisions. Although not applied here, the proposed methodology is fully flexible and model-agnostic, being therefore potentially applicable to models with finer temporal resolutions, such as hourly or seasonal models, to capture short-term volatility effects in future research.

$$Input^t_{Sampling} = \left(1 + MC_{Sampling} \cdot \frac{t - t_{now}}{t_{end} - t_{now}}\right) \cdot Input^t_{Ref} \qquad 10$$

The formulation chosen for the implementation is represented by Equation (10), where the input reference and sampled values in the time period p are represented by $Input^t_{Ref}$ and $Input^t_{Sampling}$, respectively. $MC_{Sampling}$ is a coefficient sampled with mean value equal to zero and according to the specific probability distribution of the input. The $\frac{t-t_{now}}{t_{end}-t_{now}}$ factor is used to apply a monotonic variation of the input value from $Input^t_{Ref}$, higher as t gets closer to t_{end} along the time horizon and starting

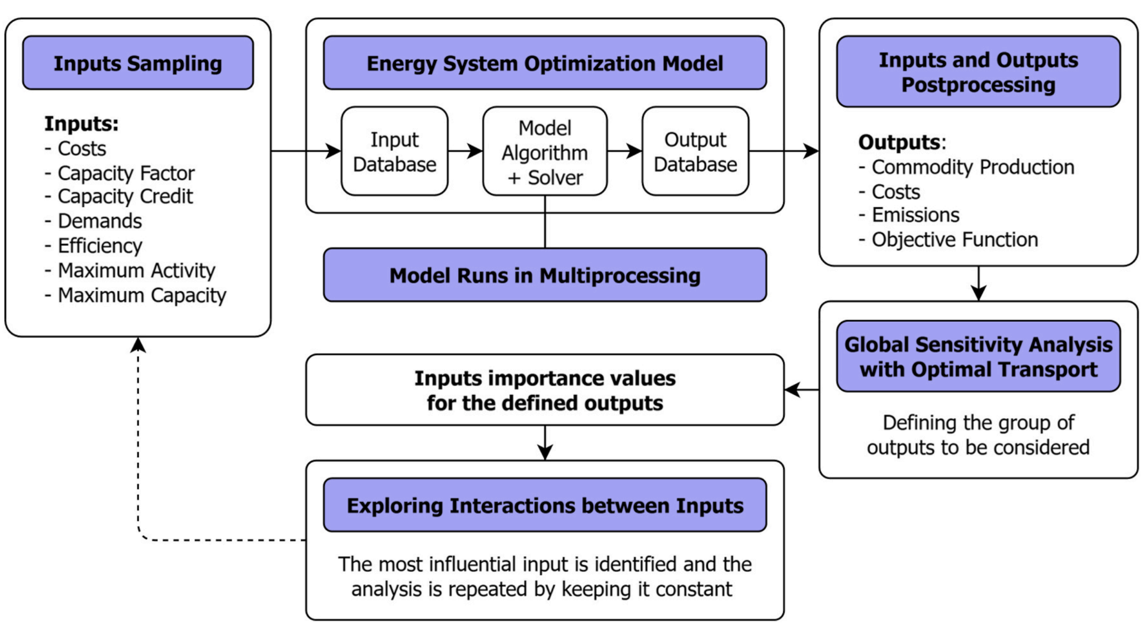

Fig. 4. Flowchart representation of the logical steps required for the application of the GSA methodology to ESOMs. The lists of inputs and outputs reported here correspond to inputs and outputs investigated in this case study (see Section 3.1) and are reported here as a non-comprehensive example of items which it is possible to include in the GSA applied to ESOMs.

from no variation applied for parameters associated with t_{now} or earlier milestone years (known data). This approach enables considering a higher uncertainty level to time periods further into the future than others, consistently with the available forecast of techno-economic parameters of energy technologies (e.g., Ref. [54]). The time periods used in the analysis coincide with the milestone years the ESOM is structured on and are therefore independent of the GSA methodology.

Concerning capacity factors and capacity credits, the possible sampled values are limited to the $\left[\frac{Input^t_{Ref}}{2}, 1\right]$ range, since they must be lower or equal to 1. The chosen number of samplings and model runs is 1000, expected to induce an error due to the sampling size limited to 3 % $\left(1/\sqrt{1000}\right)$ of the estimated importance values (IVs) [55].

Once the index $\iota(Y, X_i)$ is produced, as defined in Equation (5), one can sort the inputs by its magnitude (representing their importance). The analysis is subsequently repeated for a different set of inputs realizations and model runs, keeping constant the most influential input (as shown in Fig. 4). This is done to evaluate how the importance changes once the most important one is fixed. This analysis reveals the effect of learning one input on the model output distribution, possibly also suggesting the presence of interactions between different inputs.

3. Case study

TEMOA-Italy is a model instance focused on the representation of the Italian energy system, as accurately described in Ref. [33]. As represented in Fig. 5, the supply-side of the system encompasses the upstream sector (see Ref. [56] for more details) and the power and heat production ones (see Ref. [57] for more details). Import/export of energy carriers are also represented as a single technology for each imported/exported commodity, representing the average import/export price. The model includes technology modules for hydrogen production, as reported in Refs. [58,59], as well as carbon, capture, utilization, and storage options (see Refs. [60,61]). On the other hand, the demand-side encompasses the agriculture, residential and commercial buildings, transport, and the industrial [62] sectors aimed to satisfy the end-uses. The power sector encompasses a broad distribution of supply sources (e.g., fossil fuels, biofuels, renewables, hydrogen) to the power plants, cogeneration heat and power plants, and pure heat plants [63]. Subsequently, these plants produce intermediate commodities such as electricity and heat. The structure of the transport sector is based on two main transport categories, namely road (as described in Refs. [64,65]) and non-road transport. For each category, all their different transport options are modeled (e.g., gasoline/electric vehicles, trucks) in the same way as happens for the most relevant sectors. Each of these categories encompasses different sub-sectors that must satisfy the associated final service demands, projected according to Ref. [66].

3.1. Investigated inputs and outputs

The variety of uncertainty-affected inputs and the ESOMs data-intensity implies the necessity of defining a subset of inputs to be considered by the GSA. Similarly, ESOMs produce outputs at a high disaggregation level in terms of single commodities consumption and production by the different technologies and time and space resolution, according to the model structure. Thus, a proper postprocessing algorithm is implemented to derive results from ESOMs with a suitable aggregation level for the purposes of the conducted analyses.

As discussed below, the inputs considered in this analysis were selected based on their historical variability, supported by available data, and where applicable, on future parameter variation ranges were derived from literature. Additionally, critical inputs known to significantly influence ESOM results were included, drawing on the authors' expertise. The selected inputs cover all input groups for which future uncertainties are expected to affect technology competition and system development pathways. Some input categories, potentially subject to uncertainties, were excluded because they represent descriptive assumptions kept constant across the time horizon and thus do not influence model results in the reference configuration. Examples include the performances of building envelopes, which are assumed to be uniform across scenarios, and demand shares between different industrial products within the same sector. This selection process, necessary to limit computational cost and data processing efforts, inevitably introduces some degree of arbitrariness and remains a key limitation of the

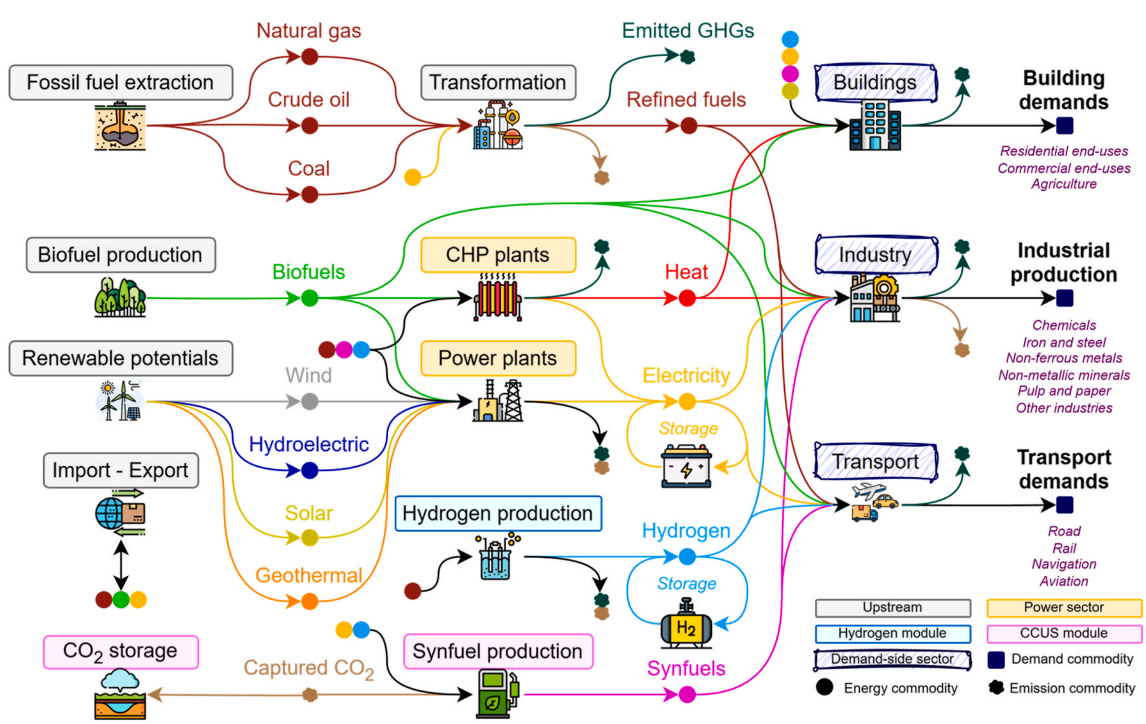

Fig. 5. Schematic representation of the main technology sectors and commodities modeled in TEMOA-Italy.

study. However, since inputs must be pre-selected before their importance can be assessed, this limitation is intrinsic to global sensitivity analyses. Moreover, the focus of this study is to propose and demonstrate a methodological framework for GSA in ESOMs rather than to provide a fully exhaustive uncertainty assessment for TEMOA-Italy.

An overview of the selected inputs is provided in Table 1. Concerning the expected probability distribution of each input, a normal distribution with mean value equal to the reference value of each input in each milestone year of the time horizon was considered. This choice is justified both by the central limit theorem, which supports the normal distribution for aggregated or average input data, and its widespread use in global sensitivity analysis when detailed empirical distribution data are unavailable [67]. Given the lack of exhaustive sources providing precise probability distribution functions or expected standard deviation values for most inputs, the normal distribution offers a reasonable and theoretically sound approach in this context. For the standard deviation, values of 10 %, 20 %, and 30 % were adopted to represent low, medium, and high uncertainty levels respectively, as reported in Table 1, based on qualitative educated guesses informed by the authors' experience and literature insights (e.g. Ref. [68] for commodity prices volatility). While 30 % standard deviation has been assigned to energy commodities price only, inputs associated with the medium standard deviation concern:

- the efficiency of synfuels production options, due to their low development level;
- investment costs of innovative vehicles and industrial technologies, classified according to Ref. [62];
- investment costs of power generation and storage plants, based on [54] (hydroelectric and geothermal excluded);
- investment costs of hydrogen, CCS-equipped and synfuels production, due to their low development level;
- demand projections and maximum constraints for renewable and CO2 storage potentials, due to the uncertainties in the literature providing them [66];
- capacity credits, since they are mostly based on assumptions in TEMOA-Italy.

The rest of the inputs have been assigned to the 10 % value. For renewables capacity factors, this choice is corroborated by ENSPRESO historical data [69].

Input-specific probability distribution shapes were not introduced because they would influence the resulting importance ranking of inputs, which is beyond the primary focus of this work. The "uniform" model configuration therefore assumes a normal distribution with a 10 % standard deviation for all inputs to provide a neutral testing ground for the optimal transport methodology, while the "different" configurations explore the impact of input-specific standard deviations only, without changing distribution shapes. Using input-specific distributions would certainly affect results: for example, assuming lognormal distributions for costs would amplify the impact of cost increases depending on the specific coefficients adopted (which are difficult to rigorously define for all technologies), while adopting uniform distributions for resource potentials would increase their importance especially under decarbonization scenarios. These aspects represent relevant extensions for future studies focused on quantitative probabilistic assessments.

Coming to the outputs considered by the analysis, three different categories of outputs have been investigated: costs, physical commodities production and GHGs emissions. The technologies capacity is not considered, being strictly correlated with the activity, represented by commodities production values. The specific outputs chosen to comprehensively represent the model response are reported in Table 2. The selection of the outputs determines the sectoral scope of the GSA, which may be focused on evaluating the importance of inputs in determining the model results at system or sectoral level.

Similarly to the selection of inputs, also the selection of outputs implies a certain degree of arbitrariness. To examine to what extent the selected outputs are representative of the general behavior of the model, the IV of the inputs for the objective function alone are evaluated. Then, inputs are ranked according to their importance at sectoral level, giving the possibility of precisely understanding the direct correlations between specific inputs and outputs of the same sector. Finally, the whole set of outputs is considered, to investigate its representativeness of the general model by comparing results to those obtained when looking at the objective function only.

Table 1
List of the inputs considered by the sensitivity analysis, sorted by input category, sector and sub-sector, and the adopted standard deviation with the related source of data.

Input Categories	Sector	Sub-sector	Standard Deviation	Source of Standard Deviation
Efficiency	Transport	Cars, Trucks	10 %	Assumption
	Industry	Iron and Stell, Non-metallic Minerals, Chemicals		
	Buildings	Space Heating		
	Electricity	Natural Gas, Coal, Oil, Biofuels, Hydrogen, Storage		
	Hydrogen and CCUS	Hydrogen Production, CCS-equipped technologies		
		Synfuels Production	20 %	
Costs	Transport	Cars, Trucks	10 ÷ 20 %	Assumption
	Industry	Iron and Stell, Non-metallic Minerals, Chemicals	10 ÷ 20 %	[62]
	Buildings	Space Heating, Insulation	10 %	Assumption
	Electricity	Hydroelectric, Geothermal		
		Photovoltaic, Wind, Natural Gas, Coal, Oil, Biofuels, Storage	20 %	[54]
		Hydrogen Fuel Cells		Assumption
	Hydrogen and CCUS	Hydrogen Production	20 %	
		CCS-equipped technologies		
		Synfuels Production		
	Upstream (Import Prices)	Coal, Oil, Gas, Biofuels, Electricity	30 %	[68]
Demands	Transport	Cars, Trucks	20 %	Assumption
	Industry	Iron and Stell, Non-metallic Minerals, Chemicals		
	Buildings	Space Heating		
Capacity Factor	Electricity	Photovoltaic, Wind, Hydroelectric	10 %	[69]
Capacity Credit	Electricity	Photovoltaic, Wind, Hydroelectric, Biofuels, Storage	20 %	Assumption
Maximum Activity and Capacity	Electricity	Photovoltaic, Wind, Hydroelectric, Biofuels	20 %	Assumption
	Hydrogen and CCUS	Biofuels, Underground CO2 Storage		

Table 2
List of the outputs considered by the sensitivity analysis and short labels adopted to represent them, sorted by sector and output category.

Sector	Output Categories	List of Single Outputs
System	Total Costs	Objective Function
Upstream	Total Primary Energy Supply	Biofuels
		Coal
		Electricity
		Natural Gas
		Geothermal
		Hydroelectric
		Oil and Oil Products
		Solar
		Wind
	Variable Costs	Imports of Coal
		Imports of Natural Gas
		Imports of Oil and Oil Products
Power Sector	Costs	
	Electricity Production	Biofuels
		Fossil
		Fossil with CCS
		Geothermal
		Hydrogen
		Hydroelectric
		Solar
		Wind
	Electricity Storage	
	Emissions	
Transport	Costs	
	Final Energy Consumption	Diesel Fuel
		Electricity
		Gasoline
		Hydrogen
		LPG
		Natural Gas
	Emissions	Cars
		Trucks
Industry	Costs	Iron and Steel
		Non-metallic Minerals
		Chemicals
	Final Energy Consumption	Electricity
		Hydrogen
		Natural Gas
	Emissions	Iron and Steel
		Non-metallic Minerals
		Chemicals
Buildings	Costs	Space Heating
	Final Energy Consumption	Electricity
		Natural Gas
	Emissions	Space Heating
Hydrogen and CCUS	Costs	Hydrogen Options
		CCUS Options
	Hydrogen Production	Biofuels
		Biofuels with CCUS
		Fossil
		Fossil with CCS
		Electrolysis
	Hydrogen Storage	
	Synfuels Production	
	CO2 Capture	
	CO2 Storage	

3.2. Model configuration

Once the list of inputs, their standard deviations and the list of outputs to be involved in the GSA have been defined, four different model configurations have been selected. From one side, they aim at exploring the results variation considering a reference scenario (Base) and a decarbonization scenario (Net0). While the reference scenario includes the minimum set of constraints required to represent technical limitations of technologies and produces the cost optimal future evolution of the system, the decarbonization scenario applies an emission limit driving the model to net zero emissions in 2050 assuming a linear emission reduction pathway starting on the historical emission levels of 2020. This is done to measure the impact on the IVs of the inputs of applying a stringent policy target compared to those associated with optimal model behavior (least-cost logic only).

On the other hand, as discussed in Section 3.1, the inputs sampling is performed both using uniform standard deviations ("Uniform") equal to 10 % and adopting the differentiated values for each of the inputs as listed in Table 1 ("Different"). This is done to explore how the variability of input standard deviations influences the outcomes. Specifically, increasing the range of variability for the inputs can reveal hidden interactions or correlations between inputs that remain undetected when stricter, narrower ranges are applied. By widening the "window" of input variability, the analysis becomes more sensitive to complex interdependencies, shedding light on how multiple inputs might interact to influence model outputs. As represented in Fig. 6, the combination of Base and Net0 scenarios with the Uniform and Different set of standard deviations leads to the four Base_Uniform, Base_Different, Net0_Uniform and Net0_Different configurations, which results are discussed in Section 4.

The IVs (computed as defined by Equation (5)) presented Section 4 are computed as the excess importance of specific inputs compared to a reference value. This reference is determined by the importance assigned by the GSA with the OT algorithm to a fictitious input that is not linked to the model outputs. Such a fictitious input – named "noise" hereafter – is sampled with a normal distribution with mean equal to 1 and standard deviation equal to 10 %. Its inclusion in the analysis allows the establishment of a threshold below which the IVs can reasonably be considered negligible, since it is associated with the importance of a non-influential input, by construction.

4. Analysis and results

This section presents the IVs of the five most important inputs in determining the model objective function taken as a single output, while the IVs of all the inputs are reported in the supplementary material. The probability distribution of the objective function value for the different model configurations presented in Section 3.2 is shown in Fig. 7. The effect of increasing the standard deviations of some inputs on the amplitude of the explored range of objective function value (Base_Different and Net0_Different configurations compared to Base_Uniform and Net0_Uniform, respectively) is highlighted, as well as the cost increase due to the application of the emission reduction pathway (Net0_Uniform and Net0_Different configurations compared to Base_Uniform and Base_Different.

IVs results for the four model configurations presented in Section 3.2 are shown in Fig. 8. By comparing the analysis outcomes in the four configurations, two main considerations concerning the categories of inputs identified as the most influential and the associated IVs emerge.

Focusing on the most influential input categories, demands and economic parameters are the most influential in the Base configurations, while maximum technology potentials and technical parameters (capacity factors and efficiencies) are the most important in Net0. Specifically, in Base the two most important inputs are the kilometers driven by cars and trucks, the first one presenting an importance excess with respect to noise approximately 8 times higher than the other inputs, and the introduction of different standard deviations does not affect this outcome. The high importance attributed to inputs belonging to the transport sector and to cars specifically is explained by the high share of the total system costs due to cars and transport in general. Indeed in Ref. [64] the transport sector was found contributing for approximately 67 % of the total costs and 73 % of the total investment costs over the 2030–2050 period, due both to capital and operational expenditures within the sector. Moreover, demand plays a crucial role in Base_Uniform and Base_Different, with technologies capacity and activity levels directly determined by final service demand levels and the technology competition being driven by economic parameters in the absence of constraints modeling strict future targets to be achieved.

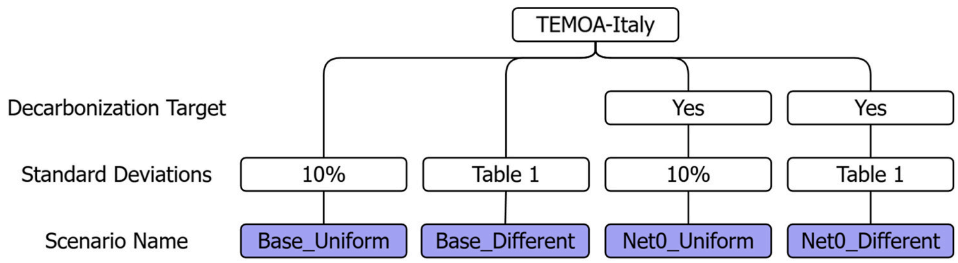

Fig. 6. Features of the four model configurations in terms of decarbonization targets and standard deviations considered for inputs sampling.

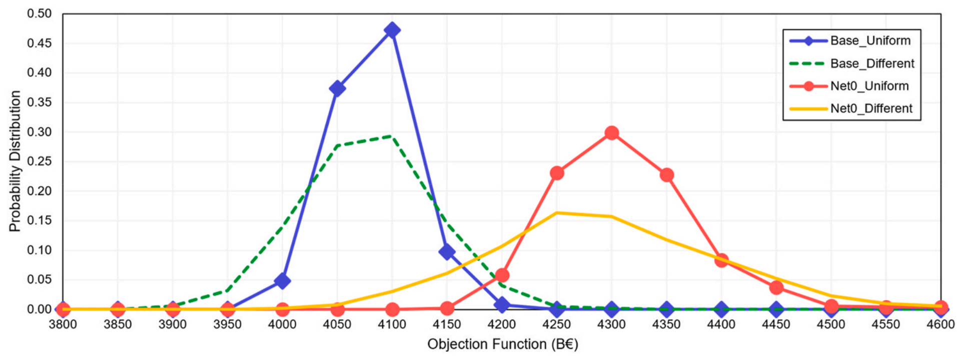

Fig. 7. Probability distribution of the objective function value in the four model configurations.

On the contrary, the most influential inputs in Net0 are technical parameters and constraints determining the capability of technologies to help in the emissions reduction towards net zero emissions in 2050, but the specific rankings here depend on the assumption made for the standard deviations. Specifically, inputs associated with renewable energy sources in the power sector are the most important. This finding corroborates the outcomes of [70], where the power sector is identified as the first sector achieving net zero emissions while applying progressively decreasing emission constraints to the system. Indeed, renewable potentials are fully saturated to substitute electricity production from fossil fuels in the power sector and to support higher electrification of the end-uses. Thus, Fig. 8 shows that solar capacity factor and maximum potential of solar, wind, biomass and CO2 storage emerge to be among the most important inputs in Net0 as they directly determine the capability of the associated generation plants in contributing to the electricity production and, consequently, emission reduction.

Additionally, the comparison between IVs of Base and Net0 highlights a different distribution of importance among the inputs. Indeed, the Base configurations assign a much higher importance to the first input with respect to the other ones, while the differentiation is lower in the Net0 configurations. This suggests that, while studying the free model behavior the single cars demand input plays the most relevant role, on the other hand, constraining the optimization process makes interactions between inputs more relevant. This is reflected in the lower importance of the first input in Net0_Uniform and Net0_Different for the first inputs and a lower differentiation for the less important one in the ranking.

In other to verify this hypothesis, the model runs have been repeated keeping constant in the four configurations the most important inputs as discussed in Section 2.4, namely this applies to: cars demand for Base_Uniform and Base_Different, solar capacity factor for Net0_Uniform and solar maximum potential for Net0_Different. The outcomes are reported in Fig. 9 for the same inputs considered by Fig. 8, while Fig. 10 presents a quantitative evaluation of the probability distribution of importance variation for the complete set of inputs once the most influential is not include in the sampling process.

Focusing on the Base configurations, the ranking does not significantly change with respect to sampling all the inputs (see Fig. 8), while it completely changes for Net0. Moreover, the probability distributions of importance variations for all the inputs shown in Fig. 10 confirm a general stability of IVs while removing the first input from the sampling for the Base cases, with importance variations within the ± 0.01 interval for 97 % of inputs for Base_Uniform and 96 % for Base_Different. On the contrary, the probability distributions for Net0 configurations (Fig. 10) show non negligible variations in the IVs for most of the inputs when removing the first one, with absolute variations higher than 0.01 for 73 % of inputs in Net0_Uniform and for 61 % of inputs in Net0_Different. This outcome confirms higher interactions between inputs in Net0 with respect to Base, as commented above. Since deepening interactions between inputs would require a specific analysis which is not in the aim of this paper, the following sections will focus on the results associated with Base configurations.

As discussed in Section 2.4, in order to explore the role played by the selected set of outputs in identifying the most important inputs for the general response of the energy system, the inputs importance ranking in influencing the objective function is compared here with the inputs importance ranking in influencing the complete set of outputs presented in Table 2 for the Base configurations (see Fig. 11). Values of importance

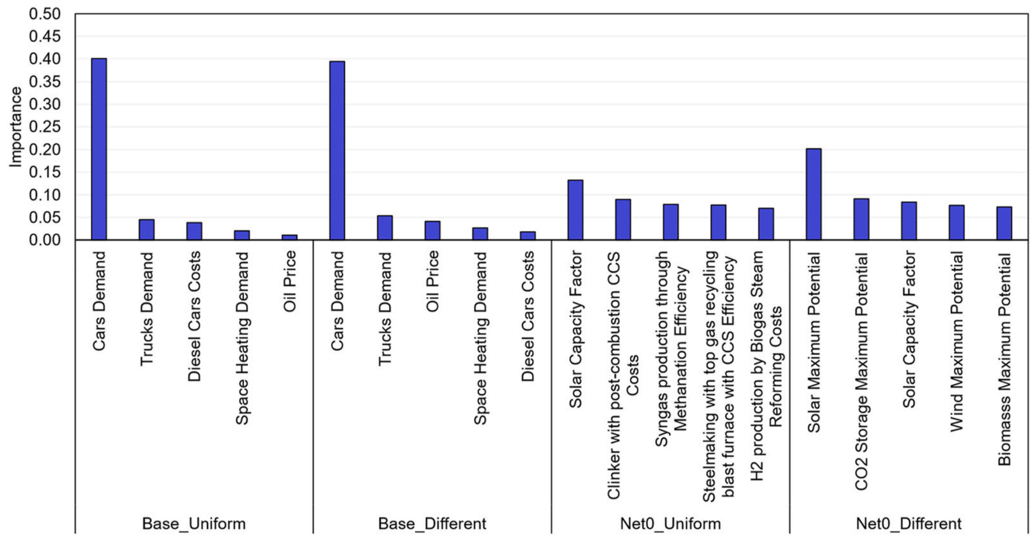

Fig. 8. Ranking and importance values of the five most important inputs in determining the model objective function taken as a single output in the four model configurations.

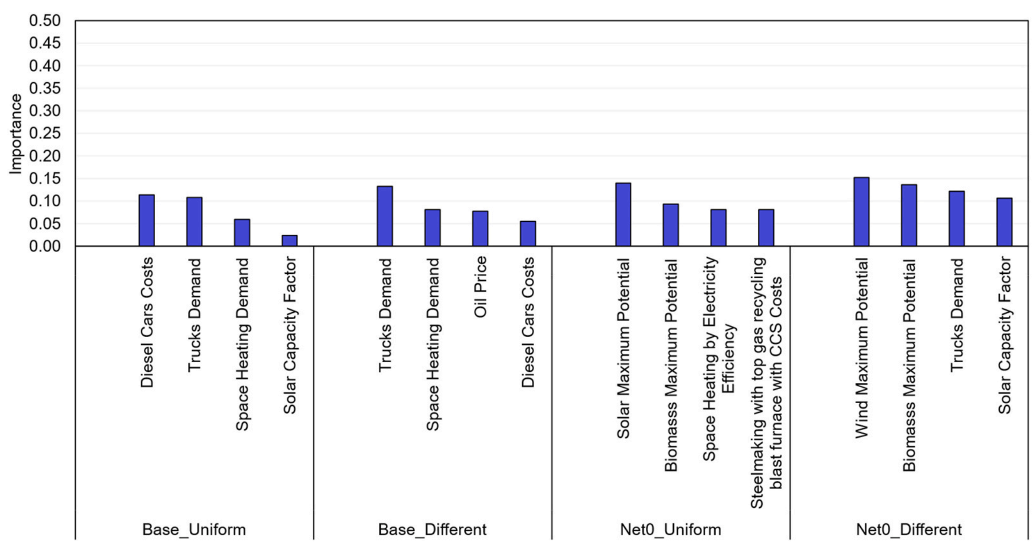

Fig. 9. Ranking and importance values of the five most important inputs in determining the model objective function taken as a single output in the four model configurations, while keeping constant the most influential input according to the ranking of Fig. 8.

do not dramatically change when including the complete set of outputs in the analysis, meaning that the objective function dependency on inputs well reflects on the group of selected outputs. However, some changes are observed: in the Base_Different configuration, cars demand remains dominant, with an importance of 0.40 for the objective function and 0.28 for the complete set of outputs. At the same time, the importance of oil price nearly doubling the objective function importance due to the high share of energy imports in the Italian total primary energy supply [71]. Similarly, diesel cars costs gain slightly in importance in both configurations. Focusing on the differences, the importance of final energy service demands decreases while that associated with the costs of energy technologies and commodities increases. At the same time, the distance between the importance of the first input and the other is reduced. This outcome suggests that applying GSA to a group of several outputs rather than one allows the identification of more inputs playing a role in affecting the model outputs.

4.1. Inputs importance for single sectors

This section deepens the effects of inputs sampling on the model outputs at sectoral level. Since the most important inputs for the model's objective function belong to the transport sector, the analysis will be performed on outputs belonging to the transport sector.

Fig. 12 presents the importance of the five most important inputs for the set of transport sector outputs. As reported in Table 2, the considered outputs are road transport costs, sectoral final energy consumption of specific commodities (diesel fuel, electricity, gasoline, hydrogen, LPG and natural gas), CO2 emissions by cars and trucks. As expected, the input ranking shown in Fig. 12a is similar to that shown in Fig. 8 concerning the importance for the objective function, since sectoral inputs influence the general optimization process through their influence on sectoral outputs.

A few exceptions emerge and, specifically, electric cars costs turn out to be the second most important input after. This is due to the inclusion in the analysis of other output categories that economic outputs only. Indeed, the cost of electric cars presents a negligible influence on sectoral and systemic costs in most of the input samplings. This is because, in most cases, electric cars are not competitive compared to alternative ICE vehicles. However, in the few subsets of input samplings where electric cars do become competitive, their deployment causes significant

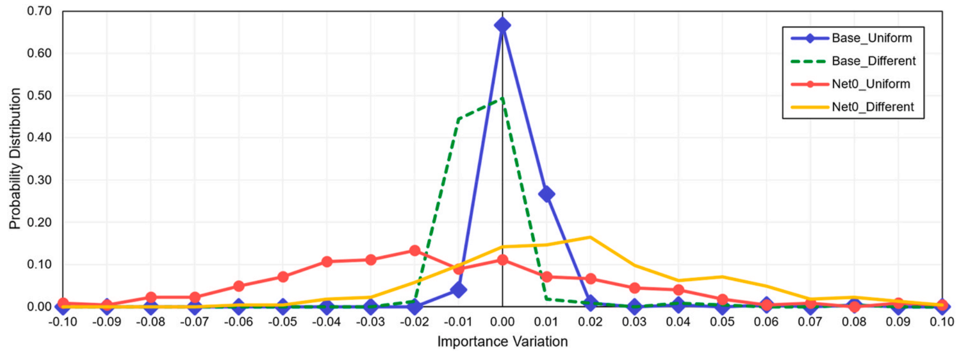

Fig. 10. Probability distribution of single inputs importance variation in determining the model objective function while sampling all the inputs and all the inputs except for the most important one.

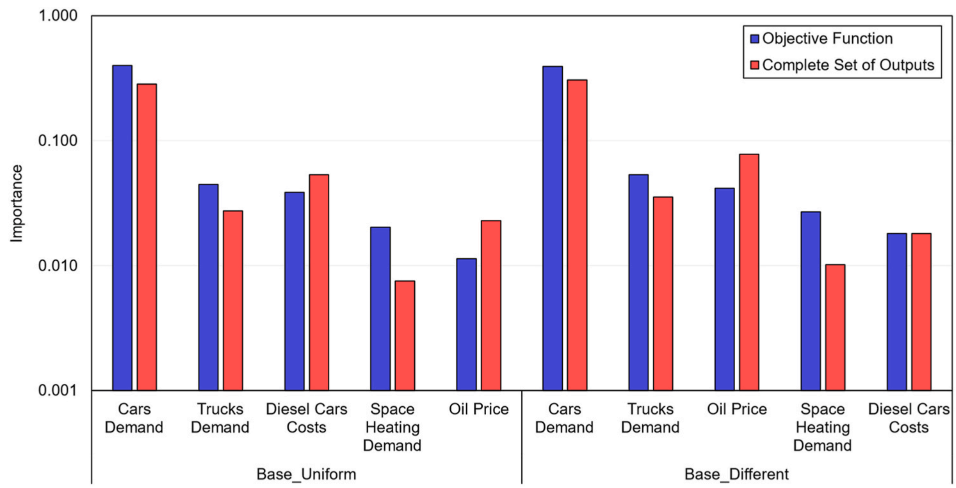

Fig. 11. Comparison between GSA with OT results when including a single output (objective function) and the complete set of outputs in the analysis.

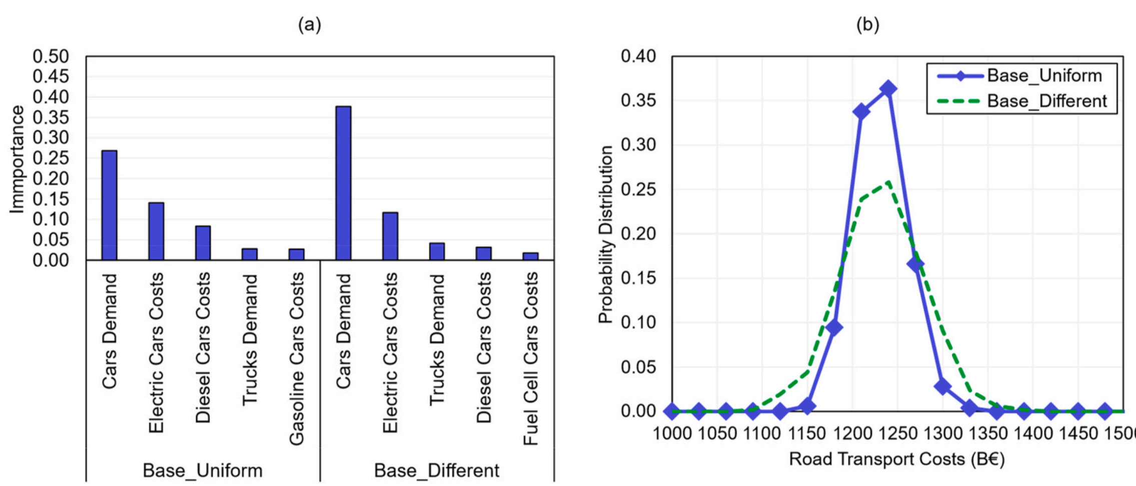

Fig. 12. Ranking and importance values of the five most important inputs in determining the model objective function taken as a single output in the Base configurations (a). Probability distribution of the output road transport costs in the Base configurations (b).

changes in both the final energy consumption mix and the emission levels. This is also confirmed by correlation matrixes shown in Fig. 13, showing negligible correlation coefficients between electric cars costs and road transport costs but relevant correlations with the other outputs.

Inputs importance associated with the Base_Different samplings present higher values for demands with respect to other input categories (see Fig. 12a), due to the higher standard deviation applied (see Table 1). Moreover, the higher standard deviations also determine a wider range for the probability distribution of outputs, as shown in Fig. 12b with an example for road transport costs and in the outputs distributions of Fig. 13. In this regard, the higher standard deviations used for inputs samplings in Base_Different also allow exploring new clusters of results not included in the outcomes of Base_Uniform. For instance, the electricity consumption distribution clearly presents a peak

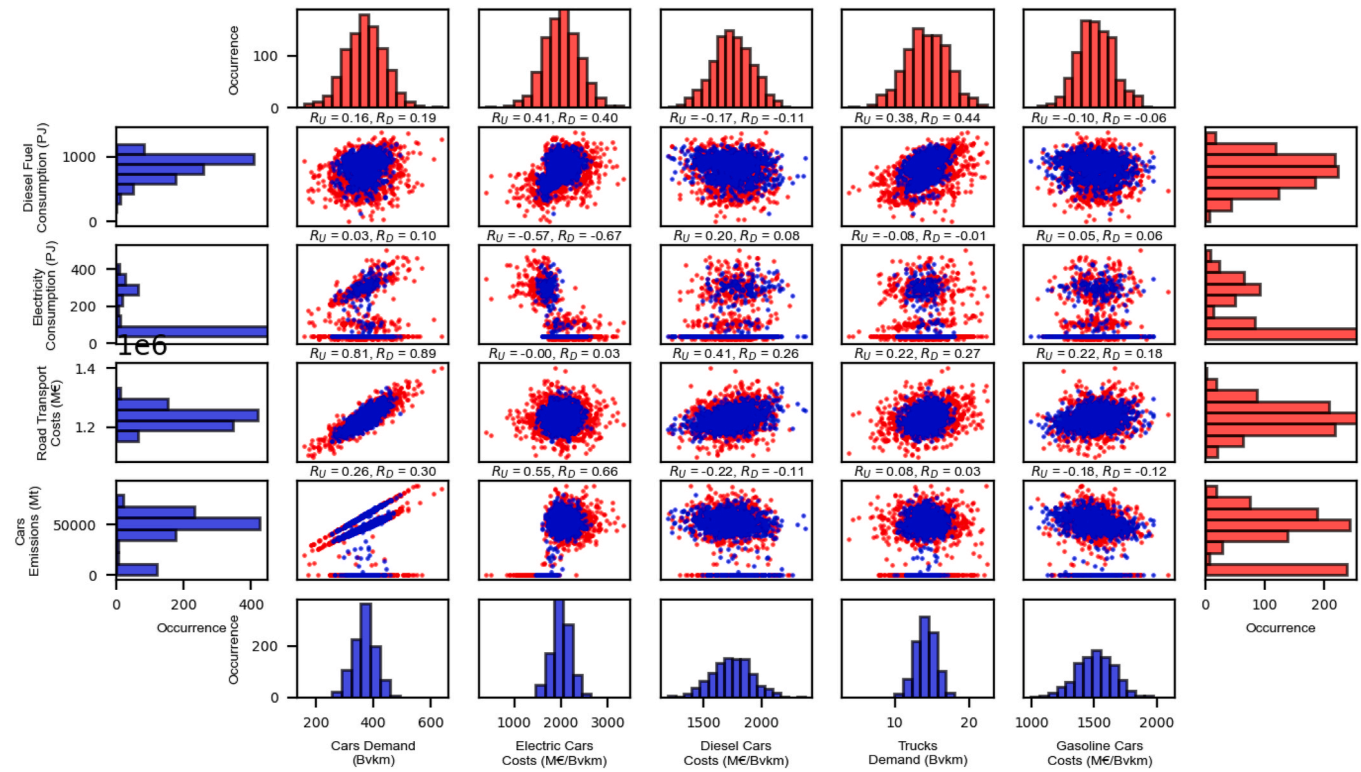

Fig. 13. Probability distributions of the five most important inputs for the transport sector, probability distributions for a selection of transport sector outputs and scatter plots and correlation coefficients (R_U for Base_Uniform, R_D for Base_Different) for the couples of inputs and outputs in the Base_Uniform (blue items) and Base_Different (red items) samplings.

at the lowest bin of the chart (corresponding to 38 PJ in 2050, which is the electricity consumption due to railways only) and another set of possible values around 300 PJ (corresponding to the penetration of electric vehicles in the cars technology mix) in Base_Uniform. On the other hand, Base_Different presents a more variegated distribution profile for electricity consumption, also including some results around 100 PJ. In general, the two model configurations produce variations in the observed clustering of results. In some cases, the red and blue points remain largely overlapping, suggesting that the assumption on standard deviation has minimal impact on correlation structure. However, in other cases (such as the relationship between diesel car costs and electricity consumption) the two sets of points show distinct distributions, implying that differentiating input uncertainty significantly alters the range of feasible outcomes.

Finally, Fig. 13 shows a high correlation between cars demand and road transport costs, thus justifying the high importance of cars demand in determining the objective function as the total costs of transport sector account for approximately 67 % of total system cost [64]. The correlation structure reveals distinct clustering patterns. Some input-output relationships exhibit well-defined linear correlations (e.g., the strong positive correlation between electricity consumption and both road transport costs ($R_U = 0.81$, $R_D = 0.89$) and CO2 emissions by cars, although with the presence of different clusters ($R_U = 0.26$, $R_D = 0.30$)). Conversely, other relationships, such as those involving diesel fuel consumption, display more scattered distributions, indicating weaker or non-linear dependencies with vehicle techno-economic parameters. Although clustering techniques were not formally applied in this study, due to the computational effort required for the entire set of outputs, the observed clustering patterns also highlight the model's non-linear behavior under uncertainty.

4.2. Comparison with feature importances of a random forest regressor

The outcomes of GSA with OT are compared here to feature importances of a surrogate model of TEMOA-Italy based on Random Forest Regression (RFR). This is done to provide an example of how a surrogate model could be used in substitution of an actual ESOM while keeping similar importance rankings for model inputs, which could be a valuable option to increase the number of samplings for GSAs with a limited computational cost.

RFR was chosen as the surrogate method due to its robustness in capturing complex, nonlinear relationships between inputs and outputs [72], without requiring prior assumptions about data distribution or functional forms, which is advantageous for the diverse input–output structures typical of ESOMs. Additionally, RFR is model-agnostic and thus potentially applicable to any ESOM framework, enhancing the generalizability of this methodology. Feature importance in RFR is estimated by analyzing the reduction in prediction error (Gini impurity) whenever a specific input is used to split the data, offering a measure of each input's influence on the output. To interpret the RFR model and ensure transparency, an Explainable Artificial Intelligence (XAI) approach is applied. XAI techniques decompose the model's predictions, quantifying the contribution of each input to the output. This allows for a more detailed and robust understanding of feature importance, addressing potential biases in RFR's built-in importance measures and capturing both linear and nonlinear dependencies, as well as input interactions. Together, RFR provides a predictive framework, while XAI ensures interpretability and validation, enabling a comprehensive comparison with the results obtained from GSA with OT.

Fig. 14 reports the comparison of IVs evaluated by GSA with OT and RFR with XAI techniques for the five most important inputs in Base_Uniform and Base_Different. Both the inputs rankings and the significantly higher importance attributed to the first input (cars demand) with respect to the others are similar. Additionally, the RFR with XAI

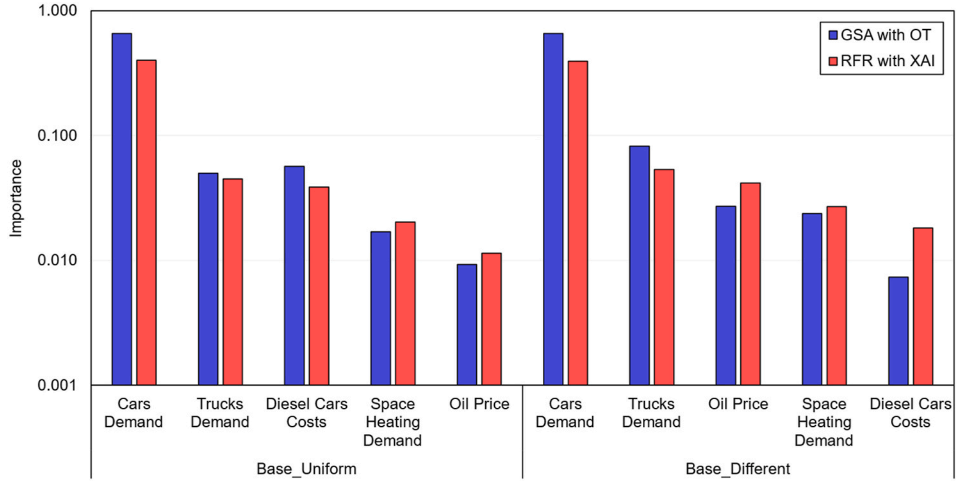

Fig. 14. Comparison between inputs importance values by GSA with OT and RFR with XAI.

produces higher coefficients of determination (R-squared), used to measure how well the model explains the variance in data [73], for Base than Net0. Namely R-squared equals 0.81 for Base_Uniform, 0.78 for Base_Different, 0.20 for Net0_Uniform and 0.03 for Net0_Different. The low R-squared value for Net0 confirms that RFR with XAI is not capable of properly predicting ESOM's outputs with its linear approximation, thus suggesting once again the presence of high interactions between inputs in Net0_Uniform and Net0_Different which deserves further investigations which are out of the scope of this paper.

4.3. Implications for long-term energy planning

The proposed methodology provides energy system models with a ranking of key influential input parameters and a quantitative evaluation of their importance in determining the outcomes of long-term energy planning. The findings of this analysis and the discussed examples of applications have several implications for stakeholders. Indeed, the differentiation in the inputs importance structure between Base and Net0 configurations highlights the relevance of aligning energy policies to address future uncertainties based on specific objectives. In the Base configurations, where the system operates without stringent decarbonization targets, demand-side management and economic parameters play a significant role. Thus, investments in technologies and strategies that shift demand patterns could yield significant cost and energy savings, for instance promoting carpooling in the transport sector or renovating buildings to improve their energy efficiency.

On the other hand, the Net0 configurations underscore the critical role of renewable energy potentials and technical parameters in achieving net-zero emissions. The importance of renewable capacities and associated parameters is because achieving deep decarbonization will require substantial investments in renewable energy infrastructure, grid flexibility, and energy storage systems, and constraints on these technologies in ESOMs are binding for the energy transition, reflecting in the high influence of such inputs. Therefore, policymakers should prioritize removing barriers to renewable deployment, such as regulatory constraints or lack of financial incentives. For instance, they can streamline permitting procedures for renewable energy projects to reduce administrative delays and implement clear and stable long-term policy frameworks that reduce investment risks. Additionally, introducing targeted financial incentives can stimulate market confidence, while investing in grid expansion and digitalization can further ensure that new renewable capacities can be effectively utilized within the power system.

The interaction effects observed in the Net0 configurations also point to the increasing complexity of energy systems under stringent decarbonization goals. This complexity calls for integrated planning approaches that account for cross-sectoral interactions and co-optimization of resources. Moreover, the notable change in the inputs important ranking emerged when removing the most important input may constitute a promising tool to establish a sequential order to address uncertainties from the policy-maker perspective.

Finally, the analysis underscores the importance of addressing uncertainty in energy planning. The varying importance of inputs under different standard deviations suggests that robust strategies should accommodate a range of potential future scenarios. Decision-makers should adopt adaptive strategies and incorporate flexibility to adjust policies as new information and technologies emerge. Addressing uncertainty effectively will enhance the resilience of energy systems in the face of evolving technological, economic, and policy landscapes.

5. Conclusions

This study introduced a framework for applying global sensitivity analysis (GSA) to energy system optimization models (ESOMs), demonstrated through the TEMOA-Italy case study. The findings highlight the varying importance of the selected inputs across different scenarios, with demands and economic parameters dominating under unconstrained configurations, whereas renewable energy potentials and technical parameters prevail under net-zero constraints. In this regard, the application of GSA with OT to the ESOM results helped in identifying the most critical constraints for achieving the energy transition, and specifically the maximum capacity of solar, wind and biomass power plant for the investigated Italian case study. Additionally, the results underline the significant interactions between inputs in constrained scenarios, emphasizing the need for comprehensive GSA methods to capture these dynamics. By quantifying the influence of uncertainties at system-wide, sectoral, and output-specific levels, the adopted methodology provides insights into the robustness of energy system designs and policy recommendations.

The proposed framework advances the field of energy planning by addressing gaps in sensitivity analysis for ESOMs. Indeed, traditional methods often fail to capture interactions between inputs or consider the multidimensional nature of model outputs. In contrast, this framework leverages the capabilities of OT theory to provide a systematic and robust analysis of uncertainty impacts. Its application to TEMOA-Italy demonstrates its potential to uncover key drivers of system behavior, enhancing transparency and reliability in long-term energy planning. The methodology offers a practical tool for policymakers to evaluate the resilience of proposed strategies, as shown in the paper.

Despite its contributions, this study has limitations that need further exploration. For instance, the computational cost associated with GSA remains a challenge, especially for high-dimensional models with extensive input-output mappings. Additionally, while the framework effectively identifies influential inputs, it does not directly address the effects of parametric uncertainties on output distributions. Future research should focus on optimizing computational efficiency and exploring its applicability to other ESOM instances and geographical contexts. Moreover, a deeper investigation into input-output interactions and the role of emerging technologies would certainly lead to valuable insights. In particular, studying the impact of adopting different input-specific probability distribution shapes could refine the understanding of input importance rankings and output risks. For example, assuming lognormal distributions for investment costs could amplify the perceived risks of cost escalations depending on the skewness parameters adopted, while using uniform distributions for resource potentials would likely increase the importance of such constraints, especially under stringent decarbonization scenarios. Furthermore, future research could extend the proposed OT-based sensitivity framework to explore input interactions, for instance by analyzing joint OT-indices to detect potential synergies, especially under input independence assumptions. Finally, an interesting avenue of future research is to extend the proposed OT-based sensitivity framework to explore interactions. For instance, by analyzing joint OT-indices and considering the variance-based components, one can detect deviations from additivity, especially under an input independence assumption. These extensions would enhance the robustness and practical relevance of model-based sensitivity analyses.

In conclusion, the integration of systematic GSA into ESOMs represents a critical advancement in energy planning, enabling more informed and adaptive strategies for navigating the uncertainties of the energy transition. By quantifying input importance and interactions, this approach enhances the robustness of scenario analyses, supporting the design of resilient, cost-effective, and sustainable energy systems. As energy systems continue to evolve in response to global challenges, the adoption of advanced analytical tools like GSA will be essential for guiding policymakers and stakeholders toward the energy transition.

CRediT authorship contribution statement

Matteo Nicoli: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Emanuele Borgonovo:** Writing – review & editing, Validation, Supervision, Software, Methodology, Formal analysis, Conceptualization. **Valeria Di Cosmo:** Writing – review & editing, Visualization, Supervision, Investigation, Funding acquisition, Conceptualization. **Daniele Mosso:** Writing – review & editing, Validation, Software, Data curation. **Elmar Plischke:** Writing – review & editing, Validation, Supervision, Software, Methodology, Formal analysis, Conceptualization. **Laura Savoldi:** Writing – review & editing, Validation, Supervision, Investigation, Conceptualization. **Anderson Rodrigo de Queiroz:** Writing – review & editing, Validation, Supervision, Methodology, Formal analysis, Conceptualization.

Declaration of generative AI and AI-assisted technologies in the writing process

During the preparation of this work the authors used ChatGPT® in order to revise the text grammar and readability. After using this tool/service, the authors reviewed and edited the content as needed and take full responsibility for the content of the published article.

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Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Matteo Nicoli reports financial support was provided by European Union. Valeria Di Cosmo reports financial support was provided by European Union. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Supplementary material

Supplementary material to this article can be found online at https://doi.org/10.1016/j.energy.2025.138788.

Data availability

The global sensitivity analysis with optimal transport methodology adopted in this paper is implemented in MATLAB scripts available at https://github.com/emanueleborgonovo/OTsensitivity. The algorithms developed for the application of the methodology to TEMOA models are implemented in Python scripts available in the supplementary material. The TEMOA model version used for the analysis presented in this paper is available at [74], while the TEMOA-Italy model instance version adopted is available at [23].

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