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Beyond the "bottom-up" and "top-down" controversy: A methodological inquiry into hybrid modeling methods for hydrogen supply chains☆

Cayet Pierre [a,b], Azzaro-Pantel Catherine [b], Bourjade Sylvain [c,*], Muller-Vibes Catherine [c]

[a] PERSEE, 26 rue Pierre Robin 69 007 Lyon, France
[b] Laboratoire de Génie Chimique, Université de Toulouse, CNRS, INPT, UPS, 4 Allee Emile Monso, 31030 Toulouse, France
[c] TBS Business School, 1 Place Alfonse Jourdain, 31000 Toulouse, France

ABSTRACT

Following the fast growth of the hydrogen economy, properly modeling the Hydrogen Supply Chain (HSC) becomes pivotal for a successful take-off. While recent review papers focus on the hydrogen engineering literature, this paper is the first to our knowledge to include economics approaches into a complete assessment of the models and mathematical formulations used to answer a variety of hydrogen-related research questions. Based on a thorough analysis of modeling choices and tools found in the HSC literature, we provide a refined classification of research papers through clustering and discriminant analysis. Using original measurement methods, we quantify the difficulty of associating existing modeling choices within a single methodology and identify opportunities and methodological blind spots for the hybridization of HSC-related research approaches.

1. Introduction

1.1. Motivation

Energy policy has become pivotal to guide the transition towards low-carbon societies and comply with decarbonization objectives such as defined in the 2020 European Green Deal. With more than 27% of total 2019 GHG emissions in EU-28 (European Environmental Agency, 2021), the transportation sector is responsible for more than a quarter of European emissions. With 72% of all domestic and international transport GHG, road transport is the biggest contributor to transport emissions (International Energy Agency, 2021). In this context, green hydrogen is considered as a key enabler of the energy transition for most recent national energy roadmaps to reach carbon neutrality by 2050. Yet, for hydrogen to play a significant role in the future energy mix, improved infrastructure design and operations, along with lower production costs, are required. For green hydrogen to take off, coordinated decisions and support are thus needed along the hydrogen supply chain (HSC), which integrates all processes from hydrogen production and storage to transportation.

Proper modeling, including various echelons and actors involved along the HSC, is thus essential to derive optimal policies. Mathematical models have been progressively introduced to inform policy decisions by providing valuable system-level insights to policy makers (see (KOPPELAAR Rembrandt et al., 2016)). However, due to the increasing complexity of energy systems, hydrogen contribution to different national or global modeling scenarios is extremely inconsistent (QUARTON J. Christopher et al., 2020). Capturing the interactions of various echelons of the HSC, along multiple spatial and temporal scales, within a unified methodological framework is a challenging exercise. Moreover, several promising uses of H_2, such as energy storage and sector-coupling, require a good representation of temporal variability, which has been traditionally poorly modeled. Capturing these details, within transparent, reproducible, and credible energy scenarios (see (Karl-Kiên et al., 2016)), is methodologically and computationally complex.

Each discipline has thus tried to develop types of modeling approaches to solve the energy demand satisfaction problem. On the one hand, most papers model the HSC following a "Bottom-up" (BU) methodological approach, traditionally used in engineering sciences. These

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* Corresponding author.
E-mail addresses: Pic@Pers-Ee.Com (C. Pierre), Catherine.Azzaropantel@Ensiacet.Fr (A.-P. Catherine), s.bourjade@tbs-education.fr (B. Sylvain), catherine.Muller@Tbs-Education.Fr (M.-V. Catherine).

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models explicitly model end-use technologies and different echelons of the supply chain. More precisely, they integrate the technical limits of the various technologies considered, in addition to the physicochemical constraints associated with the modeled processes. By focusing on the supply-side, this family of models investigates how energy demand, considered as an exogenous factor, should be optimally satisfied, generally through cost minimization.

On the other hand, "Top-down" (TD) models are traditionally associated with the economic approach of HSC modeling. They describe the (strategic) interactions between market actors, who seek to optimize their individual objective (expressed in terms of utility or profits). They may be partial-equilibrium or general equilibrium models, with a multi-sectoral formulation. This family of models may include principal-agent models in which a principal optimizes her objective (or a social planner maximizing social welfare) subject to the constraints representing each individual agents' maximization of his objective function. These models determine the optimal use of energy and other inputs to optimize social welfare and the economic efficiency of firms, while satisfying consumer preferences. The demand for energy is usually assumed to be endogenous, while the H_2 available production technologies, installed capacities, in addition to economic costs, consumption of natural resources and GHG emissions, are considered exogenous. For instance, coupling a dynamic Material Flow Analysis (MFA) with a system dynamics approach, (XUN et al., 2022) investigate the regional evolution mechanism of a fuel cell vehicle (FCV) supply chain, complexified by the impacts from domestic industrial competitiveness against foreign industries and commodities trading possibilities.

Following (HOURCADE Jean-Charles et al., 2006), BU models are often criticized for lacking realistic description of microeconomic decision-making by economic agents, or inexistent macro-economic feedback of the energy pathways on the general economic structure. In addition, TD models lack technological flexibility, and represent technological change as an aggregate phenomenon with difficulties in assessing the combined effects of technology-specific and price-based policies. The gap between the two methodological approaches has become especially strong with the recent focus of policy debate on transition towards low-carbon societies. Comprehensive HSC models should thus be technologically explicit, behaviorally realistic, and include macroeconomic feedback loops between the energy sector and other sectors. We thus define hybrid models as mergers between BU and TD approaches, which seek to compensate for the above limitations by articulating methodological elements from both model types within a single integrated formalization.

However, most review papers attempting to classify the HSC literature focus on articles formulated according to the BU methodology. (LeiMANIER HervéMANIER Marie-Ange, 2019) provide an optimization-oriented review, and classify HSC models based on their decision variables, performance measures, uncertainties, or solution methodologies. Likewise, and to identify research gaps, (Han and Jing, 2020) analyze and classify HSC system planning models based on problem types, modeling techniques and solution methods. However, none of those review papers include HSC models formulated using a TD approach. The weaknesses of BU models identified above, which are pervasive to the quasi-totality of BU HSC models, are completely overlooked by those review papers. More importantly, they completely wipe a significant share of HSC models using a TD formulation, in addition to hybrid models trying to reconcile BU and TD approaches in the case of HSC modeling.

1.2. Research gaps

The objective of this paper is to identify, classify, and analyze the importance of key factors for properly modeling the Hydrogen Supply Chain. We contribute to this literature in identifying opportunities and methodologies allowing to integrate existing economics and engineering models into hybrid models of the HSC. A systematic literature review and content analysis of relevant Bottom-Up engineering and Top-Down economics models are performed in several steps detailed in the next section. Contrary to most of previous studies, we therefore include Top-Down literature into our complete assessment of the models and mathematical formulations used to answer a variety of hydrogen-related research questions. In this paper, we present a comprehensive and structured classification, both qualitative and quantitative, of the existing methodological approaches for modeling HSC and hydrogen markets. It is worth noticing that we not only include the BU-HSC literature but also the TD-HSC literature. The analysis results in identifying five main methodological families classified depending on the research questions they address, their preferred methods, their analytical strengths and weaknesses, allowing us to better understand how they could complement each other. We also highlight the methodological gaps specific to each class and the degree of difficulty of combining several methodologies within a single model.

More precisely, we first seek to categorize existing modeling trends pertaining to HSC design, hydrogen markets and the broader macroeconomic interactions of hydrogen technologies with other sectors. Indeed, existing HSC literature reviews only include research papers formulated according to the Bottom-up methodology, with a focus on the modeling of supply-side end use technologies and technical constraints, while papers adopting a Top-down economic modeling of the HSC are systematically excluded. To our knowledge, our paper is the first to review HSC articles by including both types of approaches (BU and TD). **We investigate the relevance of applying the traditional BU-TD opposition to the HSC literature**. In particular, we explore how the differences between these two approaches are translated in terms of research questions, methodological choices, and modeling tools. This implies identifying a set of features and methodological building blocks that characterize the two approaches in the field of HSC modeling.

Second, using hierarchical clustering tools, we propose a comprehensive methodological classification of the HSC, going beyond this binary opposition. Combining this approach with the identification of a set of features that characterize the strongest discrimination between model categories, we define a set of five HSC methodological families. This allows us to spot the specific research questions, preferred methods and analytical strengths and blind spots associated with each family and pinpoint how these different approaches could complement each other. As some authors appear more than once in our sample, they are more likely to adopt similar methods across their papers. Thus, the modeling choices made by those authors may be overrepresented and may cause potential selection biases regarding the repartition and classification of modeling approaches in the HSC community. We provide robustness checks in Section 3 by measuring the Jaccard distance between papers from identical authors, and randomly drop a subset of those papers if their distance is below a fixed threshold. We then compare the clustering obtained from this reduced sample and our original sample. This allows us to conclude that our results are robust to these potential selection biases.

Finally, we investigate **the functional and formal interactions of the methodological features identified above.** Some methodological choices are unlikely to be made together, as they may be associated with different research questions, or theoretically and formally incompatible. We propose original quantitative tools to evaluate the interactions, in terms of joint occurrence, between observed methodological choices (or features) within investigated models, in addition to the dependency structure between these choices. We also explore the potential methodological and theoretical grounds that may impede the development of more comprehensive models and hinder the potentially beneficial integration of seemingly contrasting research approaches. Our classification strategy allows us to chart the connections between methodological choices, identify methodological gaps specific to each paper class, and proxy the degree of difficulty of associating various modeling choices within a single mathematical model. Indeed, as no single methodological approach may include all relevant variables and parameters for a comprehensive modeling of HSCs, integrating existing models into hybrid models is required but raises some methodological challenges that this paper explores.

This paper is the first to our knowledge to simultaneously propose a comprehensive classification of the BU and TD methods, applied to the study of the HSC and hydrogen market design. By constructing methodological categories using statistical and clustering methods, it provides a quantitative and qualitative characterization of existing modeling trends. Using original tools to quantify the complexity of articulating various modeling elements into a single framework, our approach also allows us to provide some directions for developing promising hybrid models applied to hydrogen at the intersection of BU and TD methods.

Moreover, it is worth noticing that many practitioners are interested in the economic and technological impact of the application of different policy instruments within the HSC. According to a Boston Consulting Group report from 2021,[1] "Many technological, economic, and policy challenges remain before hydrogen can offer a truly cost-effective way to lower greenhouse gas (GHG) emissions. To realize its complete potential, hydrogen must become more cost-effective and efficient in its production, distribution, and utilization." The EU strategy on hydrogen (COM/2020/301), adopted in 2020, also suggests policy action points in 5 areas: investment support, support production and demand, creating a hydrogen market and infrastructure, research and cooperation and international cooperation. These key economic challenges need to tackle the "chicken-and-egg" problem of H_2 supply and demand actual realization, and policy makers as well as industry leaders and manufacturers may strongly benefit from modeling demand more structurally, as a function of H_2 price (or Levelized Cost of Hydrogen, LCOH) and infrastructure development. As underlined by the consultancy company McKinsey in its "Hydrogen Insight 2022" report: "Both investment and project development have ramped up. However, a funding gap remains.[2]" A better understanding of economic mechanisms is needed for industry leaders and financial institutions to make thorough and better-informed decisions.

Our original categorization approach could also guide further research, enabling to develop comprehensive and promising hybrid models applied to hydrogen at the intersection of BU and TD methods. This could also help practitioners to understand what the most critical economical and technical determinants are (and how to manage them) to design an efficient hydrogen supply chain.

Our paper is organized as follows. We describe our data and methodology in Section 2. Section 3 presents our clustering analysis and the results. Section 4 discusses the opportunities and challenges for developing hybrid methodological approaches in HSC modeling. Finally, Section 5 concludes, both from a theoretical and managerial perspective. Limitations and suggestions for future research are also highlighted.

2. Data & methodology

2.1. Selection of papers and classification features

A systematic literature review (SLR) was conducted to build a representative sample of papers, to ensure replicability and validity of the results obtained in this paper. Our review was conducted according to the PRISMA protocol introduced in (LIBERATI Alessandro et al., 2009), which provides an item-checklist to improve the transparency of systematic reviews and has imposed itself as the standard procedure for reporting evidence in systematic reviews and meta-analyses.

We first collected relevant papers using the Science Direct database, which provides a broad coverage of engineering, management, decision sciences and environmental sciences papers, and then implement the same selection procedure on Google Scholar.[3] The identification of relevant papers was carried out using the following list of keywords string: ("hydrogen" AND "supply chain") OR "hydrogen infrastructure" OR "hydrogen network" OR "hydrogen supply network" OR "hydrogen-fuel infrastructure" OR "hydrogen refueling station" OR "hydrogen market" OR "hydrogen value chain". The logical operator 'OR' was used to generate full search strings for articles containing at least one keyword string in their title, abstract or keyword. The keyword string "hydrogen vehicle" was deliberately omitted to filter out papers concentrating on the physicochemical or engineering technical aspects of hydrogen mobility. Our focus is specifically on hydrogen mobility within the context of the HSC. Since we are mostly interested in the methodological approaches regarding the modeling of future hydrogen production, storage and distribution facilities, our selection procedure is supply oriented. However, our list of keywords allows the inclusion of methodologies that propose and endogenously model market characteristics, such as demand and prices, in addition to market interactions between various economic agents within the HSC. This first search resulted in a total of 16532 references found. Only peer-reviewed research articles written in English and belonging to the following subject areas were kept: 'energy,' 'engineering', 'chemical engineering', 'environmental science', 'social sciences' and 'decision sciences'. We should notice that papers published in 'business/management' are included into either the 'social sciences' or the 'decisions sciences' categories. A total of 9937 papers were removed, leaving a total of 6595 records for screening.

Selected articles sought for retrieval were then included based on the following criteria, which were assessed based on the screening of titles and abstracts:

- Topic relevance: articles with explicit physicochemical topic were systematically rejected. Moreover, articles must include at least one search keyword in their title.
- Hydrogen supply chain: only articles focusing on part or the whole HSC were included.

This screening procedure resulted in a set of 307 articles assessed for eligibility. The reduction in the initial pool can be explained by the low number of articles that model the hydrogen supply chain or the hydrogen market. Indeed, many articles in the initial pool correspond to publications in physics, chemistry, biology, and other hard sciences (even when restricting to subject areas likely to contain articles meeting our criteria). Other papers model the hydrogen supply chain within refinery activities, which is not consistent with our analysis. This rigorous screening process ensures that our final selection of articles is aligned with our research objectives. Eventually, we excluded papers which did not satisfy both following conditions: (I) include an HSC model; (II) provide an explicit mathematical formulation of the HSC model. This leaves us with a total of 75 papers included in our final sample. The steps followed in our selection procedure are summarized in Fig. 1. However, a careful analysis of our sample shows most papers are engineering-like oriented and HSC papers adopting an economic approach are underrepresented, despite the inclusion of the 'hydrogen market' keyword. To complement our initial sample, we implement the same selection procedure on Google Scholar, removing duplicates. We obtained a list of 12 papers, resulting in a full sample of 87 records included.

Interestingly, when comparing with the sample of papers

[1] https://www.bcg.com/publications/2021/capturing-value-in-the-low-carbon-hydrogen-market.

[2] https://www.mckinsey.com/capabilities/sustainability/our-insights/five-charts-on-hydrogens-role-in-a-net-zero-future.

[3] We have decided not to include Web of Science and Scopus. Indeed, as (MARTIN-MARTIN et al., 2018) (MARTIN-MARTIN et al., 2018) show, Spearman correlations of citation counts between Google Scholar and Web of Science/Scopus are strong across all subjects (0.78–0.99).

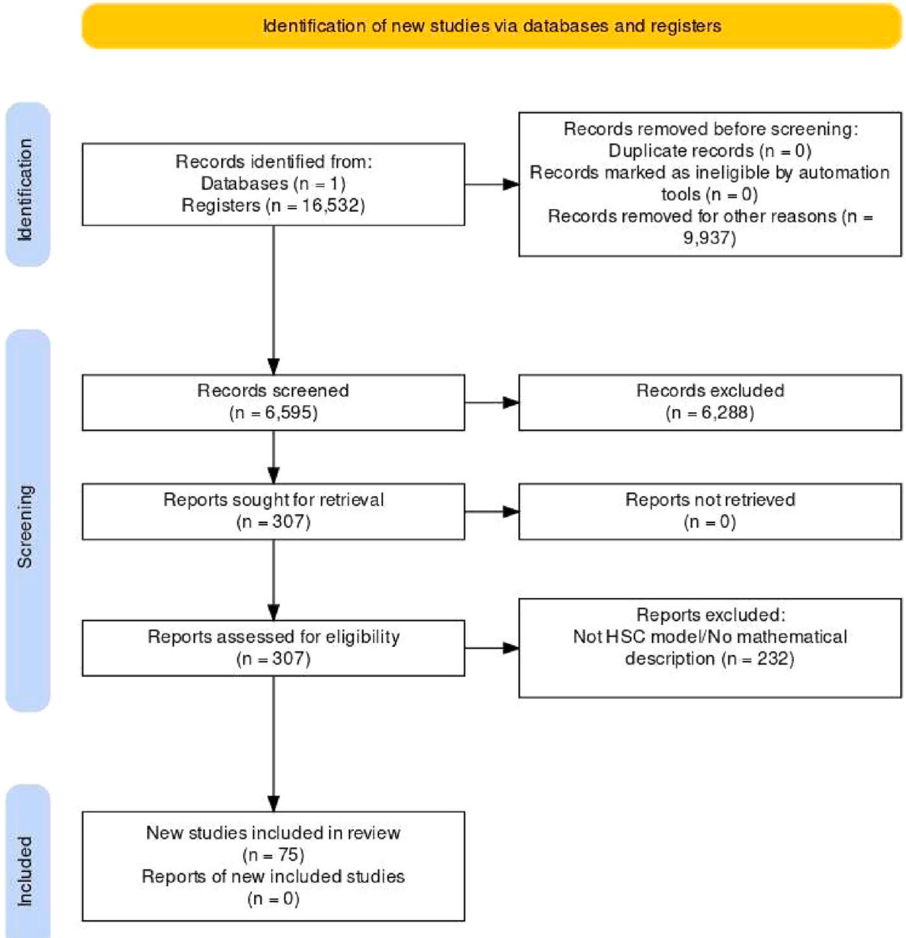

Fig. 1. PRISMA protocol diagram.

investigated in (LeiMANIER HervéMANIER Marie-Ange, 2019), 80% of selected papers obtained from Science Direct with our methodology and published before 2020 are also surveyed in (LeiMANIER HervéMANIER Marie-Ange, 2019). We should notice that we obtain such an important similarity even though we also add papers using a top-down economic approach in our analysis while (LeiMANIER HervéMANIER Marie-Ange, 2019) only include bottom-up engineering approaches. The sample constructed in (SGARBOSSA Fabio et al., 2023) includes an even much higher share of our sample. As our sample shares a significant proportion of articles with other review papers, we can be confident that our research objectives and data sources converge with existing review papers which use Web of Science and Scopus as their primary databases. We thus think that we are working with a similar set of articles which serves as a strong validation of our results' robustness.

Papers are drawn from a collection of 25 different journals. However, their repartition is clearly heterogeneous regarding the number of papers published per journal. Within our sample, only 7 journals count strictly more than 1 publication. Like (LeiMANIER HervéMANIER Marie-Ange, 2019), the *International Journal of Hydrogen Energy* clearly dominates our sample with 33 publications, which accounts for roughly 46% of papers included in our classification. *Applied Energy* ranks second, with 12% of papers, followed by *Chemical Engineering Research & Design*, *Energy* and *Computers & Chemical Engineering*, which all respectively account for 5% of selected papers. Overall, approximately 70% of papers included in our sample are drawn from only 5 journals.

We may expect papers published within a given journal to be more likely to share methodological features than when comparing papers published by different journals. Thus, clustering may capture differences between journals or journals' editorial preferences instead of pure methodological divergences between articles. However, following a SLR for constructing our sample ensures our results accurately reflect the editorial structure driving HSC papers publication process and may shed an interesting light on publication preferences of journals.

2.2. *Selection of methodological features*

In order to build a self-contained and clear list of methodological features used for our analysis (going beyond the traditional BU/TD categorization), we only use features that appear at least once in our sample. We use the term "feature" as a neutral and general terminology referring to individual modeling choices. Indeed, a given feature may either be modeled as a parameter, or a variable depending on the methodological approach. For instance, technology subsidies may be modeled as an exogenous parameter or as a decision variable set by a social planner agent. The formulation of a mathematical problem as a MILP is also a methodological feature. We then identified 15 principal features categories with 138 methodological features.

2.2.1. *"Bottom-up" model types*

Seven types of BU formulations or models are identified: Linear Programming (LP), Mixed Integer LP (MILP), location models (mainly *p*-median models), Value Web Models (VWM), Mixed Complementarity Problems (MCP) and physicochemical models. These features are not exclusive and may be combined within a single paper. Although they use LP formulation for representing techno-economic aspects of the energy system, MARKAL models stand as a specific model family and are thus distinguished. Following (ROSENBERG et al., 2010), this demand-driven model type allows a detailed representation of the demand for energy services addressed by each economic sector, while accounting for available energy sources, energy carriers and conversion technologies. Introduced in (SAMSATLI Sheila and SAMSATLI Nouri, 2015), VWM is a general MILP spatio-temporal model of energy systems including technology production, conversion, transport, storage, and transportation infrastructures. However, this model uses a specific representation of time, exploiting periodicity via a non-uniform hierarchical time discretization, which allows the inclusion of multiple temporal and spatial scales while controlling the computational efficiency of the model. Thus, for the sake of classification, we further distinguish MILP from MARKAL and VWM. Mixed Complementarity Problems (MCP) arise as a specific type of variational inequality problem, allowing for the incorporation of mixtures of equations and inequalities in square systems of nonlinear equations. They involve Karush-Kuhn-Tucker (KKT) conditions of constrained nonlinear programs, regime-switching behavior, and market equilibrium situations. Finally, physicochemical models integrate equations modeling physical and chemical constraints of H2, such as its storage temperature and pressure.

2.2.2. "Top-down" model types

Seven types of TD modeling approaches are used within sample papers: dynamic system models (mostly used for modeling diffusion processes like in (BENTO, 2010) and (HEINZ et al., 2013)), game theoretical approaches, discrete choice models, market equilibrium models, Cournot models (for oligopolistic competition), Hotelling/Salop models (used for spatial competition) and (dynamic) computable general equilibrium (CGE) models.

2.2.3. Optimization objectives

Most papers adopt a single agent setting, which optimizes either a single or, more rarely, a multi-objective function. The most frequent metrics to be optimized are costs, environmental performance, HSC reliability and risk level, social welfare, economic agents' profits, or distance of refueling stations from end-users. In multi-agent settings, the pursued objectives for the social planner are either profit or social welfare, while individual agents optimize their utility or profit.

2.2.4. Economic agents' behavior and interactions

"Soft variables" and parameters regarding the behavior and preferences of economic agents are rarely mentioned nor included in HSC models. A set of recurrent economic echelons can yet be identified, corresponding to distinct types of economic agents involved in the HSC. We assume a model is multi-agent if it includes more than one distinct objective function. Four types of economic agents appear in our sample: the government/social planner, households/final consumers, firms, and retailers. A rather limited set of behavioral features is found to characterize these agents: our features include foresight quality, rationality, and risk preferences. The interactions between agents are mostly determined by strategic interactions, network effects, externalities, while their investment decisions may benefit from learning effects and economies of scale.

2.2.5. Hydrogen supply chain composition and spatio-temporal characterization

The HSC is traditionally decomposed into a collection of key building blocks. These building blocks correspond to various homogeneous "functional" echelons within the supply chain. Six to seven echelons can be identified: feedstock sources, production, storage (potentially in addition to long-term storage), distribution, transportation, and consumption. Binary and integer decision variables are typically used to model the investment decisions and timing, location and size of production and storage facilities, transportation, and distribution modes, among available technologies considered in the model.

2.2.6. More specifically, HSC echelons are found to be characterized by the following sets of features respectively

- Feedstock echelon: type of feedstock considered (natural gas, biomass, coal, water, grid electricity, hydroelectricity, solar electricity, wind electricity, nuclear), in addition to the attention paid to its logistics (availability, storage, transportation) and their associated costs.
- Production echelon: CO2 emission constraints, techno-physical constraints on the production process, including technology and unit size (SMR, electrolysis, coal, and biomass gasification), onsite production, presence of Carbon Capture and Storage (associated with coal and biomass gasification).
- Storage echelon: techno-physical constraints on storage dynamics, unit size, physical state of stored hydrogen (liquid, gaseous or through Liquid Organic Hydrogen Carriers absorption)
- Transportation/distribution echelon: technical constraints, unit size, included transportation technology (LH_2 tanker truck, LH_2 railway, LH_2 ship, GH_2 tube trailer, GH_2 pipeline), included distribution technology (LH_2 tanker truck, GH_2 tube trailer, GH_2 pipeline).
- Refueling stations echelon (specific to papers studying hydrogen mobility): included distribution technology, unit size.

HSC models also differ by the type of H_2 physical state and uses considered, including industrial use, heat production, light-duty, and heavy-duty mobility. Furthermore, the HSC models can be implemented at various spatio-temporal scales (international, national, regional, or urban), potentially combining multiple geographic and time scales. Geographical explicit models focus on the deployment of hydrogen infrastructure and can be combined with geospatial analysis using the GIS module to even model real geographic regions.

2.2.7. Uncertainty sources and treatment

The consideration, sources and treatment of uncertainties are also important modeling choices for HSC analysis. In our sample, uncertainty-related features mainly pertain to H2 demand level, production costs and hydrogen price, renewable energy sources (RES) generation level, electricity price for electrolysers using grid electricity. The uncertainty is either treated via the introduction of scenarios (an isolated optimization run is performed for each scenario), stochastic, chance-constrained, robust, or fuzzy optimization formulations.

2.2.8. Government intervention

The modeling of public intervention is quite sparse in our sample and translates into taxes and price subsidies, capital grants to investments in hydrogen production technologies, procurement obligations, carbon taxes and carbon budgets. These features are always formulated as exogenous parameters in our sample.

2.2.9. Hydrogen demand modeling

The modeling of hydrogen demand, either as a parameter or a variable, is pivotal. In the former case, the level and dynamic profile of H_2 demand can be based on consumers' socio-economic characteristics and according to an exogenously defined penetration rate of H_2 uses. When endogenous, demand is mostly defined as a function of prices, number of H_2 vehicles in the and refueling stations in the relevant geographic area, in addition to the distance with respect to the latter. Endogenous formulations also allow to model the competition of H_2 with alternative fuels and consumer relative preferences for various fuels, that better capture the change in consumption habits from existing technologies to H_2 based ones. When accounting for its geographical distribution, demand may either be translated into node-based or flow-based formulations. Following (LeiMANIER HervéMANIER Marie-Ange, 2020), node-based models consider each node as a demand point, which implied customers must make specific trips to facilities to consume H_2. Flow-based formulations, such as (HUANG et al., 2015), model demand as flows on a network and customers consume H_2 on their way. While less realistic, node-based formulations are relatively easier to calibrate and allow lower computational complexity.

2.2.10. Interactions of HSC with other supply chains

Eventually, the HSC is often coupled with other supply chains, to model their interactions and feedback loops. The most frequently modeled supply chains are the electricity and gas networks, carbon sequestration and storage chain, and biomass supply chain. The oxygen market is considered in (OGUMEREM Gerald et al., 2018) and (WON et al., 2017) as a valuable outlet for electrolysis, while H_2 supply is modeled as a by-product from chlor-alkali industries in (HAN et al., 2013).

We summarize our results in Table A1 in Appendix. Based on this set of methodological features, we provide *a priori* categories corresponding to "Bottom-up," "Top-down" and "Hybrid" papers as shown in the References section. Papers are allocated to one of the three categories if they respectively include at least one model from the "Bottom-up,"," "Top-down" or both types of models. Following the example of (BUENO et al., 2020), Fig. 2 proposes an analytical framework based on BU and TD mathematical models and formulations identified above. It summarizes how statistical and clustering methods allow us to relate and compare, qualitatively and quantitively, both modeling approaches and provide a characterization of existing modeling trends, research gaps and directions for hybrid HSC model development.

2.3. Summary statistics and main characteristics of the sample of HSC papers

Before getting into cluster analysis, it is worth investigating the main statistical characteristics of our sample. Fig. 3A and 3B Show how the repartition of various BU and TD mathematical models in our sample evolves in time. For all publication years included in our sample (corresponding to the period 2004–2022), we measure the cumulative frequency of each model between 2004 and this publication year, for each *a priori* category identified in the above subsection. As several different model types may be included within a single paper, percentages are computed with respect to the total number of models observed in our sample.

Before 2010, MILP, MARKAL and physicochemical model types appear as exclusive mathematical modeling approaches. They respectively account for 80%, 10% and 10% of all modeling choices for BU formulations. From 2010, the cumulative share of models using physicochemical constraints increases from roughly 8%–13.5% in 2022. Linear programming and *p*-median location models are progressively employed in the literature from 2012 to 2015 respectively, accounting for respectively 7.5% and 8.5% in 2022. Finally, VWM formulation is introduced in 2018 and represents 3.5% of chosen mathematical formulations over 2004–2022. Globally, the number and diversity of BU mathematical models have globally increased over the last decade, although MILP models still account for an overwhelming 57% of all papers over the whole period. From 8.5% in 2010, the cumulative share of papers adopting a MCP formulation has slowly decreased, representing only 3.5% of all investigated papers overall.

Similarly, to BU models, we see from Fig. 3B. that the choices of TD mathematical models evolve towards increasing diversity, with more evenly distributed choices. During the 2004–2009 period, dynamic systems, discrete choice, game theoretical and Hotelling-Salop models respectively account for 20%, 20%, 40% and 20% of observed modeling choices. CGE models start being employed in 2010 and account for 11% of model choices for whole period. Cournot-Stackelberg models, used to model oligopolistic competition between economic actors of the HSC, are only introduced in 2017. Yet, their cumulative share steadily increased to reach 14.5% of all model choices. Overall and during the 2004–2022 period, dynamic systems and market equilibrium models appear as the favored choice, corresponding to 24% of modeling choices each, followed by game theoretical and Cournot-Stackelberg models, both accounting for 14.5% of observed models. Hotelling-Salop model evolves as the least common choice of mathematical model, representing only 7% of models.

Considering the repartition of mathematical model choices within the full sample, MILP is by far the most frequent type of mathematical formulation, accounting for 54% of HSC modeling choices over the 2004–2022 period. By comparison, MARKAL and physicochemical models are chosen by 6% and 12.5% of papers, respectively. Similarly, only 7% of HSC papers use market equilibrium models, while 4.5% and 3.5% use game theoretical or CGE models, respectively. As already noted, several mathematical models might be used within a single paper. Within our full sample, approximately 30% of papers employ more than one of the identified mathematical models. However, this result is likely to be positively biased, as some models may be considered as belonging to subsets of larger families of models. In this respect, MARKAL models are designed using MILP formulation, while Cournot models are strongly associated with formulations that include market equilibrium constraints.

Yet only 15% of papers include both BU and TD model types within a single methodological framework. Within this subset of papers, the most frequent associations are the MILP-Cournot, MARKAL-CGE and MCP-Market equilibrium approaches. Interestingly, the MCP formulation is only found within this subset. In terms of *a priori* categories, 73% of these papers belong to the "Hybrid" class of HSC papers, while the remaining is included in the TD class. This suggests the relevance of identifying an intermediary category of papers, potentially corresponding to more synthetic methodological approaches.

As shown in Fig. 4, the distribution of methodological features is strongly uneven: 50% of features have a probability lower than 11.5% of being observed. Conversely, less than 13% of features appear in more than 50% of our sample. Only 30% of features are observed in more than 20% of papers. This suggests that there are few characteristics that cut across the methodological approaches found in the literature.

Geographic explicitness and light-duty H_2 vehicles are the most frequent features, included in respectively 79% and 77% of papers. A large majority of our sample is thus focused on the transportation applications of hydrogen. A case study is included in 86% of papers, 56% of which apply to a national case. The review shows that 59% of the papers adopt a single-objective or multi-objective optimization approach, with cost being the most frequently optimized features, followed by GWP reduction. H_2 production is the most common functional echelon, modeled within 70% of papers, with electrolysis being the dominant production technology in modeling choices (61% of papers). 60% and 65.5% of articles include the storage and transportation echelon.

A multi-period formulation is adopted by 64.5% of papers. In terms of demand modeling, node-based formulations clearly dominate the subset of geographically explicit models. Finally, considering interactions with other supply chains, we find that the electricity network is the most frequent choice, modeled in 22% of our sample. Similarly, identifying the least frequent methodological features provides valuable information on rare or original modeling choices. Only 22% of the articles with a single-agent framework use multi-objective optimization, and less than 7% of them use social-welfare as an objective. Less than 15% of papers use a multi-agent formulation, with 61% of this subset including network effects. Regarding functional echelons, only 34.5% and 19% of sampled papers consider H_2 refueling stations and distribution. Moreover, less than 40% of articles include four or more distinct functional echelons in their model, while only 8% of articles include all types of echelons. Moreover, if the distinction between storage and long-term H_2 storage holds, we find that no article includes all functional echelons in a single framework.

In terms of demand modeling, only 21% of papers formulate demand as a model variable (endogenous demand), and 9% consider the competition of alternative fuels. The flow-based formulation remains marginal, as it accounts for approximately 10.5% of geographically

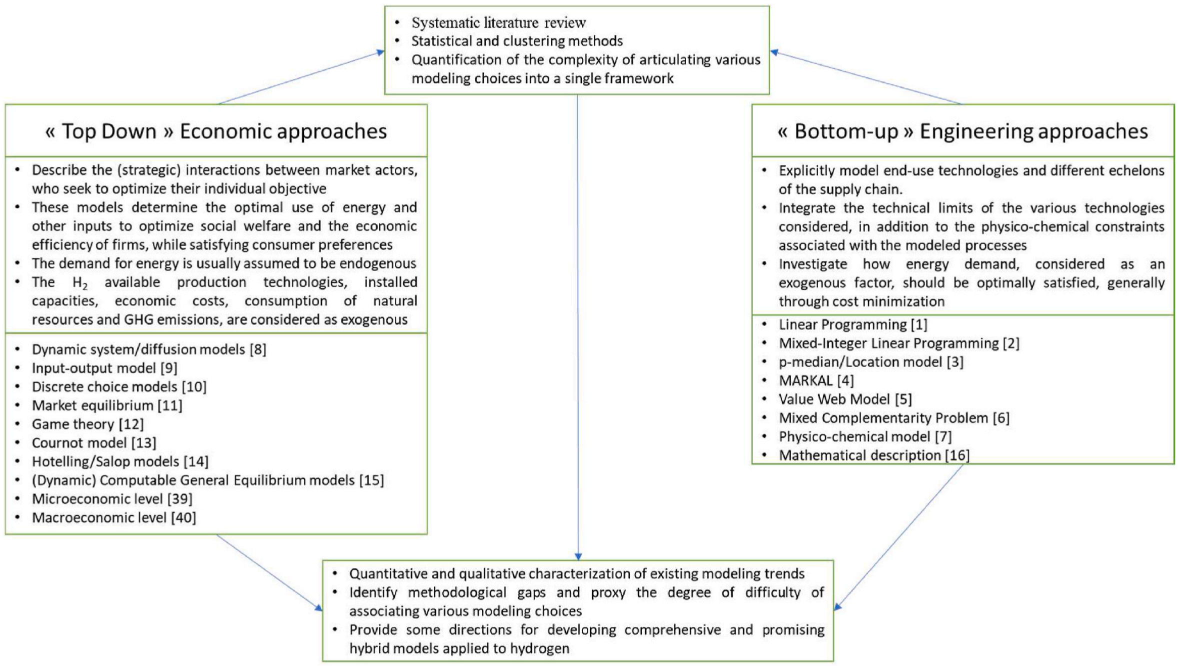

Fig. 2. Analytical framework of research methodology and objectives.

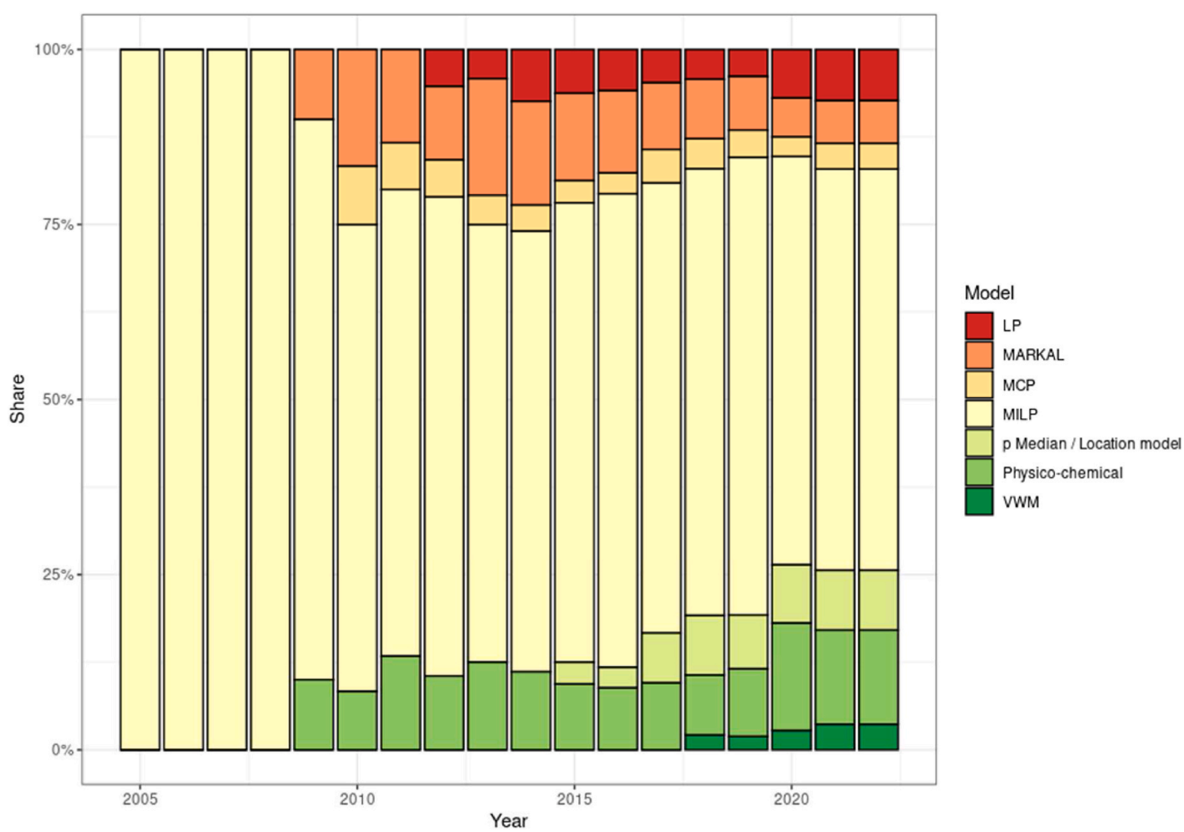

Fig. 3A. Evolution of the repartition of "Bottom-up" mathematical models from 2004 to 2022 (Cumulative shares).

explicit articles (8% of the whole sample). Only 11.5% of articles include socio-economic factors in their modeling of demand, either as an exogenous parameter or a variable. Government intervention is also rarely accounted for: less than 20% of papers consider at least one policy instrument (taxes being the most frequent) and only 3% consider more than three different instruments. Finally, uncertainties related to model parameters are mostly overlooked as less than 26% of papers account for at least one source of uncertainty, with respectively 84%, 25% and 5% of them modeling H_2 demand, RES generation and electricity price uncertainty. Yet, the level of renewable production and electricity price are pivotal components of the total cost of "green" hydrogen, as they significantly influence the unit cost of hydrogen. Thus, omitting these

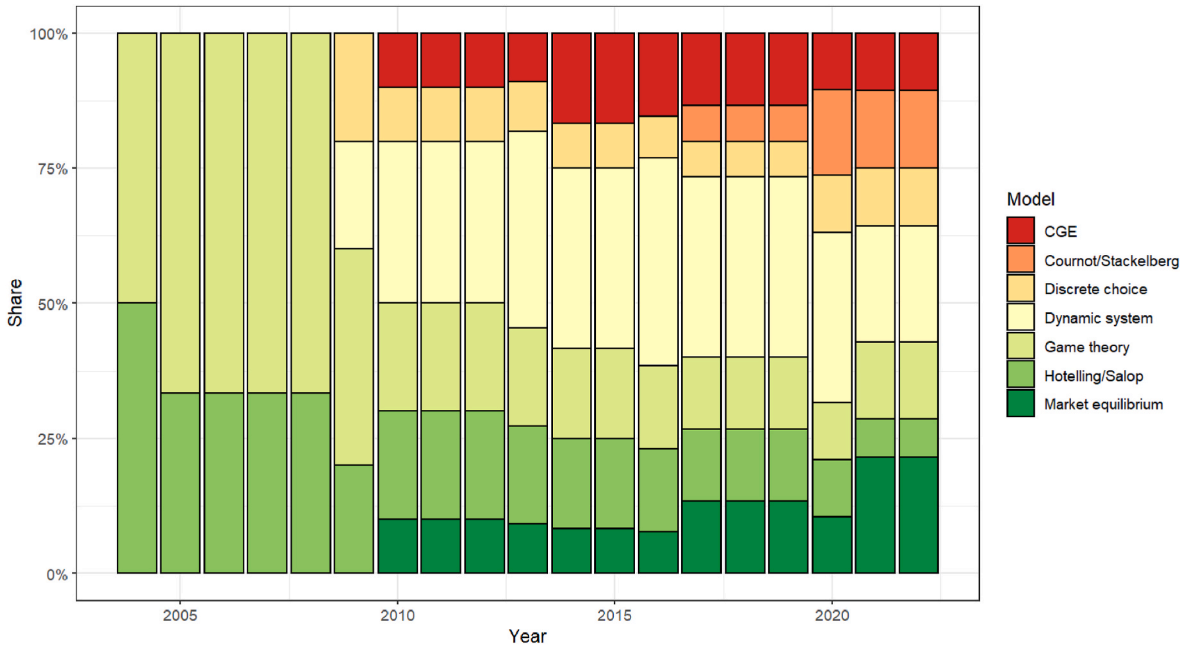

Fig. 3B. Evolution of the repartition of "Top-down" mathematical models from 2004 to 2022.

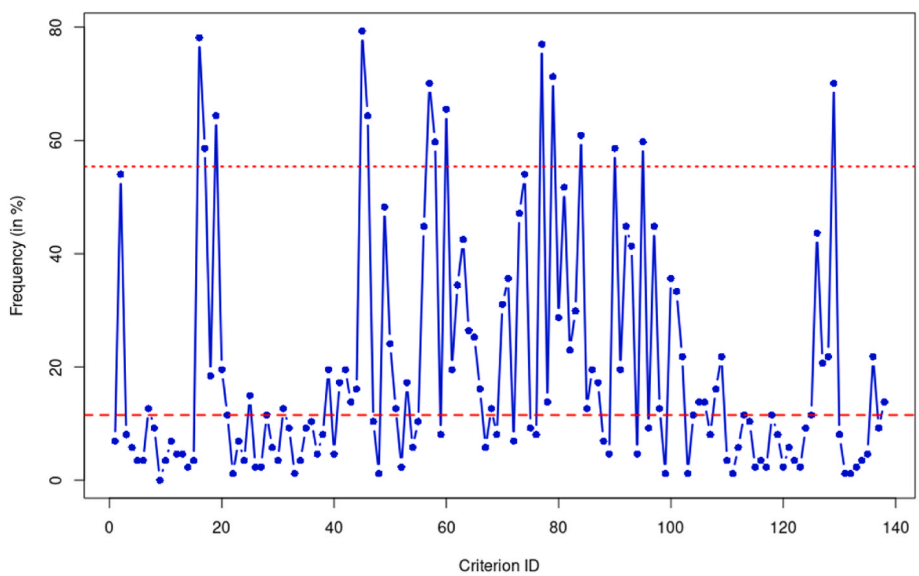

Fig. 4. Frequency of individual methodological feature. **Note:** For each feature, the blue dot corresponds to the proportion of papers verifying the feature. The dashed (resp. dotted) red line corresponds to the median (resp. 9-th decile) of the cumulative probability distribution.

sources of uncertainty may result in clearly underestimating the expected total cost of electrolysis. Moreover, uncertainties pertaining to the price of gas are not mentioned within our sample, while gas prices both affect SMR and electrolysis variable costs.[4] Furthermore, we note stochastic and scenario-based formulations are the preferred approaches to account for uncertainty, while robust and fuzzy optimization methods are chosen by only 13.5% and 8% of papers modeling uncertainty (3.5% and 2% of all sampled papers). Yet, as H_2 consumption time series are still only virtual due to insufficient development of HSC infrastructures and H_2 market, non-probabilistic methods may provide a safer way for quantifying hydrogen demand uncertainties.

[4] Although indirectly for the latter as the price of gas only affects the price of electricity during peak hours when gas turbines are dispatched by the network operator.

3. Clustering analysis & results

3.1. Clustering methodology and performance comparison

Our dataset is formulated as a complete disjunctive table, where each feature is expressed as a binary variable. The absence of continuous variables makes difficult the application of traditional clustering techniques such as *k*-means clustering, which requires defining *a priori* cluster centroids. Hierarchical ascendant classification (HAC) appears as an appropriate method. The aim of HAC is to group individuals following a predefined similarity feature, where the set of all pair-wise distances (computed between each pair of papers) is written as a distance matrix. HAC iteratively classifies individuals by producing a dendrogram, starting from individual observations and producing nested classes of increasing size.

The choice of an adequate distance metric, to measure similarities between papers, is thus pivotal to account for the specificity of our data. We compare three types of distance metrics: the Manhattan distance (or L^1 norm), the Jaccard distance and the Φ^2 distance. The Manhattan distance metric computes the distance between two vectors as the sum of the absolute differences of their Cartesian coordinates. The Jaccard index, which varies between 0 and 1, measures the similarity between two papers as the cardinal of their intersection (equal to the number of common features) divided by the cardinal of their union. The Jaccard distance is then equal to one minus the Jaccard index. The Φ^2 distance is mostly used in multiple correspondence analysis and computes the average of the squared difference between two vectors of features, where each feature is weighted by its frequency within the sample. For instance, if two papers share a methodological feature that is rare, this indicates they are more likely to share similar characteristics.

For each distance metric, we can represent the distance between each pair of papers with a heat map. Using Manhattan distance, Figure A1 ain Appendix displays the existence of at least two distinct classes of papers, which correspond to the green areas located near the corners of the map. Figure A1 b, and A.1. c, respectively corresponding to the heat maps obtained from the Jaccard and Φ^2 distances, are also disclosed in Appendix.

Our clustering strategy uses the Ward method, which maximizes (resp. minimizes) the inter-cluster (resp. intra-cluster) inertia. By measuring how total cluster inertia varies with the number of clusters associated with each distance metric, we find the optimal number of clusters is either 2, 3 or 5. Figures A2 a, A.2. b and A.2. c. (in Appendix) respectively plot the dendrograms associated with the Manhattan, Jaccard and Φ^2 distances. Some relevant similarities can be noted between the three metrics: first, cutting the dendrograms into 2 clusters results into strongly uneven categories. When using the Manhattan distance (resp. the Jaccard or Φ^2 distances), we find the two clusters include 75% and 25% of papers (resp. 76%/24% and 44%/56%).

Furthermore, to compare the different clustering methods and quantify their similarity, we use the Jaccard distance to measure how papers are allocated between clusters when comparing two clustering methods. Indeed, the simpler Hamming distance may result in wrong results as two paper partitions may be identical up to cluster index permutation. For each pair of clustering approaches (corresponding to a couple of distance metric and number of clusters), Figures A3 a, A.3. b and A.3. c. in Appendix show the corresponding Jaccard similarity, normalized between 0 and 1, as a heat map. For 2 clusters, we note the Manhattan and Jaccard distance metrics yield almost identical clustering results, with a Jaccard similarity of 0.975. Interestingly, as foreshadowed by Figure A2 b and Figure A2 c, the Jaccard similarity between the pair J5/P5 (0.658) is equivalent the one between J5/M5 (0.669), which shows the classification of papers resulting from the Jaccard and Manhattan distance metrics are quite similar.

Finally, to choose the most appropriate clustering methodology, we measure the degree of inter-cluster and intra-cluster dissimilarity using a comprehensive set of measurements. For each candidate distance metric, we quantify the inter-cluster dissimilarity using two distinct measures: the complete-linkage and average-linkage distances. Similarly, we use the complete diameter and average diameter distances for measuring intra-cluster dissimilarity. Note that for consistency, both inter-cluster and intra-cluster distance measures must be computed using a single distance metric, in our case being the Jaccard distance. Eventually, to compare the overall clustering quality associated with our different approaches, we introduce a weighted-score metric based on the set of performance measures defined above. Additional details and formal definitions are given in Appendix.

Clustering performance metrics corresponding to 2, 3 and 5 clusters are given in Table A2 a, A.2. b and A.2. c, respectively in Appendix. By comparing the clustering scores, we note that classifying our sample into 5 paper categories using the Jaccard distance yields the highest clustering quality.

3.2. *Identification of the most discriminatory features for HSC classification*

Instead of comparing the paper clusters resulting from HAC based on the 137 methodological features identified above, we first restrict the number of candidate variables used to characterize our clusters. This analytical step amounts to dimensionality reduction. We select the most discriminant variables (the subset of features which best discriminate paper categories) to better identify the main differences between clusters.

Two complementary methods are tested to assess the discriminatory power of features. First, we measure the inter-cluster variance of each feature, measured as the variance of a given feature across clusters. We weight the variance by the ratio of the relative frequency of each feature (relatively to the average frequency of occurrence of all features, equal to 20%). Fig. 5a displays the significant gaps in the inter-cluster variance of our methodological features, which suggests only a reduced number of variables are required to characterize the clusters.

Second, we use Fisher linear discriminant analysis (LDA), which aims at finding the linear combination of features that maximizes the separateness between categories of the projected data. We proxy the discriminating power of each feature by measuring its correlation with respect to the first two canonical components. We use the vector of cosine similarity related to each canonical component and their associated eigenvalues.[5]

Fig. 5b confirms the intuition that most variables have similar proportions across paper clusters and are not discriminant, i.e., do not provide additional information on clusters' exclusive characteristics. Finally, for both methods, we rank the features by decreasing order of discriminatory power and keep only two-thirds of the joint list of most discriminating features. After removing duplicates, we have compiled a list of 45 unique features.

3.3. *HSC paper categories and methodological pattern analysis*

It is worth noticing that there are few differences between the two classifications resulting from *a priori* and clustering approaches, although the *a priori* one solely relies on mathematical models. Although a binary classification quite accurately reflects the BU/TD opposition, it fails to capture the specificities of hybrid approaches.

By passing from the 2 clusters (C1 and C2) reflecting the BU/TD opposition to 5 clusters (K1 to K5), C1 is roughly split into three uneven clusters, counting respectively 15%, 37% and 14% of sampled papers. C2 is split into two equal sized clusters: this suggests categories K1 to K3 encompass more methodological diversity and modeling variety. The specific status of hybrid papers is well captured as 88% of papers identified as "Hybrid" belong to category K4 and count for 64% of the total number of papers included in the cluster.

For each cluster and each feature in the vector of most discriminatory features, Table 2 reports the proportion of papers verifying this feature (see also Table 1). The strong similarities between clusters K1 and K2 suggests that most methodological diversity is found within clusters K3 to K5.

Cluster K1 can be referred to as the family of *Diverse HSC planning and*

[5] We define the first two canonical components resulting from LDA, Z_1 and Z_2 (with their associated eigenvalues λ_1 and λ_2). For each criterion $Y \in Y$ where Y is the set of methodological criteria, we define as follows the degree of discriminating power associated with Y noted β_Y:

$$\beta_Y = \left(\frac{\lambda_1}{\lambda_1 + \lambda_2}\right) \times cos^2(Z_1, Y) + \left(\frac{\lambda_2}{\lambda_1 + \lambda_2}\right) \times cos^2(Z_2, Y)$$

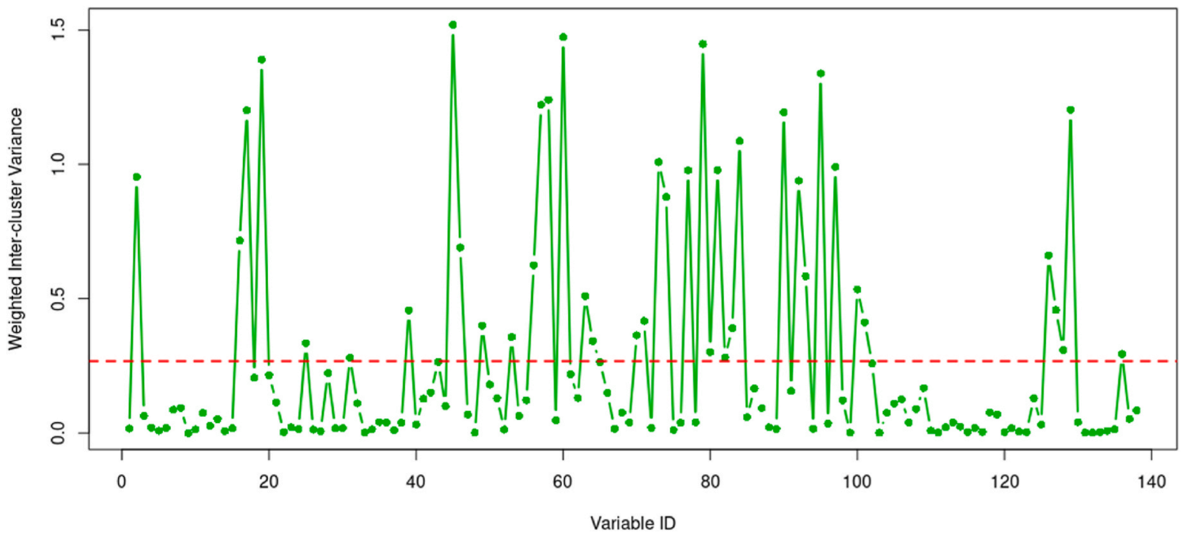

Fig. 5a. Weighted inter-cluster variance plot. **Note:** The red dashed line corresponds to the average weighted variance.

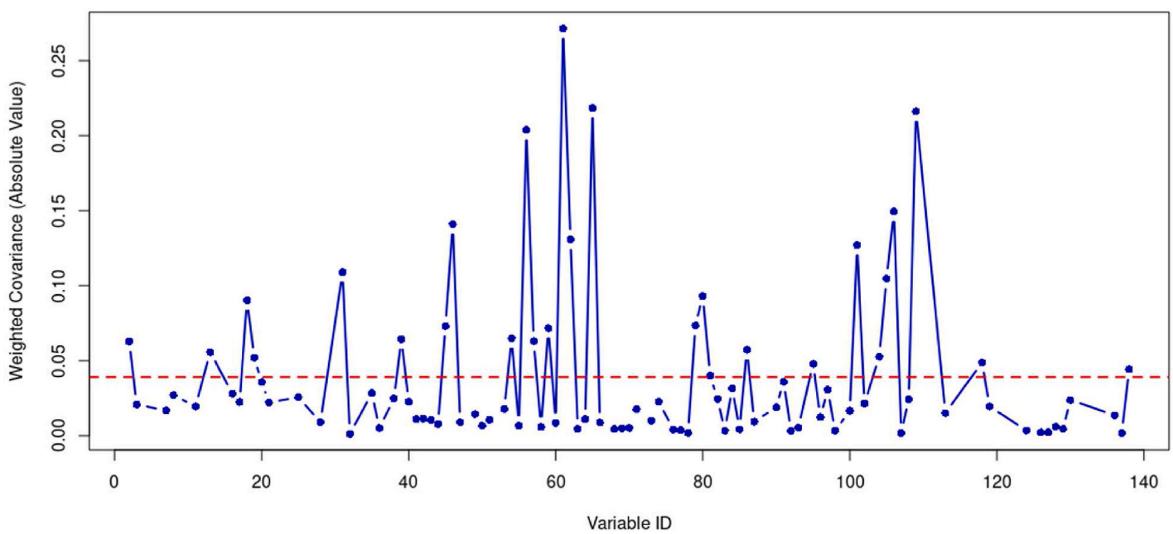

Fig. 5b. Weighted linear-discriminant analysis covariance plot **Note:** The red dashed line corresponds to the average covariance.

operation optimization models. Indeed, alternative mathematical formulations, such as MARKAL and VWM, only appear in K1, respectively accounting for 15% and 11% of papers. A social-planner takes operational decisions and optimizes a mono-objective function in 78% of papers, corresponding to costs in 85% of cases. Note that location/investment decisions remain rare (26% of papers), most articles focusing on HSC operational decisions. Multi-objective papers also remain marginal (11% of clustered papers). MILP is adopted by 56% of papers, concurrent with a strong emphasis on mathematical description. Cluster K1 is thus characterized a variety of Bottom-up planification models that minimize the total energy system cost, often using carbon emissions as an additional performance metric for model results. A proper modeling of feedstock types, availability and transportation constraints is found in 67% of model. These features are concomitant with dominant geographically explicit and node-based demand formulations (89% and 78% respectively). These models often explicitly include sets of constraints for each functional echelon. Finally, a strong emphasis is put on the detailed modeling of time and demand dynamics: multiple timescales are introduced (30%), allowing to model fine-scale changes in demand profiles with monthly, daily, and even hourly variations (59%). The increase in model complexity is controlled through original formulations of time scales like in VWM.

Cluster K2 shares many similarities with K1 but appears less general and flexible in terms of modeling choices. Most noticeably, this cluster regroups papers that use multi-objective optimization within a MILP framework. We refer to papers belonging to K2 as *Classical multi-objective HSC design and planning optimization models*. These models propose an integrated approach to design the optimal hydrogen network mainly in terms of the optimal trade-off between conflicting objectives. A multi-objective function is proposed in 52% of papers, while respectively 87%, 52% and 44% of them include cost, CO_2 emissions and risk in their objective function. However, MILP dominates mathematical formulation choice (96 % of papers included), the only alternative formulation being physicochemical in 4% of papers. Like K1, this family of models strongly relies on geographically explicit formulation of investment location, physical flows, in addition to node-based demand definitions. Finally, multiple production technologies are included, with a strong emphasis on electrolysis and SMR. Ideally, these models tend to consider all functional levels and types of infrastructures (feedstock, production plants, refueling stations, transportation network), all types of technologies and associated features (size, type of output), in addition to the geographical distribution of feedstock, its logistics and associated procurement constraints for H_2 production plants. These models seek to determine the optimal investment planning, typically over a long-term

Table 1a
Allocation of HSC papers with 2 clusters.

Cluster ID	Size	Authors/Paper ID
C1	**38**	Agnolluci P. et al. (AGNOLLUCI Paolo et al., 2013); Almansoori A. & Shah N. (ALMANSOORI and SHAH, 2006); Almansoori A. & Shah N. (ALMANSOORI and SHAH, 2009); Almansoori A. & Shah N. (ALMANSOORI and SHAH, 2012); Almansoori A. & Betancourt-Torcat A. (ALMANSOORI and BETANCOURT-TORCAT, 2016); Balta-Ozkan N. & Baldwin E. (BALTA-OZKAN Nazmiye and BALDWIN, 2013); Cantu et al. (CANTU Victor and AZZARO-PANTEL CatherinePONSICH Antonin, 2021); Dayhim M. et al. (DAYHIM Muhammad et al., 2014); De Leon Almaraz S. et al. (DE LEON ALMARAZ Sofia et al., 2013); De Leon Almaraz S. et al. (DE LEON ALMARAZ Sofia et al., 2014); De Leon Almaraz S. et al. (DE LEON ALMARAZ Sofia et al., 2015); Fazli-Khalaf M. et al. (FAZLI-KHALAF Mohamadreza et al., 2020); Güray Güler M. et al. (GÜRAY GÜLER MehmetGECICI EbruERDOGAN Ahmet, 2021); Han J. et al. (HAN et al., 2013); Hugo A. et al. (HUGO et al., 2005); Kim J. et al. (KIM et al., 2008); Kim J. et al. (KIM and MOON, 2008); Kim J. et al. (KIM et al., 2011); Li L. et al. (LeiMANIER HervéMANIER Marie-Ange, 2020); Li Z. et al. (Zheng et al., 2008); Moreno-Benito M. et al. (Moreno-Benito MartaAgnolucci Paolo and Papageorgiou Lazaros, 2017); Murthy-Konda N.V.S.N. et al. (MURTHY-KONDA et al., 2011); Ochoa-Bique A. & Zondervan E. (OCHOA BIQUE AntonZONDERVAN Edwin, 2018); Ochoa-Bique A. et al. (OCHOA BIQUE Anton et al., 2019); Ochoa Robles J. et al. (ROBLES JesusAZZARO-PANTEL CatherineAGUILAR-LASSERE Alberto, 2020); Quarton C. J. & Samsatli S. (QUARTON Christopher and SAMSATLI Sheila, 2020); Quarton C. J. & Samsatli S. (QUARTON Christopher and SAMSATLI Sheila, 2021); Reuss M. et al. (Markus et al., 2017); Reuss M. et al. (Markus et al., 2019); Rosenberg Eva et al. (ROSENBERG et al., 2010); Sabio N. et al. (SABIO Nagore et al., 2012); Samsatli S. & Samsatli N. J. (SAMSATLI Sheila and SAMSATLI Nouri, 2015); Samsatli S. & Samsatli N. J. (SAMSATLI Sheila and SAMSATLI Nouri, 2018); Seo S.-K. et al. (SEO et al., 2020); Stöckl F. (STÖCKL FabianSCHILL Wolf-PeterZERRAHN Alexander, 2021); Strachan N. et al. (STRACHAN Neil et al., 2009); Talebian H. et al. (TALEBIAN Hoda and HERRERA Omar, 2019); Tlili O. et al. (Olfa et al., 2020)
C2	**49**	André J. et al. (ANDRE Jean et al., 2013); Bae S. et al. (BAE et al., 2020); Ball M. et al. (BALL et al., 2007); Baufumé S. et al. (BAUFUME Sylvestre et al., 2011); Chen Q. et al. (CHEN et al., 2021); Cho S. & Kim J. (CHO and KIM, 2019); Coleman D. et al. (COLEMAN et al., 2020); Dagdougui H. et al. (DAGDOUGUI HananeOUAMMI AhmedSACILE Roberto, 2012); Deng Z. & Jiang Y. (DENG and JIANG, 2020); Gabrielli P. et al. (GABRIELLI Paolo et al., 2020); Gim B. et al. (GIM et al., 2012); Hajimiragha A. et al. (HAJIMIRAGHA Amirhossein et al., 2009); He C.et al. (HE et al., 2017); Huang Y. et al. (HUANG et al., 2015); (HWANGBO Soonholee et al., 2017) (HWANGBO SoonhoLEE In-Beum and HAN, 2017); Li Y. et al. (LI et al., 2018); Nunes P. et al. (Moreno-Benito MartaAgnolucci Paolo and Papageorgiou Lazaros, 2017); Obara S. & LI J. (OBARA and LI, 2020); Ogumerem G. S. et al. (OGUMEREM Gerald et al., 2018); Park K. & Koo J. (PARK and KOO, 2020); Rosa L. & Mazzotti M. (ROSA and MAZZOTTI Marco, 2022); Sun H. et al. (SUN et al., 2017); Tao Y. et al. (TAO et al., 2020); Wang B. et al. (WANG et al., 2020); Won W. et al. (WON et al., 2017); Woo Y. et al. (WOO et al., 2016); Wu X. et al. (WU et al., 2019); Yang G. (YANG et al., 2020); Bae J. H. & Cho G. (BAE et al., 2010); Bento N. (BENTO, 2010); Conrad K. (CONRAD, 2004); Espegren K. et al. (ESPEGREN Kari et al., 2021); Greaker M. & Heggedal T. (GREAKER MadsHEGGEDAL Tom-Reiel, 2010); Heinz B. et al. (HEINZ et al., 2013); Köhler J. et al. (KÖHLER et al., 2010); Li W. et al. (LI et al., 2020a); Li Y. et al. (LI et al., 2020b); Li Y. et al. (LI et al., 2020c); Meyer P. E. & Winebrake J. J. (MEYER Patrick and WINEBRAKE James, 2009); Sartzetakis E. S. & Tsigaris P. (SARTZETAKIS Eftichios and TSIGARIS Panagiotis, 2005); Silva C. M. et al. (SILVA Carla, 2014); Crönert T. & Minner S. (CRONERT TobiasMINNER Stefan, 2021); Guo Z. et al. (GUO et al., 2021); Koirala B. et al. (KOIRALA et al., 2021); Khojasteh M. (KHOJASTEH Meysam, 2020); Li X. & Mulder M. (LI and MULDER, 2021); Liu H. et al. (LIU et al., 2021); Michalski J. (MICHALSKI Jan 2017); Thiel D. (THIEL, 2020)

Table 1b
Allocation of HSC papers with 5 clusters.

Cluster ID	Size	Authors/Paper ID
K1	**27**	Agnolluci P. et al. (AGNOLLUCI Paolo et al., 2013); Balta-Ozkan N. & Baldwin E. (BALTA-OZKAN Nazmiye and BALDWIN, 2013); (BAUFUME Sylvestre et al., 2011); Cho S. & Kim J. (CHO and KIM, 2019); Coleman D. et al. (COLEMAN et al., 2020); Dagdougui H. et al. (DAGDOUGUI HananeOUAMMI AhmedSACILE Roberto, 2012); Deng Z. & Jiang Y. (DENG and JIANG, 2020); Li L. et al. (LeiMANIER HervéMANIER Marie-Ange, 2020); Moreno-Benito M. et al. (Moreno-Benito MartaAgnolucci Paolo and Papageorgiou Lazaros, 2017); Murthy-Konda N.V.S.N. et al. (MURTHY-KONDA et al., 2011); Ogumerem G. S. et al. (OGUMEREM Gerald et al., 2018); Quarton C. J. & Samsatli S. (QUARTON Christopher and SAMSATLI Sheila, 2020); Quarton C. J. & Samsatli S. (QUARTON Christopher and SAMSATLI Sheila, 2021); Reuss M. et al. (Markus et al., 2017); Reuss M. et al. (Markus et al., 2019); Rosenberg Eva et al. (ROSENBERG et al., 2010); Samsatli S. & Samsatli N. J. (SAMSATLI Sheila and SAMSATLI Nouri, 2015); Samsatli S. & Samsatli N. J. (SAMSATLI Sheila and SAMSATLI Nouri, 2018); Stöckl F. (STÖCKL FabianSCHILL Wolf-PeterZERRAHN Alexander, 2021); Strachan N. et al. (STRACHAN Neil et al., 2009); Talebian H. et al. (TALEBIAN Hoda and HERRERA Omar, 2019); Tlili O. et al. (Olfa et al., 2020); Won W. et al. (WON et al., 2017); Woo Y. et al. (WOO et al., 2016); Wu X. et al. (WU et al., 2019); Yang G. (YANG et al., 2020); Koirala B. et al. (KOIRALA et al., 2021)
K2	**23**	Almansoori A. & Shah N. (ALMANSOORI and SHAH, 2006); Almansoori A. & Shah N. (ALMANSOORI and SHAH, 2009); Almansoori A. & Shah N. (ALMANSOORI and SHAH, 2012); Almansoori A. & Betancourt-Torcat A. (ALMANSOORI and BETANCOURT-TORCAT, 2016); Cantu et al. (CANTU Victor and AZZARO-PANTEL CatherinePONSICH Antonin, 2021); Dayhim M. et al. (DAYHIM Muhammad et al., 2014); De Leon Almaraz S. et al. (DE LEON ALMARAZ Sofia et al., 2013); De Leon Almaraz S. et al. (DE LEON ALMARAZ Sofia et al., 2014); De Leon Almaraz S. et al. (DE LEON ALMARAZ Sofia et al., 2015); Fazli-Khalaf M. et al. (FAZLI-KHALAF Mohamadreza et al., 2020); Güray Güler M. et al. (GÜRAY GÜLER MehmetGECICI EbruERDOGAN Ahmet, 2021); Han J. et al. (HAN et al., 2013); Hugo A. et al. (HUGO et al., 2005); Kim J. et al. (KIM et al., 2008); Kim J. et al. (KIM and MOON, 2008); Kim J. et al. (KIM et al., 2011); Li Z. et al. (Zheng et al., 2008); Nunes P. et al. (NUNES et al., 2015); Ochoa-Bique A. & Zondervan E. (OCHOA BIQUE AntonZONDERVAN Edwin, 2018); Ochoa-Bique A. et al. (OCHOA BIQUE Anton et al., 2019); Ochoa Robles J. et al. (ROBLES JesusAZZARO-PANTEL CatherineAGUILAR-LASSERE Alberto, 2020); Sabio N. et al. (SABIO Nagore et al., 2012); Seo S.-K. et al. (SEO et al., 2020)
K3	**16**	André J. et al. (ANDRE Jean et al., 2013); Bae S. et al. (BAE et al., 2020); Ball M. et al. (BALL et al., 2007); Baufumé S. et al. (BAUFUME Sylvestre et al., 2011); Gabrielli P. et al. (GABRIELLI Paolo et al., 2020); Gim B. et al. (GIM et al., 2012); Hajimiragha A. et al. (HAJIMIRAGHA Amirhossein et al., 2009); He C.et al. (HE et al., 2017); Huang Y. et al. (HUANG et al., 2015); Hwangbo S. et al. (HWANGBO SoonhoLEE In-Beum and HAN, 2017); Li Y. et al. (LeiMANIER HervéMANIER Marie-Ange, 2020); Obara S. & LI J. (OBARA and LI, 2020); Park K. & Koo J. (PARK and KOO, 2020); Rosa L. & Mazzotti M. (ROSA and MAZZOTTI Marco, 2022); Sun H. et al. (SUN et al., 2017); Wang B. et al. (WANG et al., 2020)
K4	**8**	Tao Y. et al. (TAO et al., 2020); Crönert T. & Minner S. (CRONERT TobiasMINNER Stefan, 2021); Guo Z. et al. (GUO et al., 2021); Khojasteh M. (KHOJASTEH Meysam, 2020); Li X. & Mulder M. (LI and MULDER, 2021); Liu H. et al. (LIU et al., 2021); Michalski J. (MICHALSKI Jan 2017); Thiel D. (THIEL, 2020)
K5	**13**	Bae J. H. & Cho G. (BAE et al., 2010); Bento N. (BENTO, 2010); Conrad K. (CONRAD, 2004); Espegren K. et al. (ESPEGREN Kari et al., 2021); Greaker M. & Heggedal T. (GREAKER MadsHEGGEDAL Tom-Reiel, 2010); Heinz B. et al. (HEINZ et al., 2013); Köhler J. et al. (KÖHLER et al., 2010); Li W. et al. (LI et al., 2020a); Li Y. et al. (LI et al., 2020a); Li Y. et al. (LI et al., 2020c); Meyer P. E. & Winebrake J. J. (MEYER Patrick and WINEBRAKE James, 2009); Sartzetakis E. S. & Tsigaris P. (SARTZETAKIS Eftichios and TSIGARIS Panagiotis, 2005); Silva C. M. et al. (SILVA Carla, 2014)

Table 2
Proportion of most discriminating features by cluster.

Feature ID	Cluster ID				
	1	2	3	4	5
MILP	**0.56**	**0.96**	0.43	0.37	0
p-median/Location model	0	0	0.31	0.25	0
Physico-chemical model	0.11	0.04	0.31	0.25	0
Market equilibrium	0.04	0	0	**0.5**	0.08
Cournot model	0	0	0	**0.5**	0
Mathematical description	**0.63**	**0.96**	**0.81**	**1**	**0.62**
Mono-objective	**0.78**	**0.52**	**1**	0.25	0
Cost minimization	**0.85**	**0.87**	**0.75**	0.12	0
Multi-agent	0	0	0	**1**	0.38
Agent – Profit/utility	0	0	0	**0.86**	0.23
Strategic interactions	0	0	0	**1**	0.23
Network effects	0	0	0.06	0	**0.54**
Microeconomic level	0.04	0	0	**1**	**0.61**
Macroeconomic level	0	0	0	0	0.31
Externalities	0.04	0	0	0	**0.85**
Geographically explicit	**0.93**	**0.96**	**0.94**	**0.75**	0.08
Multi-period	**0.89**	**0.56**	0.31	0.62	**0.69**
Urban scale	0.07	0	0.25	**0.5**	0.08
Economic echelon - Households	0	0	0	0.37	**0.92**
Economic echelon - Firms	0	0	0	**0.5**	0.08
Echelon – Sources	**0.67**	**0.61**	0.25	0.37	0.23
Echelon – Production	**0.93**	**1**	0.37	**0.5**	0.24
Echelon – Storage	**0.85**	**0.91**	0.19	**0.62**	0
Echelon – Transportation	**0.81**	**1**	**0.69**	0.12	0
Investment decision	0.26	**0.78**	0.44	0.25	0.23
Liquid H_2	**0.59**	**0.96**	0.19	0	0
Gaseous H_2	**0.70**	**0.74**	**0.56**	0.25	0
Light-duty vehicles	**0.85**	**0.87**	0.44	**0.5**	**1**
Production – Technical constraints	**1**	**1**	0.44	**0.5**	0.08
SMR	0.48	**1**	0.44	0.12	0.08
Electrolysis	**0.89**	**0.87**	0.25	0.37	0.15
Storage – Technical constraints	**0.81**	**0.91**	0.19	**0.62**	0
Liquid storage	**0.59**	**0.91**	0.12	0	0
Gaseous storage	**0.63**	**0.61**	0.19	0.25	0
Transportation – Technical constraints	**0.81**	**0.91**	**0.56**	0	0
LH_2 tanker truck	**0.52**	**1**	0.12	0	0
GH_2 trailer	0.48	**0.65**	0.19	0	0
Price subsidies	0.07	0	0	0	0.38
Alternative fuel competition	0	0	0	0	**0.61**
Demand – penetration rate	**0.59**	**0.70**	0.25	0	0.15
Endogenous demand	0.04	0	0	**0.75**	**0.85**
Demand – dynamic profile	**0.59**	0	0	0.37	0
Node-based demand	**0.78**	**0.96**	**0.75**	**0.62**	0.08
Flow-based formulation	0.04	0.04	0.25	0.12	0
Electricity network included	0.33	0	0.31	**0.62**	0

Note: For each feature, we underline the highest value. Moreover, for each cluster, bold values correspond to cases where at least 50% of papers include the feature.

horizon, i.e., the number, size, location and technology types of production plants, storage units and refueling stations, the optimal physical form of H_2, in addition to the optimal transportation and distribution infrastructures in terms of size, available technologies and physical flows. Overall, this class of papers uses a finer modeling (in terms of spatio-temporal resolution) of operational constraints than K1, and focuses on the multiple trade-offs, investigated through -constrained and Pareto front methods, between concurring objectives in the development of green and safe hydrogen infrastructures.

We refer to cluster K3 as the set of *General energy-system level HSC models*. Included papers display more mathematical formulation diversity than K1 and K2: only 44% of models use a MILP formulation, while *p*-median models account for 31% of clustered papers. Moreover, 31% of articles include physico-chemical constraints in their mathematical formulation of H_2 production, compression, storage, and transportation. Papers in K3 focus more often on interactions with other energy systems and diverse uses of H_2: respectively 31% and 25% of included papers model incorporate the electricity grid and the CO_2 capture and storage network. In addition, this family of models is characterized by its stronger emphasis on multiple H_2 usages (19% of papers consider hydrogen demand for heating) and interactions with other energy networks. Compared to K2, papers in K3 are three times more likely to model the coupling with carbon captures and storage (CCS) supply chains, while the electricity network is only modeled in K1 and K2. In summary, K3 investigates how the development of hydrogen infrastructures and spatial network interacts with and impacts the operations of other energy sectors. More specifically, most papers seek to co-optimize the investment and operational decisions of the HSC and other energy supply chains through an integrated modeling framework.

As mentioned, cluster K4 mostly includes papers identified as “hybrid”. We refer to it as *Strategic interactions investment and operation optimization models*. With a majority of geographically explicit formulations (75%), this class of papers is distinct from the previous ones by its focus on the urban scale (50%), and a limited attention to national scale case studies (25%). As in K3, a strong focus is put on interactions with other energy supply chains, mostly electricity (62%) and gas networks (25%). Models with investment decisions mostly pertain to refueling station location and size, in a context of retailer competing for optimal location with strategic interactions (61%). Moreover, 61% of papers adopt a multi-agent framework. It is significant that also the MCP, which is exclusive to K4, is used by 25% of clustered papers. Moreover, K4 articulates large proportions of both Bottom-up and Top-down models, especially *p*-median models (25%), physico-chemical models (25%), market equilibrium and Cournot models (both 50% of papers). The hybrid aspects of this class of papers are better represented in operational decision models with technical constraints on decision variables in a multi-agent framework. They explore the strategic uses of H_2 storage for profit maximization, associated to an explicit modeling of production and storage constraints. Through market clearing and equilibrium conditions, producers/retailers make production, investment and storage decisions that are constrained by technical limitations of technologies (storage state of charge, ramping limit, minimum generation volume) and influence other agents through the price channel. Due to this focus on agents’ decision making and operational constraints, those models are uniquely formulated at the microeconomic level (100%). The research questions tackled by this class of papers are multiple: how do market interactions influence the investment, production, storage decisions and prices of H_2 under operational constraints? How does hydrogen storage impact the operations and behavior of economic agents on the electricity and gas markets? Regarding location decisions, these models investigate how retailer competition affects the emergence of a H_2 refueling stations network and how policy-makers should intervene. Yet, this category of papers is characterized by the extremely poor accounting of the transportation echelon (12 %), while transportation constraints are totally absent.

Finally, cluster K5 is a composite family referred to as *Technological diffusion, spatial competition, and socio-economic assessment models*. Diffusion and dynamic system models (46% of papers) are essentially found in cluster K5. Frequently formulated in a multi-agent framework (38%), this set of papers is the only one to investigate and investigate the interactions between the hydrogen network structure (in terms of density of refueling stations) and economic agents’ spatial distributions and their impact in terms of network effects (54%) and externalities (85%). The models are exclusively focused on the transportation sector. With the frequent exception of the production echelon, none of the identified functional echelons nor associated technical constraints are modeled. Competition between “fossil-fueled” gasoline cars and hydrogen cars is distinctive of K5 (61% of papers), and mostly pertains to the choice of transportation technologies made by consumers and its interactions with the economic and geographic development of (available) refueling infrastructures. Demand modeling is strongly endogenous (85%), as it depends on model variables such as relative prices of competing fuels, shares of users of each technology, refueling stations density and distance for each technology, in addition to consumers’ preferences such as environmental concern. The existence of network effects creates lock-in effects in favor of the incumbent gasoline refueling stations or gasoline vehicle fleet. Many papers belonging to cluster K5 investigate the existence of barriers to entry for H_2 vehicles and refueling stations in the presence of existing gasoline infrastructures. They model the classical "chicken-and-egg" problem and study what factors may create a lock-in in favor of dirty technologies and whether policy intervention, under the form of taxes and subsidies, is required to speed up the diffusion rate of hydrogen refueling infrastructures. The coordination and potential synergies between economic echelons (producers, retailers, and consumers) through multi-side market models are also investigated. Finally, K5 is the only cluster to investigate the macroeconomic effects of the hydrogen economy, with a strong microeconomic basis (61%). A significant proportion of papers, namely 23%, employ a multi-sectoral approach associated with CGE models, wherein sectors are frequently grouped into energy, transportation, and industrial clusters. In terms of research questions, this subset of papers investigates the economy-wide repercussions of the introduction of hydrogen production and transportation technologies: how does hydrogen substitute for existing energy sources? What are the inter-sectoral effects of pro-hydrogen policies and how does hydrogen production affect the sectoral final energy consumption, production, and profits? Finally, on an aggregate level, these models investigate the impact of hydrogen on macroeconomic variables like sectoral employment, investment demand, real aggregate consumption, wage rates, export demand and carbon emissions. However, even within K5, the number of macroeconomic models remains modest.

Overall, each cluster corresponds to a set of research questions with its associated methodological strengths and blind spots: cluster K1 and K2 offer the most comprehensive modeling of HSC functional echelons and technical constraints, with extensive use of MILP formulations. K3 proposes more diverse mathematical formulations and a general approach by investigating the interactions between the HSC and other energy supply chains. Yet, these three groups of papers ignore how non-cooperative behavior and market interactions influence the optimal investment and operational decisions. Taking demand as exogenous neglects the importance of network effects and expectations on the development of hydrogen demand, in addition to feedback effects on hydrogen producers and retailers expected profits. Finally, except a subset of K5, all models are formulated as partial-equilibrium models, or focus on the interaction of hydrogen technologies with other types of supply chains within the energy sector.

Our goal is thus to find pathways to integrate these pivotal modeling features into more classical HSC formulations, such as found in K1, K2 and K3, which are characteristic of BU models. Hybridization efforts must thus concentrate on how to articulate the research questions identified above into a single framework. However, as found in K4, several directions are possible, either by adapting the classical MILP framework or using original mathematical formulation such as the MCP framework. The feasibility of such methodological hybridization and the pros and cons associated to existing pathways are thus investigated in the next section.

3.4. Robustness checks

Yet, as some authors appear multiple times within the sample, this might lead us to overestimate the relative importance of some methodological approaches. They would indeed correspond to the preferred modeling choices and research questions of authors who appear frequently in the sampled literature. Thus, we control for authors publishing multiple articles within the sample by computing the Jaccard distance between each pair of papers. If the distance is below some fixed threshold for papers, we assume the two papers are roughly identical and randomly drop one of them from our sample. Surprisingly, only two pairs of papers have a Jaccard distance below 0.25. Choosing this threshold level and dropping two papers from our sample, we apply our classification method on the reduced sample. The Jaccard distance remains the distance metric associated with the highest clustering score all number of clusters (0.0992), significantly above the scores associated to the Manhattan and Φ^2 distances (0.0764 and 0.664).

When comparing the robust clustering to baseline ones, we note very strong similarities with basically a reshuffling of cluster labels. Regarding cluster compositions, robust cluster K1 and baseline K2 share 78% of papers. Similarly, 83% of papers in robust K3 are included in baseline K1. Finally, we note that robust K2 is identical to baseline K3, while K4 and K5 from both approaches are identical. Robust and baseline clusters thus strongly overlap and result in a remarkably similar classification of our sample. Moreover, 87% of features found in the "robust" vector of most discriminatory features are found in the baseline vector. Checking for multiply authorship thus does not significantly affect our clustering results and has a limited impact on the set of features used to analyze their differences.

4. A discussion of the opportunities and challenges for developing hybrid methodological approaches in HSC modeling

Following (HELGESEN Per Ivar, 2013; TAALBI Josef and NIELSEN, 2021), soft-linking corresponds to a framework in which the processing and exchange of information between several models is controlled by the user. The user evaluates the models on a set of Common Measuring Points (CMPs), within the subset of variables where models overlap[6] and for which models should yield identical results. If not, the user manually modifies models' input to make them converge. With hard-linking, information exchange and processing between models is done automatically through computer programs. An algorithm negotiates the results over the subset of overlapping variables. Finally, integrated models directly influence each other into a single framework.

Soft-linking offers more transparency and learning about how models behave and react to changes in inputs. Hard-linkage provides higher productivity, especially as the volume of model runs increases, uniqueness, and better control on models' output. However, for both types of linkage, the control of noise resulting from divergent measures at CMPs is difficult as most of the useful sets of CMPs are *non-exclusive*, which makes uncertainty analysis quite tricky. Hybrid models, which correspond to the type of integrated model linkage, avoid these convergence issues, and thus appear as the best option.

4.1. Identification of "polarizing" methodological choices

Considering the classification from Section III, we use a features-based approach to quantify the difficulty of hybridizing methodological approaches from various clusters. We proxy it by measuring the methodological uniqueness associated with each feature, corresponding to the degree of "methodological" proximity with alternative features within a given model formulation. The interpretation is simple: a low divergence score $\Delta_{Y,Y'}$ means that features Y and Y' are strongly related in methodological choices. Intuitively, two features with a low divergence score consistently appear jointly in models, which indicates associating these features within a single broader methodological framework is frequent. This may either mean that associating these two modeling choices is simple, or that one methodological choice implies making the other one.

Finally, we introduce a repulsion score to quantify polarizing methodological choices: intuitively, a feature with a low score can be utilized in various methodological frameworks without requiring

[6] CMPs reacting to changes everywhere within the overlapping area are called *inclusive*. CMPs that are independent, i.e., have non-overlapping influence areas, are said to be *exclusive*. The influence area of a CMP corresponds to the set of variables for which a change causes a change of the value measured at the CMP.

significant modifications of the model. For instance, a multi-agent formulation is expected to be highly polarizing as the possible mathematical formulations, choice of variables and parameters are *a priori* quite incompatible with a MILP formulation. The formal description of both scores is given in Appendix.

The distribution of the resulting pair-wise normalized divergence scores is plotted in Fig. 6a. Strikingly, 56% of all features pairs have normalized divergence score below the average, equal to 0.79. With a standard deviation of 0.46, less than 18% of feature pairs have a score one standard deviation above the mean, as suggested by the fat-tailed distribution. This suggests most features play non-polarizing methodological roles within investigated models, and thus do not significantly drive formalization and modeling choices. For instance, it is relatively simple to add taxes or technology-specific subsidies as additional cost parameters in both a MILP and a Cournot model. Likewise, other energy supply chains are easily integrated within optimization models by minimizing the summed costs of both the HSC and additional network through co-optimization. On the opposite, a minority of features pairs exhibit a large divergence, which optimistically suggests only a small subset of methodological features might be difficult to associate within a single framework.

When plotting the normalized repulsion scores in Fig. 6b, the distribution of scores exhibits a strong right-skew, with 68% of features having a score below the average. Only 17% of features scores are above one standard deviation. Intuitively, features with high scores polarize formalization choices because they are only strongly associated with some subset of modeling features. Thus, we may rank features by decreasing repulsion score in order to establish a hierarchy in terms of driving methodological choices. We identify three classes as presented in Table 3.

On the one hand, unsurprisingly, alternative fuels competition, associated with the modeling of economic households' decision making and multi-agent approaches, are the strongest driving features. Considering alternative fuels to H_2 (typically gasoline for mobility uses) implicitly requires formulating substitutability patterns between competing fuels. Strategic interactions have a strong influence as they imply defining hydrogen demand as a function of competing network sizes (expressed as the results of interactions between users and potential users in the Baas model, see (HEINZ et al., 2013)), in addition to several measurable characteristics including, but not limited to, relative prices of alternative fuels, relative vehicle price, CO_2 price, and consumer preferences. Still, dynamic systems and diffusion models do not precisely account for the detailed topology of competing networks. A proper modeling of hydrogen demand must thus satisfy two conditions: first, because the hydrogen refueling network is a spatial phenomenon, hydrogen demand must be defined on a (discrete) metric space, such as a graph; second, it can be equal to zero if the hydrogen refueling network is inexistent or the cost of hydrogen mobility is too high compared to alterative options. Indeed, papers included in our sample suffer from a teleological bias as none allows the case where no investment occurs at optimality and hydrogen demand remains null.

In this respect, using a multi-period model makes little sense if the transition dynamics from early to developed stages of the HSC are not well represented. Modeling future demand dynamics using a deterministic sequence of values based on future projections, or probabilistic scenarios, makes the implicit assumption that the evolution of hydrogen demand is exogenous and independent from the development of the HSC and refueling stations network. As stated in (BAKKER, 2021) and (TAALBI Josef and NIELSEN, 2021), electric vehicles in the early 20th century were comparable to gasoline ones on a cost basis when adjusting prices for performance and range. Yet, the limited development of the electricity network constrained electric cars manufacturers to urban areas, helping to lock the industry into a carbon-intensive technology choice. Policy instruments like carbon tax or subsidies may be ineffective in practice without sufficient refueling infrastructures (see (SARTZETAKIS Eftichios and TSIGARIS Panagiotis, 2005) for a modeling of their interactions). H_2 demand should thus be formulated as a function of the station network structure, associated with a measure of users' "range anxiety" (see (HUANG et al., 2015)).

When possible, expressing the optimal price and number of refueling stations (like in (CONRAD, 2004) and (GREAKER MadsHEGGEDAL Tom-Reiel, 2010)) as linear combinations of the above features would be compatible with BU approaches. Yet, it may not be possible to get linear or closed form expressions when incorporating technical limits for production, storage, and transportation units as inequality constraints on decision variables. These modeling objectives are typically unfeasible in conventional BU formulations. Indeed, BU traditionally use shadow prices associated with programming constraints to proxy energy prices. Yet, following (BÖHRINGER ChristophLÖSCHEL Andreas, 2006), the shadow price may actually not coincide with market prices, which

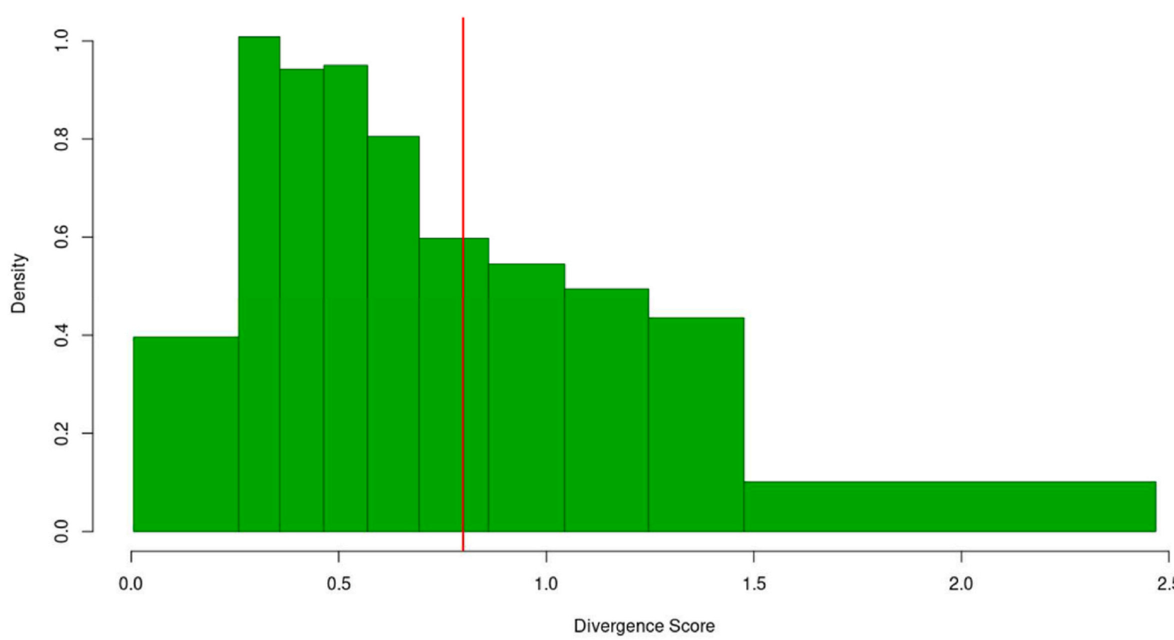

Fig. 6a. Distribution of normalized pairwise divergence scores. **Note:** The divergence score is normalized by subtracting the mean and dividing by its standard deviation. Each column corresponds to 10% of all potential pairs of methodological features. The red vertical line equals the mean divergence score.

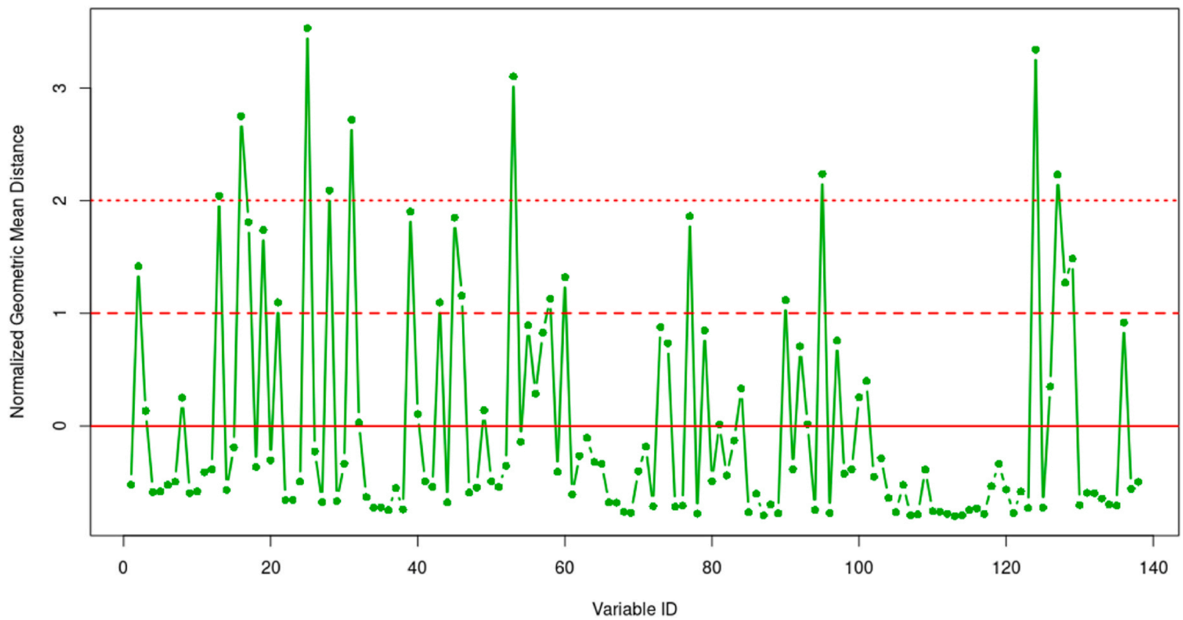

Fig. 6b. Normalized repulsion score by methodological feature. **Note:** The plain (resp. dashed and dotted) line corresponds to the mean value (resp. one and two standard deviations above the mean).

Table 3
Categories of polarizing methodological features based on repulsion score ranking.

Feature Group Type	Size	Feature/Feature ID
"Strong" driving features	**9**	Multi-agent; Alternative fuel competition (); Economic echelon - Households; Mathematical description; Strategic interactions; Transportation – Technical constraints; Endogenous demand; Agent – Profit/utility; Cournot model
"Moderate" driving features	**14**	Microeconomic level; Light-duty vehicles; Geographically explicit; Mono-objective; Cost minimization; Node-based demand; MILP; Echelon – Transportation; Demand – penetration rate (); Multi-period; Echelon – Storage; Storage – Technical constraints; Risk/reliability optimization; Externalities
"Low" driving features	**20**	Electricity network included; Echelon – Retailers; Liquid H_2; Production – Technical constraints; Echelon – Production; LH_2 tanker truck; Gaseous H_2; Liquid storage; GH_2 pipeline; Demand – penetration rate; Electrolysis; Echelon – Sources; GH_2 trailer; Dynamic system/diffusion models; National scale; *p*-median/Location model; Macroeconomic level; Network effects; Gaseous storage; SMR

Note: The "strong" driving features correspond to the class of features with normalized repulsion score above two standard deviations. Similarly, "moderate" (resp. "low") driving features include features with normalized repulsion score between one and two standard deviations (resp. between zero and one standard deviation).

violates the "integrability" condition required to use conventional production functions, such as CES functions in CGE models. MCP appears as a more general and flexible formulation that guarantees "integrability" and endogenously model prices.

In addition, the high repulsion scores associated to mono-objective, cost optimization and geographically explicit models is characteristic of BU models. As pointed in Table 2, those features have a much lower probability of occurrence in clusters K4 and K5. HSC "functional" echelons are also absent from K5 and are very poorly modeled in K4, which explains the moderate driving strength of these features in terms of repulsion score. A realistic HSC must both account for various functional echelons, from feedstock and hydrogen production to delivery to final consumers or refueling stations, and explicitly model the technical constraints associated with each of them. We note that the quasi totality of modeling features analyzed in (LeiMANIER HervéMANIER Marie-Ange, 2019), considering only the set of features relevant for K1 to K3, are low driving features: they pertain to the choice of technologies, technological characteristics (unit sizes available), H_2 physical state for production and storage, in addition to non-driving features such as inclusion of CCS for CO_2 emitting H_2 production technologies. All those features, in addition to exogenous subsidies and taxes, can be simply included within a MILP formulation, at the price of higher model complexity and resolution time.

Based on the above requirements, a subset of promising modeling approaches can be identified in our sample, more specifically from papers included in K4. Two main types of mathematical formulations can be distinguished: extensions based on linear and non-linear programming, and MCP models.

4.2. Existing hybrid approaches and future hybridization perspectives

The first family of hybrid models encompasses various adaptations of the basic LP formulation. A first possibility is to linearize the KKT conditions of the initial problem: using a multi-agent framework, where each agent separately maximizes its individual profit, the model in (GUO et al., 2021) is reformulated into a set of market equilibrium conditions derived from the first-order conditions. The reformulated problem proposes a set of equations and inequality constraints and is transformed into a MILP using the Big-M method, which introduces auxiliary binary variables to reformulate each complementarity and non-linear constraints as a set of linear constraints. The example of (GUO et al., 2021) shows that features such as the integration of demand uncertainty (using a robust approach in this case), have a very low driving force and do not significantly modify the model formulation. Yet, linearization methods may significantly increase the model complexity, which increases exponentially with the number of nonlinear equations to reformulate. Efficient formulations, preserving high spatio-temporal resolution of the model while controlling the computational efficiency of the model such as in VWM, or reducing the number of integer variables and constraints (see (NUNES et al., 2015)), may come handy to limit the explosion of

Table 4
Methodological elements for a hybrid HSC model.

Feature Category	Modeling directions
Mathematical formulation	➢ MILP: Linearization of KKT conditions of the initial MILP problem; bilevel or multi-level formulation for hierarchical multi-agent framework. ➢ Integer Programming Games (IPG) ➢ Mixed Complementarity Problem (MCP)
H_2 demand formulation	➢ Closed-form expression: Cournot model with asymmetric costs, including transportation costs; Hotelling model; Salop model. ➢ Multinomial logit choice: multimodal choice between alternative fuel types (dependent on relative vehicle and fuel prices, in addition to consumer preferences), and between competing refueling stations located on a graph; nested multinomial model to hierarchize vehicle choice and refueling station choice. ➢ Representative consumer utility function (macroeconomic perspective): maximization of inter-temporal utility with exogenous mobility and/or heating requirements, under inter-temporal budget constraint. Model H_2 and alternative fuel vehicles as additive components in the utility function (substitutes), and distribution networks parameters as being multiplicative with respect to mobility choices (complements).
Price formulation	➢ Closed-form expression: Cournot model; Hotelling model; Salop model. ➢ Shadow value (classical MILP formulation) but entails exogenous prices. ➢ Endogenous price formulation from KKT system derived from market-clearing and zero-profit conditions.
Strategic interactions	➢ MILP with linearized KKT conditions/MCP: coordination through price and volume channels. ➢ IPG: payoff-functions, reaction functions.
Technical constraints	➢ MILP with linearized KKT conditions/MCP: reformulation of technical constraints as system of equalities and inequalities with complementarity conditions. ➢ IPG: include technical constraints in the definition of the set of strategies of each player.
Government intervention	➢ Modeling of taxes and subsidies as exogenous scalar parameters. ➢ Endogenous policy variables as decision variables of a benevolent regulator which maximizes social welfare or some other criterion (H_2 vehicle penetration, CO_2 emissions).

CPU time.

Multi-agent interactions and macroeconomic models may also be formulated as multi-player or multi-sector games in a market, with possibly contradicting objective functions, integrated within a classic MILP. The solving strategy then depends on the structure of the game. (KHOJASTEH Meysam, 2020) model a Stackelberg game with residential electricity consumers (the followers) and a Micro-grid Operator (MGO, the leader) with hydrogen storage. The hierarchical decomposition allows writing a lower-level problem (consumers minimizing the energy procurement costs) and upper-level problem (the MGO maximizes her profit under network and thermal operational constraints). Similarly, to the multi-objective optimization case (see (ROBLES JesusAZZARO-PANTEL CatherineAGUILAR-LASSERE Alberto, 2020)), this formulation allows for sequential solving with the help of genetic algorithms. Finally, if player actions are defined as integer variables (allowing both the representation of discrete investment and operational decisions under start-up or storage constraints for instance), the game can be formulated as an Integer Programming Game (IPG). IPG are a class of non-cooperative and non-convex games in which each strategic player must solve a MIP problem. The solution set of each player is described as a collection of lattice points bounded by a set of linear inequalities. Under the (strong) assumption that solution sets are neither empty nor unbounded, the existence of at least one (pure or mixed strategy) equilibrium is proven in (CARVALHO et al., 2022), which proposes two algorithmic approaches guaranteed to approximate the equilibrium under mild conditions. By encoding solution sets with short rational generating functions, (Matthias and RYAN Christopher, 2011) present efficient algorithms for enumerating all pure Nash equilibria with piecewise linear convex payoff functions.

Yet, in the presence of both complementarity conditions and inequalities, MCP appears as a natural framework for problems that are hard to formulate using classic optimization tools. Following (MURPHY FrédéricPIERRU AxelSMEERS Yves, 2016), MCP models have become commonplace for analyzing market responses to policy interventions, as in (BAE et al., 2010). MCPs are particularly adapted to situations which require explicit formulation and manipulation of the solutions to linear programs (e.g., prices). Compared to MILP approaches, MCP avoids the requirement of closed-form expressions for KKT conditions. Moreover, as in (Jan et al., 2019), bilevel MCP formulations can be used to model the interactions of a benevolent regulator, who minimizes societal energy system through optimal policy choice, with profit-maximizing agents within the HSC. This allows for an endogenous formulation of taxes and subsidies required for optimal HSC deployment. Finally, (BÖHRINGER ChristophLÖSCHEL Andreas, 2006) show MCP can articulate a BU model of the HSC with a CGE model describing other sectors at an aggregate level using CES functions. Yet, the non-convex structure of MCPs makes them particularly challenging to use. Moreover, we can notice that (LI and MULDER, 2021) and (MICHALSKI Jan 2017) only include continuous variables in their MCP formulations. As stated by (GABRIEL et al., 2021), MCPs constrained by integrality conditions are much harder than continuous MCPs and have been relatively unstudied. To address this issue, the authors propose a purely continuous reformulation of integrality constraints as complementarity constraints with promising solution time and quality.

Regarding endogenous network-dependent formulations of demand, a promising solution is proposed in (CRONERT TobiasMINNER Stefan, 2021), coupled with an IPG formulation. Using a flow-based formulation of demand on a graph, the flow of H_2 vehicles between each pair of nodes is both a function of customer preferences and refueling stations distribution on the graph. Using a multinomial logit choice model, the probability that a customer chooses an active refueling facility is a function of her preferences regarding maximum deviation distance, facility attractiveness and distance. A similar approach may be developed to model the aggregate probability of adopting H_2 vehicles as a function of relative vehicle prices when comparing technologies, autonomy, preferences, and hydrogen refueling stations network development. We leave this question open for further research.

Table 4 provides a summary of the most promising methodological choices and formulations for the modeling various elements of the HSC within a hybrid model. Although incomplete, it provides a formal basis of hybrid modeling elements that comply with the methodological requirements identified above. However, we leave it for further research how to best articulate these elements within a single framework, both in terms of mathematical complexity and performance regarding solution time and decision optimality.

5. Conclusion

5.1. Theoretical contribution

By using both qualitative and quantitative methods through clustering, or paper presents a comprehensive and structure classification of the existing methodological approaches for modeling HSC and hydrogen markets. While recent review papers such as (LeiMANIER HervéMANIER Marie-Ange, 2019) and (SGARBOSSA Fabio et al., 2023) focus on the BU-HSC literature, this paper is the first to our knowledge to include TD literature into a complete assessment of the models and mathematical formulations used to answer a variety of hydrogen-related research questions.

By first identifying a set of methodological choices found in existing HSC models, we propose a methodological classification of the literature by using hierarchical clustering. Each paper category is characterized by a set of research questions, preferred mathematical models and methodological formulations. In addition, by identifying the analytical blind-spots associated with each category, our work allows a discussion of the pros and cons associated with existing approaches and pinpoints how these could complement each other within hybrid models. Finally, we introduce original metrics that allow us to quantify statistically the dependency of methodological choices, in terms of joint frequency of occurrence within sampled papers and "repulsion" strength. This allows us to map the HSC modeling choice patterns made by authors and understand why some methodological features appear frequently together, or some features seem mutually exclusive. A careful qualitative analysis ultimately enables us to explain if those patterns are the consequence of modeling habits within the HSC modelers community, or if there exist strong mathematical and formal difficulties preventing the association of specific model elements within an integrated framework.

This analysis finally allows us to identify and provide some methodological requirements and elements for developing hybrid models of the HSC, articulating the strengths of both BU and TD models.

5.2. Managerial implications

As noted above, most methodological choices and features discussed in other HSC reviews are low driving choices and can be simply accommodated within a classical MILP framework. Thus, practitioners interested in the economic and technological impact of introduction taxes and subsidies may introduce such features as exogenous that enter the objective function and constraints, in the form of additional costs (possibly negative for subsidies) or constraints (for instance, upper CO_2 emission bounds when considering a carbon budget for the HSC).

Practitioners concerned with the "chicken-and-egg" problem of H_2 supply and demand actual realization may strongly benefit from modeling demand as exogenous, as a function of H_2 price (or LCOH) and infrastructure development at least, to identify the conditions for the emergence of a structured aggregated hydrogen demand. Considering the arbitrage between H_2 and alternative fuels technologies in the definition of the demand function is also a prerequisite to properly model the transition from carbon emitting to H_2 technologies. Coupled with a sensitivity analysis on taxes and subsidies, this provides a relevant modeling approach for identifying optimal public policies that would foster both hydrogen supply and demand.

5.3. Limitations and suggestions for future research

As previously noted, the mathematical formulations proposed for developing hybrid models may seriously increase model complexity and may be difficult to implement for large-scale case studies. The introduction of binary variables to linearize the KKT conditions of the optimization problem into a MILP is a good example. Similarly, the consideration of integrality conditions on decision variables introduces non-convexities in MCP models, which adds considerable complexity and may require formulations to ensure model tractability and solvability. Those limitations thus require for future research a careful analysis of the pros and cons associated with hybrid modeling elements identified in this paper, in terms of mathematical tractability, solvability, solution time and interpretability of results. Finding the optimal combination of those elements within a consistent framework is outside the scope of the present article but shall thus be investigated in future work.

We also think that, when developing a model to optimize HSCs using a hybrid approach combining engineering and economics, future work should include the technological aspects and the development potential of the energy system while considering the strategic interactions between the different actors in the market in order to optimize either the objective of each individual actor or the social welfare.

Data availability

Data will be made available on request.

Appendix

Table A1
Methodological features categories and list

Features Category	Size	Features Name
"Bottom-up" mathematical models	**7**	Linear Programming; Mixed-Integer Linear Programming; *p*-median/Location model; MARKAL; Value Web Model; Mixed Complementarity Problem; Physico-chemical model; Mathematical description
"Top-down" mathematical models	**9**	Dynamic system/diffusion models; Input-output models; Discrete choice models; Market equilibrium; Game theory; Cournot model; Hotelling/Salop models; (Dynamic) Computable General Equilibrium models; Microeconomic level; Macroeconomic level
Social planner's objectives	**8**	Mono-objective; Multi-objective; Cost; GWP/environmental performance; Risk/reliability; Social welfare; Profit; Distance
Economic agents' objectives	**3**	Principal – Social welfare; Principal – Profit; Agent – Profit/utility
Economic agents' features and echelons	**17**	Multi-agent; Multi-sectoral; Strategic interactions; Network effects; Perfect rationality; Perfect rationality mention; Perfect foresight; Perfect foresight mention; Risk aversion; Risk aversion mention; Learning effects; Economies of scale; Externalities; Echelon – Social planner; Echelon – Households; Echelon – Firms/producers; Echelon – Retailers
Spatio-temporal features and echelons	**15**	GIS (Geographic Information System) module; Geographically explicit; Multi-period; Multiple time scales; International scale; National scale; Regional scale; Urban scale; Echelon – Feedstock; Echelon – Production; Echelon – Storage; Echelon – Long-term storage; Echelon – Transportation; Echelon – Distribution; Echelon – Refueling stations/demand nodes; Investment decision
Feedstock echelon	**9**	Natural gas; Biomass; Coal; Water; Grid electricity; Hydroelectricity; Solar electricity; Wind electricity; Nuclear electricity
H_2 physical form and uses	**6**	Liquid H_2; Gaseous H_2; Industrial use; Heat; Light-duty vehicles; Heavy-duty vehicles
Production echelon	**10**	Technical constraints; Unit size; SMR (Steam Methane Reforming); Coal gasification; Biomass gasification; Electrolysis; Onsite SMR; Onsite electrolysis; SMR with CCS (Carbon Capture & Storage); Coal gasification with CCS; Biomass gasification with CCS
Storage echelon	**5**	Technical constraints; Unit size; Liquid storage; Gaseous storage; LOHC storage
Transportation echelon	**7**	Technical constraints; Unit size; LH_2 tanker truck; LH_2 railway; LH_2 ship; GH_2 trailer; GH_2 pipeline
Distribution echelon	**5**	Technical constraints; Unit size; LH_2 tanker truck; GH_2 trailer; GH_2 pipeline
Refueling stations echelon	**2**	Unit size; Technology type
Uncertainty sources and treatment	**9**	Demand; Costs; Price/revenue; RES generation; Treatment – Scenarios; Treatment – Stochastic; Treatment – Chance-constraint; Treatment – Robust; Treatment – Fuzzy
Government intervention	**7**	CO_2 emission constraints; Taxes; Price subsidies; Capital grants; Carbon tax; Carbon budget; Procurement obligations for refueling stations/retailers
Demand features	**7**	Alternative fuels competition; Socio-economic characteristics; Penetration rate modeling; Endogenous demand; Dynamic profile; Node-based formulation; Flow-based formulation
Integration to other supply chains	**8**	Industrial H_2; Utility; Oxygen; Heat; Biomass; Electricity network; Gas network; Carbon sequestration and storage

Note: The numerical identifier of each feature is provided between brackets.

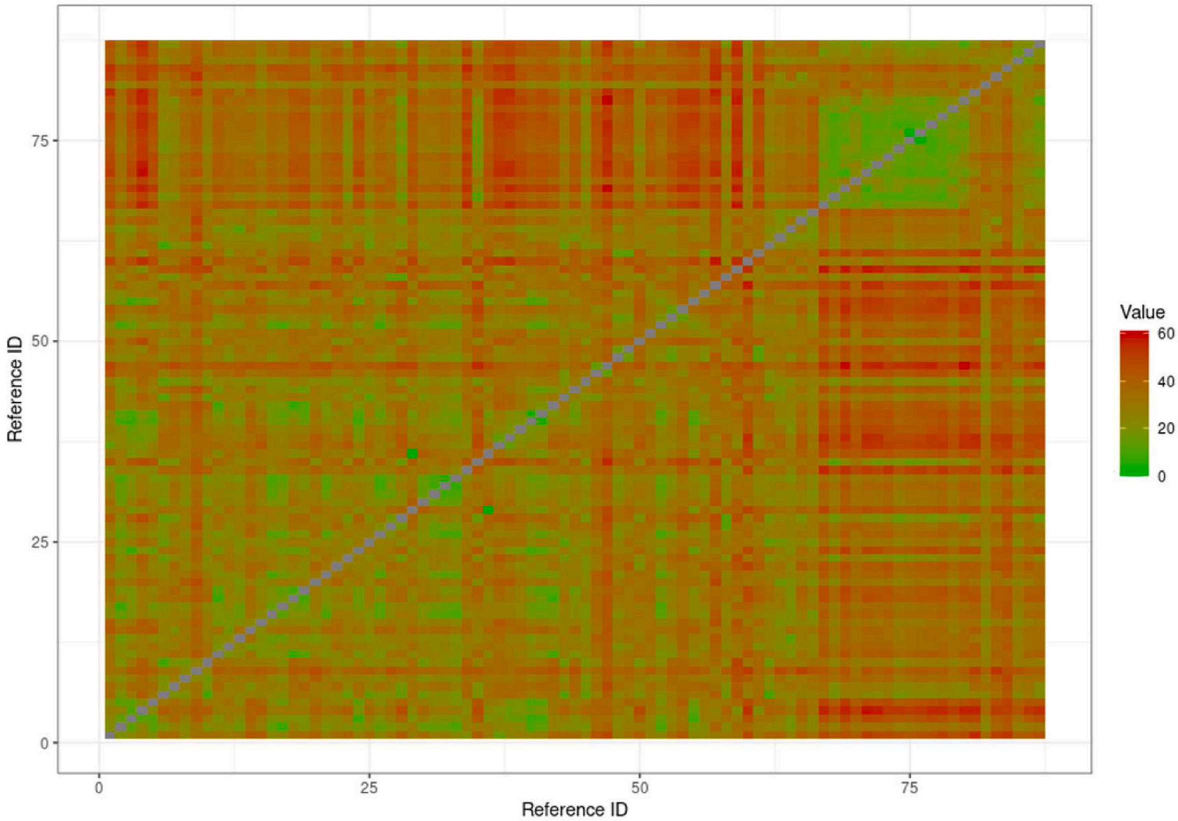

Figure A1a. Manhattan distance heat map.

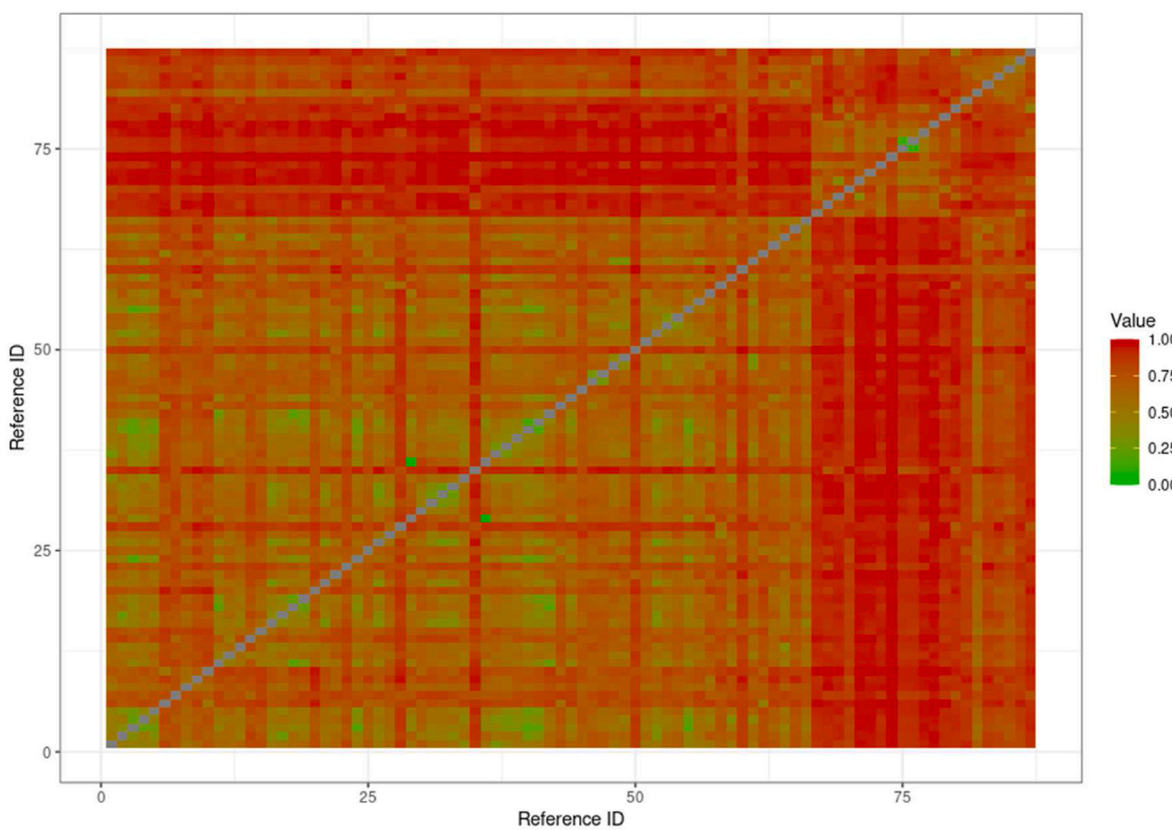

Figure A1b. **Jaccard** distance heat map.

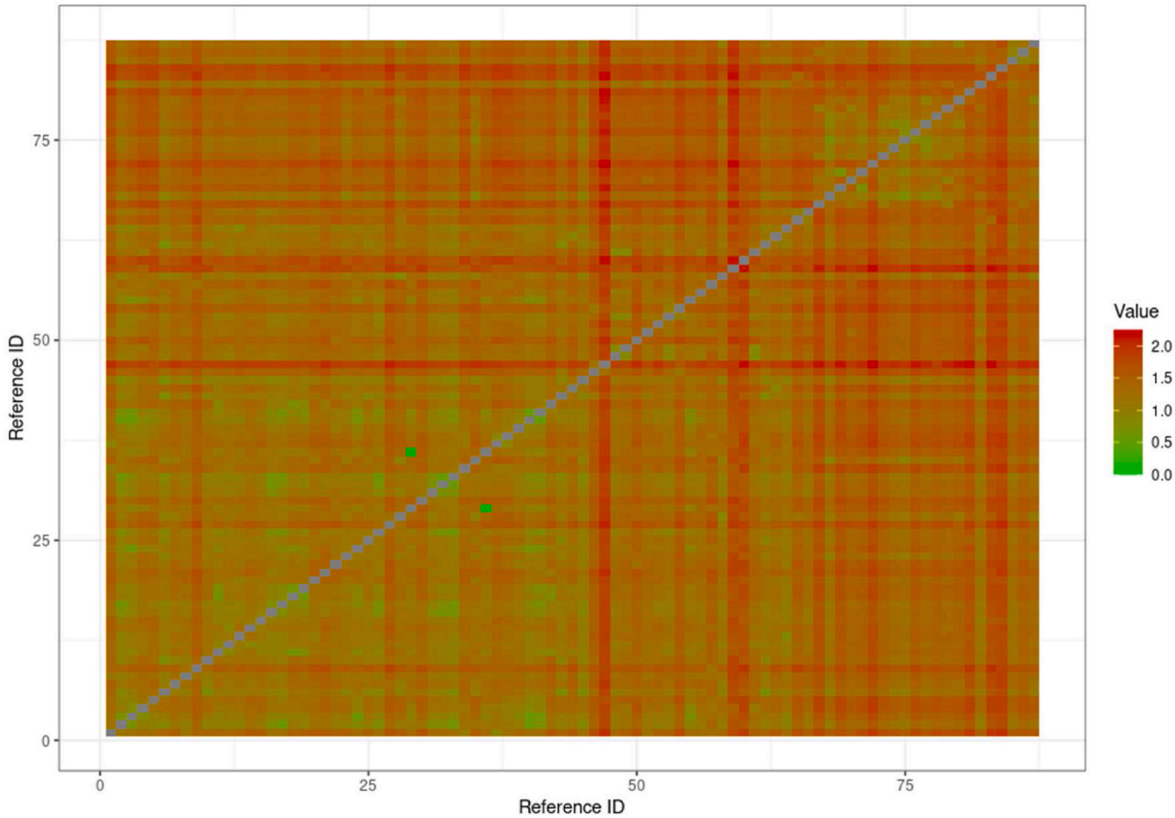

Figure A1c. Φ^2 **distance** heat map.

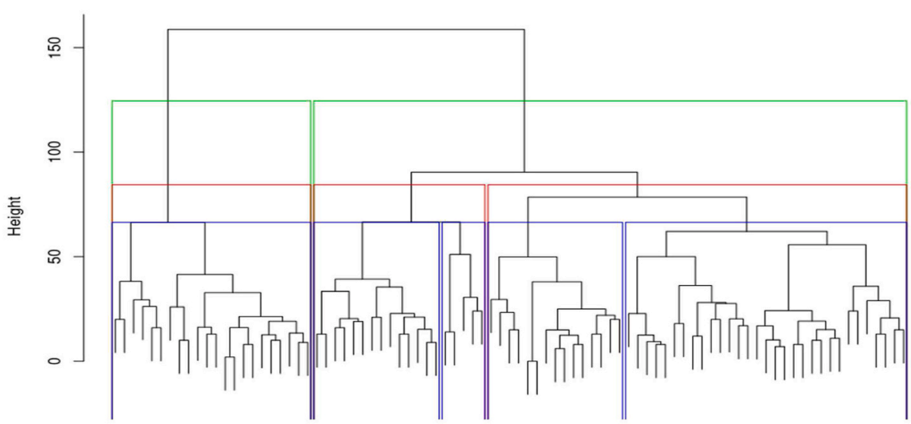

Figure A2a. Clustering dendrogram associated to the Manhattan distance metric.

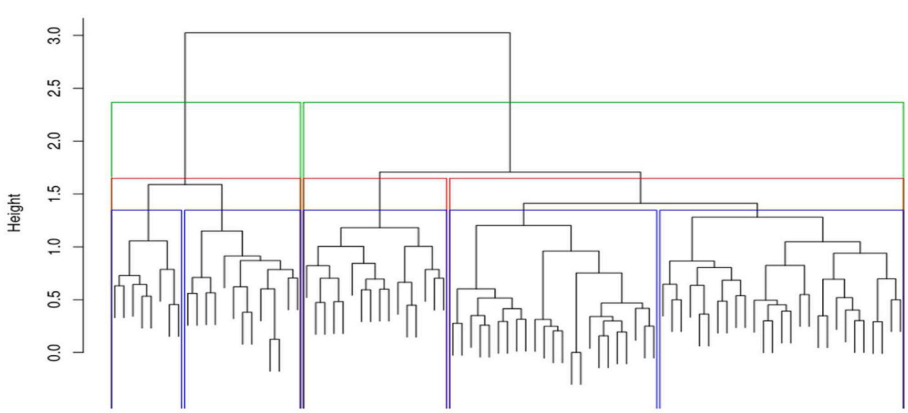

Figure A2b. Clustering dendrogram associated with the Jaccard distance metric.

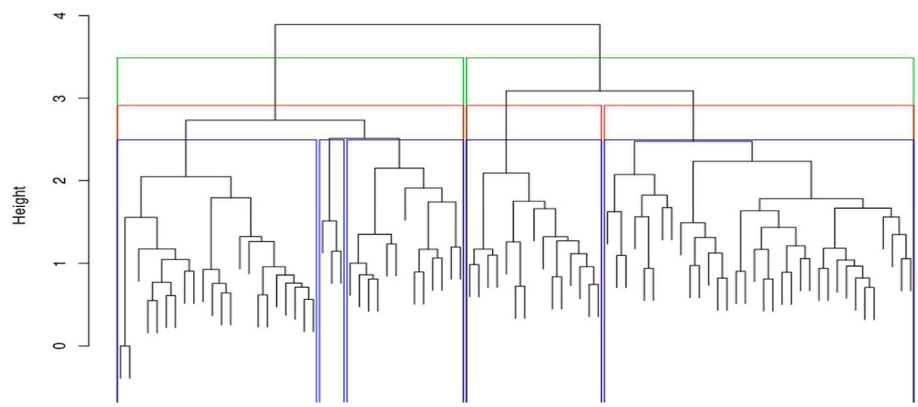

Figure A2c. Clustering dendrogram associated with the Φ^2 distance metric.

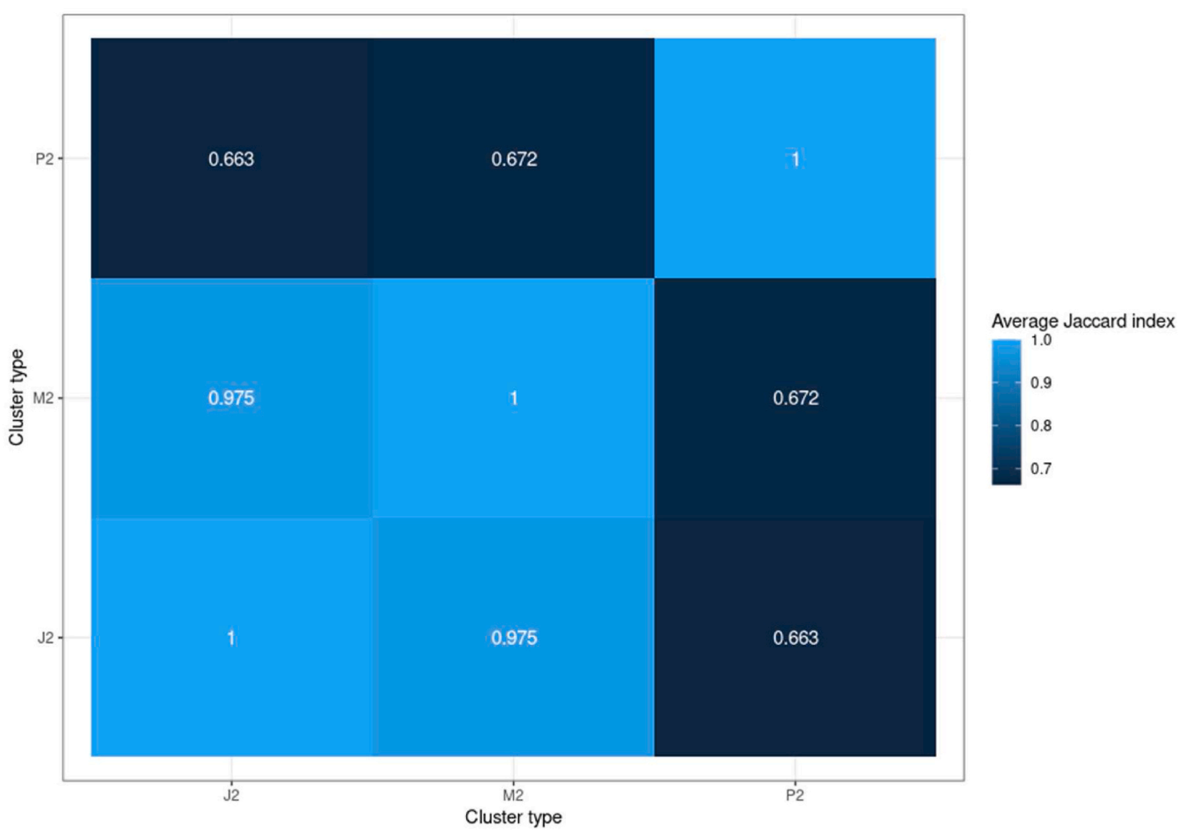

Figure A3a. Pairwise cluster Jaccard distance heat map, 2 clusters. **Note:** M2 (resp. J2 and P2) corresponds to the association of the Manhattan distance (resp. Jaccard and Φ^2 distances) with 2 clusters.

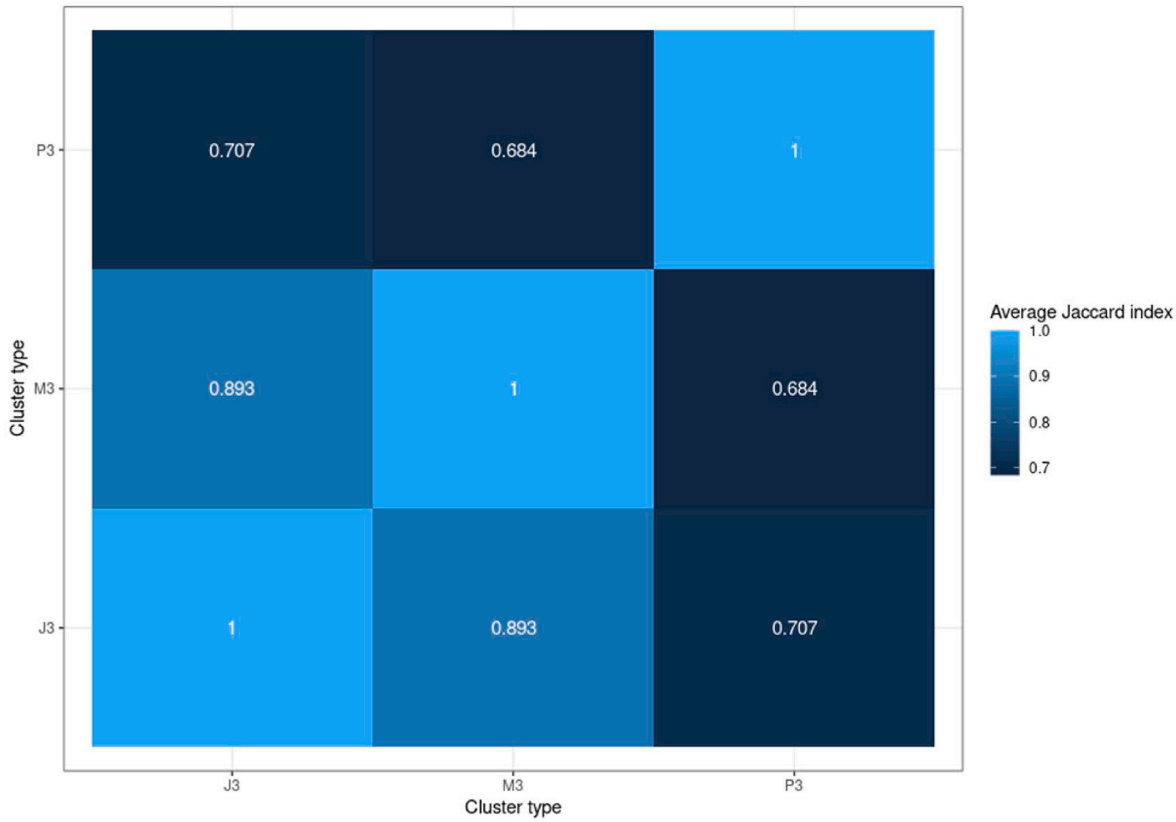

Figure A3b. Pairwise cluster Jaccard distance heat map, 3 clusters.

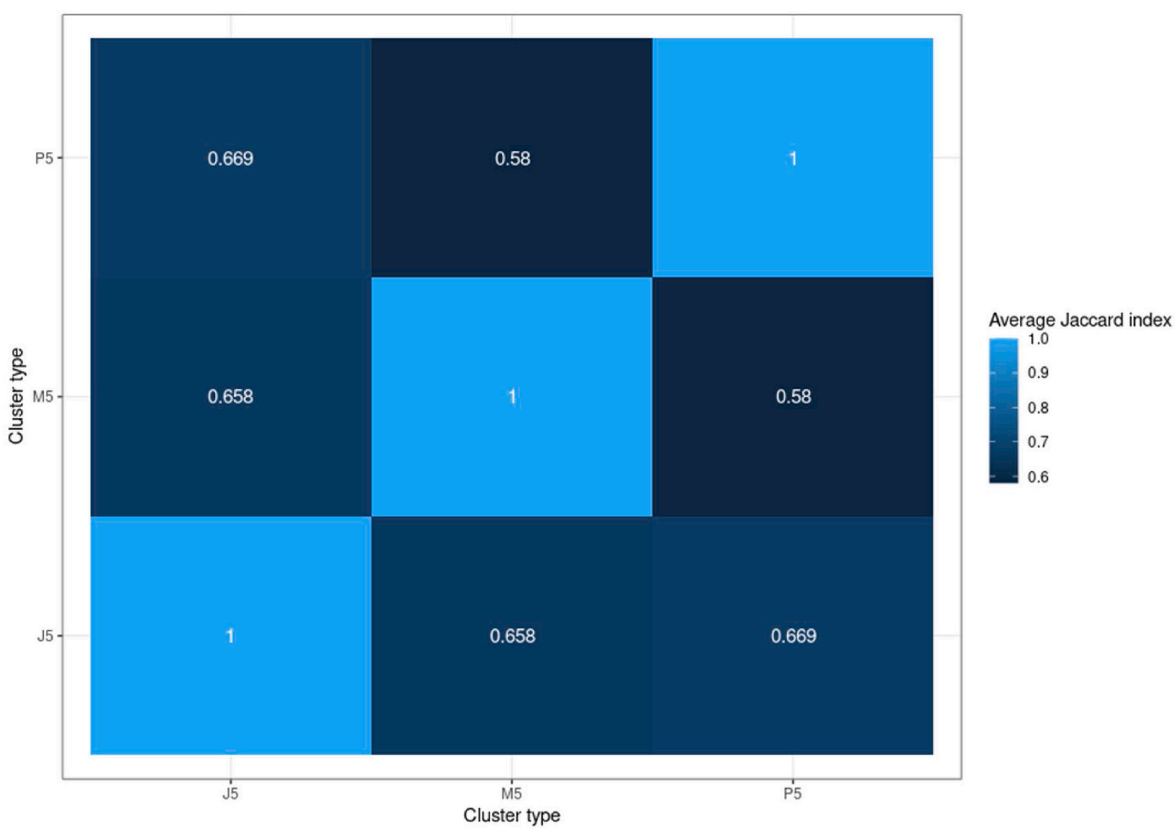

Figure A3c. Pairwise cluster Jaccard distance heat map, 5 clusters.

Appendix to 2.3.: Formal definition of clustering performance metrics.

Let us consider a pair of clusters C_k and $C_{k'}$, $1 \leq k < k' \leq K$, where K is the total number of clusters. We define $\mathscr{X}$ the set of sampled papers. We note X_k and $X_{k'}$ a pair of objects (in the present investigation, these correspond to HSC-related papers) belonging to C_k and $C_{k'}$ respectively. Then, we define the inter-cluster complete linkage and average linkage distances, noted $\delta_1^{k,k'}$ and $\delta_2^{k,k'}$, as follows:

$$\delta_1^{k,k'} = \{X_k \in C_k X_{k'} \in C_{k'}\}$$

$$\delta_2^{k,k'} = \frac{1}{|C_k||C_{k'}|} \sum_{X_k \in C_k X_{k'} \in C_{k'}} J(X_k, X_{k'})$$

Similarly, for any fixed cluster C_k, $1 \leq k \leq K$, we define the intra-cluster complete diameter distance and average diameter distance, noted Δ_1^k and Δ_2^k respectively:

$$\Delta_1^k = max\left\{J\left(X_1^k, X_2^k\right), \left(X_1^k, X_2^k\right) \in C_k \times C_k\right\}$$

$$\Delta_2^k = \frac{1}{|C_k|(|C_k|-1)} \sum_{\left(X_k^1, X_k^2\right) \in C_k X_{k'} \in C_{k'}} J\left(X_k^1, X_k^2\right)$$

The global quality of the clustering procedure increases with inter-cluster distance and decreases with intra-cluster distances. This expresses the fact that a group of observations belonging to a given cluster must share more similarities overall than with another group belonging to a different cluster. Thus, for each combination of candidate distance metric and number of clusters K, we define its performance score σ_K that we define as follows:

$$\sigma_K = \sum_{k=1}^{K} \left[\left(\frac{1}{K-1} \sum_{k'>k} \left(\frac{N_{C_k \cup C_{k'}}}{N} \right) \frac{\delta_1^{k,k'} + \delta_2^{k,k'}}{2} - \left(\frac{N_{C_k}}{N} \right) \frac{\Delta_1^k + \Delta_2^k}{2} \right) \right]$$

For any pair of clusters C_k and $C_{k'}$, $1 \leq k < k' \leq K$, $N_{C_k \cup C_{k'}}$ is equal to the cardinal of their union, while N_k corresponds to the cardinal of C_k. We easily verify that the sum of the $N_{C_k \cup C_{k'}}$, taken over all pairs of clusters (accounting for order) is equal to $(K-1)N$. The value of σ_K increases with the sum of inter-cluster distances associated with each pair of clusters, where $\delta_1^{k,k'}$ and $\delta_2^{k,k'}$ are weighted equally and decreases with the set of intra-cluster distances of each cluster. Since $0 \leq J(X_k, X_{k'}) \leq 1$, we have $-1 \leq \sigma_K \leq 1$, where σ_K increases with clustering quality. Finally, our weighting approach ensures that clusters which include a large number of observations have a stronger impact on σ_K.

Table A2a
Clustering performance metrics (2 clusters)

Distance	Cluster k	Cluster k'	$\delta_1^{k,k'}$	$\delta_2^{k,k'}$	Δ_1^k	Δ_2^k	σ_K
Manhattan	1	1	–	–	0.821	0.544	**0.0512**
	1	2	0.855	0.618	–	–	
	2	2	–	–	0.788	0.596	
Jaccard	1	1	–	–	0.821	0.547	**0.0525**
	1	2	0.855	0.618	–	–	
	2	2	–	–	0.782	0.585	
Φ^2	1	1	–	–	0.687	0.468	**0.0674**
	1	2	0.855	0.618	–	–	
	2	2	–	–	0.830	0.648	

Table A2b
Clustering performance metrics (3 clusters)

Distance	Cluster k	Cluster k'	$\delta_1^{k,k'}$	$\delta_2^{k,k'}$	Δ_1^k	Δ_2^k	σ_K
Manhattan	1	1	–	–	0.692	0.479	**0.0764**
	1	2	0.821	0.544	–	–	
	1	3	0.846	0.604	–	–	
	2	2	–	–	0.821	0.603	
	2	3	0.855	0.658	–	–	
	3	3	–	–	0.787	0.596	
Jaccard	1	1	–	–	0.790	0.498	**0.0558**
	1	2	0.821	0.547	–	–	
	1	3	0.855	0.608	–	–	
	2	2	–	–	0.760	0.580	
	2	3	0.827	0.645	–	–	
	3	3	–	–	0.782	0.585	
Φ^2	1	1	–	–	0.687	0.468	**0.0811**
	1	2	0.847	0.571	–	–	

(continued on next page)

Table A2b (*continued*)

Distance	Cluster k	Cluster k'	$\delta_1^{k,k'}$	$\delta_2^{k,k'}$	Δ_1^k	Δ_2^k	σ_K
	1	3	0.855	0.595	–	–	
	2	2	–	–	0.803	0.614	
	2	3	0.830	0.648	–	–	
	3	3	–	–	0.762	0.536	

Table A2c
Clustering performance metrics (5 clusters)

Distance	Cluster k	Cluster k'	$\delta_1^{k,k'}$	$\delta_2^{k,k'}$	Δ_1^k	Δ_2^k	σ_K
Manhattan	1	1	–	–	0.557	0.366	**0.0775**
	1	2	0.692	0.479	–	–	
	1	3	0.786	0.549	–	–	
	1	4	0.662	0.447	–	–	
	1	5	0.846	0.639	–	–	
	2	2	–	–	0.692	0.487	
	2	3	0.803	0.552	–	–	
	2	4	0.783	0.516	–	–	
	2	5	0.833	0.621	–	–	
	3	3	–	–	0.760	0.581	
	3	4	0.821	0.603	–	–	
	3	5	0.827	0.644	–	–	
	4	4	–	–	0.621	0.514	
	4	5	0.855	0.644	–	–	
	5	5	–	–	0.787	0.596	
Jaccard	1	1	–	–	0.790	0.538	**0.0875**
	1	2	0.790	0.498	–	–	
	1	3	0.821	0.587	–	–	
	1	4	0.847	0.598	–	–	
	1	5	0.855	0.637	–	–	
	2	2	–	–	0.614	0.387	
	2	3	0.786	0.524	–	–	
	2	4	0.803	0.522	–	–	
	2	5	0.841	0.580	–	–	
	3	3	–	–	0.760	0.580	
	3	4	0.804	0.628	–	–	
	3	5	0.827	0.634	–	–	
	4	4	–	–	0.737	0.568	
	4	5	0.782	0.585	–	–	
	5	5	–	–	0.658	0.496	
Φ^2	1	1	–	–	0.656	0.470	**0.0721**
	1	2	0.687	0.452	–	–	
	1	3	0.818	0.610	–	–	
	1	4	0.846	0.545	–	–	
	1	5	0.656	0.492	–	–	
	2	2	–	–	0.614	0.383	
	2	3	0.803	0.568	–	–	
	2	4	0.841	0.590	–	–	
	2	5	0.657	0.424	–	–	
	3	3	–	–	0.803	0.614	
	3	4	0.830	0.648	–	–	
	3	5	0.847	0.616	–	–	
	4	4	–	–	0.762	0.536	
	4	5	0.855	0.606	–	–	
	5	5	–	–	0.441	0.364	

Appendix to 4.1: Formal definition of the divergence and repulsion sores.

We first define $\mathscr{Y}$ as the set of methodological features. For each pair of features $(Y, Y') \in \mathscr{Y} \times \mathscr{Y}$, we note its associated modified Jaccard index $J_I(Y, Y')$ and define it as follows:

By slight abuse of notation, $Y \in X$ being true is equivalent to feature Y being included in the formulation of the paper X. The denominator is equal to the total number of papers in X which include at least one of the features Y or Y'. We define the weight ω_Y, or methodological magnitude, associated with $Y \in \mathscr{Y}$:

$$\omega_Y = \frac{\left(\sum_{k \in K}\left(\frac{1}{C_k}\sum_{X \in C_k}\mathbb{I}\{Y \in X\}\right)\right)}{\sum_{k \in K}\mathbb{I}\left\{\left(\sum_{X \in C_k}\mathbb{I}\{Y \in X\}\right) > 0\right\}}$$

The definition of ω_Y accounts for the fact that some features might be specific to a subset of clusters. We note that ω_Y is maximal when it is included in all articles of the subset of clusters where it is found, and $0 \le \omega_Y \le 1$. Finally, we define the repulsion force between for any pair $(Y, Y') \in \mathscr{Y} \times \mathscr{Y}$ as follows:

$$\sigma_{Y,Y'} = (1 - J_I(Y, Y')) \times \omega_Y \times \omega_{Y'}$$

We easily verify that $0 \leq \sigma_{Y,Y'} \leq 1$. The formulation of $\sigma_{Y,Y'}$ is inspired from the Coulomb repulsive force: for any pair of particles, the magnitude of their repulsion is proportional to the product of their individual magnitudes and is inversely proportional to their squared distance. In our case, ω_Y measures the average within-cluster proportion of articles including feature Y in their methodological framework, which approximates its relative importance in modeling choices. The parallel with the Coulomb repulsive force expresses the fact that the degree of attraction or repulsion between two features is deemed stronger if both features are frequently observed within clusters, but rarely observed together, i.e., belong to different paper clusters.

Then, for each pair of features $(Y, Y') \in \mathscr{Y} \times \mathscr{Y}$, we define its “divergence” score $\Delta_{Y,Y'} \geq 0$ as follows:

$$\Delta_{Y;Y'} = \sqrt{\sum_{y \in \mathscr{Y}, y \neq (Y,Y')} \left(\sigma_{y,Y} - \sigma_{y,Y'}\right)^2}$$

Finally, we associate to each feature $Y \in \mathscr{Y}$ its “repulsion” score ρ_Y, defined as the geometric mean of divergence computed over each pair $(Y, Y') \in \mathscr{Y} \times \mathscr{Y}$:

The use of the geometric mean ensures the influence of extreme $\Delta_{Y,Y'}$ values is smoothed out and ρ_Y better captures the central tendency of the pairwise divergence scores associated with Y. We note that $\rho_Y = 0$ if there exists at least one pair of features $(Y, Y') \in \mathscr{Y} \times \mathscr{Y}$ such that $\forall y \in \mathscr{Y}, y \neq (Y, Y')$, $\sigma_{y,Y} = \sigma_{y,Y'}$. This would imply that features Y and Y' always occur together, which is indicative of a strong dependence between these features in terms of modeling choices.

The cosine between covariates and the canonical components can be interpreted as their covariance (not their correlation as the variables are not centered). Yet, a variable which has maximal negative covariance with a canonical component accurately predicts its behavior, so it is equivalent to having maximal positive covariance. Thus, we square the cosine to obtain only positive values. Finally, in order to account for the share of the original variance explained by each canonical component, we weight the covariances by the associated eigenvalue divided by the sum of eigenvalues.

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