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A Systematic Review of Bilevel Optimization Methods Using a Meta-Synthesis Approach: Algorithms, Complexity, and Applications in Resource Allocation

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A B S T R A C T

This study seeks to provide a comprehensive overview of bilevel optimization methods through a systematic review and meta-synthesis of the literature, focusing on solution algorithms, computational complexity, and applications in resource allocation. Using a meta-synthesis approach and a systematic literature review, the study identifies 64 credible sources from Scopus, Web of Science, and Google Scholar and analyzes them within four main streams: (1) theory and exact and metaheuristic solution algorithms, (2) uncertainty modeling and robust optimization, (3) policy applications in energy and supply chains, and (4) multifollower structures and security games. The analytical criteria include computational complexity, the type of mathematical reformulation (KKT/MPCC), and the approach to uncertainty. Exact methods based on reformulations using the Karush–Kuhn–Tucker (KKT) optimality conditions and mathematical programs with complementarity constraints (MPCC) are highly effective for convex problems, but face computational challenges in nonconvex or large-scale problems. Continuous regularization and smoothing methods strike an appropriate balance between accuracy and scalability. Regarding uncertainty, scenario-based approaches and the conditional value-at-risk (CVaR) measure are less conservative than classical robust optimization and are more suitable for resource allocation problems involving discrete scenarios. A significant research gap was also identified in simultaneously integrating heterogeneous multifollower structures with downside risk control in science and technology policymaking. By proposing a conceptual framework and identifying research gaps, this study paves the way for developing robust bilevel optimization models with a multifollower approach. The proposed framework can serve as a roadmap for researchers working on optimization and its applications in national resource allocation.

Keywords: *Bilevel optimization, KKT optimality conditions, mathematical program with complementarity constraints (MPCC), conditional value-at-risk (CVaR), meta-synthesis.*

1. Introduction

The allocation of scarce resources is a central problem in public policy, industrial strategy, infrastructure planning, and research and development (R&D) management. These decisions are rarely made within a single, unified decision-making structure. In many real settings, a central authority first determines budgets, incentives, capacities, or regulatory parameters, after which decentralized organizations respond according to their own objectives and constraints. This hierarchy creates an interdependent decision process in which the effectiveness of the upper-level decision depends on the lower-level response. Bilevel optimization provides a formal representation of this process by embedding the optimization problem of one decision maker within that of another. Its intellectual foundations can be traced to Stackelberg's leader–follower model, while subsequent studies established bilevel programming as a distinct field of mathematical optimization (Bard, 1991; Ben-Ayed & Blair, 1990; von Stackelberg, 2011). Early surveys clarified its general formulation, theoretical properties, and principal application areas, laying the foundation for contemporary research on hierarchical decision systems (Colson et al., 2005, 2007).

The attraction of bilevel optimization lies in its capacity to represent strategic dependence explicitly. The leader selects a decision while anticipating that the follower will solve a separate optimization problem in response; consequently, the feasible set of the leader is implicitly determined by the follower's optimal-solution mapping. This nested structure distinguishes bilevel problems from conventional mathematical programs and explains much of their computational difficulty. Even linear bilevel programs are generally difficult to solve, and the introduction of integer variables, nonlinear relationships, multiple followers, or uncertainty further increases complexity. Research has therefore developed along two connected lines: a theoretical line concerned with mathematical structure, optimality conditions, and reformulation, and an algorithmic line concerned with exact, approximate, and evolutionary methods. Comprehensive reviews have documented the transition from classical formulations to increasingly diverse computational approaches and applications (Dempe & Zemkoho, 2020; Kleinert et al., 2021; Sinha et al., 2018).

One of the most influential solution strategies replaces the follower's problem with its Karush–Kuhn–Tucker optimality conditions, thereby transforming the bilevel model into a single-level mathematical program with complementarity constraints (MPCC). The Fortuny-Amat and McCarl formulation made it possible to linearize complementarity conditions through binary variables and a sufficiently large constant, and it remains widely used in mixed-integer implementations (Fortuny-Amat & McCarl, 1981). However, a KKT-based replacement is exact only under appropriate assumptions, particularly lower-level convexity and suitable constraint qualifications. Treating it as universally valid can therefore produce misleading solutions in nonconvex settings (Dempe & Dutta, 2012). MPCC formulations also violate standard constraint qualifications at feasible points, creating numerical and theoretical complications that require specialized analysis (Luo et al., 1996). Regularization methods alleviate these difficulties by replacing exact complementarity with a parameterized approximation, while branch-and-bound procedures exploit the geometry and discrete structure of particular bilevel models (Hansen et al., 1992; Scholtes, 2001).

The diversity of bilevel problems has encouraged the development of solution approaches beyond direct KKT/MPCC reformulation. Exact algorithms include branch-and-bound, branch-and-cut, decomposition, and value-function methods, whereas approximate approaches include nested optimization, evolutionary computation, coevolution, penalties, smoothing, and hybrid methods. Metaheuristics are especially useful when the follower's problem is nonconvex, discontinuous, black-box, or otherwise unsuitable for classical optimality-based reformulation, although reproducibility, stopping criteria, computational budgets, and the verification of lower-level optimality remain persistent concerns (Camacho-Vallejo et al., 2023). Recent work on complementarity-constrained optimization has also refined regularization, smoothing, and penalty strategies and clarified their numerical behavior (Nurkanović et al., 2024). These developments show that method selection cannot be separated from problem structure: convexity, variable type, dimensionality, follower multiplicity, and uncertainty jointly determine which algorithm is defensible and computationally practical.

Uncertainty introduces another decisive layer of complexity. In a hierarchical problem, uncertain coefficients may affect the leader, the follower, the link between their decisions, or the information available at each level. A decision that appears optimal under nominal parameters may become infeasible, inefficient, or strategically unstable when costs, demand, policy implementation, or actor capacities deviate from their expected values. Stochastic programming

represents uncertainty through probability distributions or scenarios and supports decisions that account for expected performance across alternative futures (Shapiro et al., 2009). Robust optimization instead protects decisions against adverse realizations within a prescribed uncertainty set. Foundational work on robust convex optimization and its subsequent generalization established tractable counterparts for broad classes of uncertain problems (Ben-Tal et al., 2009; Ben-Tal & Nemirovski, 1998). Budgeted uncertainty and the concept of the price of robustness further provided a means of balancing protection against conservatism (Bertsimas et al., 2011; Bertsimas & Sim, 2004), while practical guidance has helped translate robust formulations into implementable models (Gorissen et al., 2015).

Uncertainty in bilevel optimization is more intricate than in single-level models because the leader must anticipate how uncertain conditions alter both the follower's feasible set and its optimal reaction. The timing of information, the distribution of uncertainty between levels, and the leader's attitude toward risk can produce substantially different formulations and outcomes (Beck et al., 2023). Conditional value-at-risk (CVaR) offers a particularly useful means of controlling downside exposure. Rather than optimizing only expected outcomes or protecting against an absolute worst case, CVaR measures the mean loss in the adverse tail of a distribution (Rockafellar & Uryasev, 2000, 2002). In resource-allocation settings with discrete scenarios, this property enables decision makers to control severe but plausible losses without necessarily adopting the excessive conservatism associated with worst-case robust solutions. Integrating CVaR into the leader's objective can therefore connect resource efficiency with explicit risk tolerance, although its use in heterogeneous multifollower policy models remains limited.

Applications demonstrate the practical value of hierarchical modeling. In environmental and energy policy, bilevel formulations have been used to determine renewable-energy subsidies, carbon taxes, and emission-sensitive incentives while anticipating the operational responses of firms or energy systems (Almutairi & Elhedhli, 2014; Martelli et al., 2020). In green supply chains, Stackelberg and bilevel models capture how regulation affects procurement, production, and interorganizational relationships (Bao & Zhang, 2018). Water allocation models similarly represent the interaction between a central authority and subordinate users within a hierarchical system (Calvete et al., 2023). Government subsidy policy in green product markets and dynamic R&D spillover games further illustrate how leader decisions can influence investment, pricing, information use, and market evolution (Chen et al., 2024; Long & Zheng, 2025). A recent sustainability-oriented review confirms that bilevel optimization now supports a wide range of policy applications, while also identifying the need for richer behavioral, environmental, and institutional representations (Caselli et al., 2026).

Resource allocation becomes still more challenging when several followers respond to the leader. A single representative follower can conceal major differences in objectives, costs, capacities, and institutional roles. Multifollower models instead represent decentralized reactions explicitly and may incorporate cooperative, competitive, or equilibrium relationships among actors. In industrial resource coordination, such models can support transitions among products or technologies when several operational units compete for shared capacity (Khorramfar et al., 2024). The broader literature on multileader–multifollower games shows that the existence, selection, and computation of equilibria depend strongly on how followers interact and what information they possess (Aussel & Svensson, 2020). Stackelberg security games provide another mature application in which a leader allocates limited defensive resources while anticipating strategic responses (Bucarey et al., 2021; Casorrán et al., 2019). These studies demonstrate that follower multiplicity is a substantive feature of the decision environment rather than a minor technical extension.

The same insight applies to R&D and innovation portfolios. Organizations must distribute limited funds across projects with different expected benefits, technological dependencies, time profiles, and risks. Classical portfolio management emphasizes strategic balance, project interdependence, and alignment with organizational objectives (Cooper et al., 2001; Stummer & Heidenberger, 2003). Optimization models have extended this perspective by incorporating endogenous uncertainty, fuzzy constraints, imprecise information, and multiple objectives (Hassanzadeh et al., 2014; Perez & Gomez, 2016; Solak et al., 2010). A multifollower bilevel formulation has also been applied to R&D portfolio selection in a pharmaceutical holding company, showing how central portfolio decisions can be linked to the responses of subordinate units (Salehi et al., 2023). Nevertheless, much of this literature remains organization-specific and does not fully capture national-level allocation among heterogeneous implementing actors operating under shared institutional constraints.

At the national level, innovation cannot be understood as a linear progression from scientific discovery to commercial output. National innovation system theory conceptualizes innovation as the product of relationships among firms, universities, government agencies, financial structures, and supporting institutions (Edquist, 1997; Freeman, 1995; Lundvall, 1992; Nelson, 1993). Evolutionary accounts emphasize learning, selection, institutional change, and cumulative capability development (Fagerberg et al., 2005; Metcalfe, 1995). The triple-helix perspective highlights university–industry–government interaction (Etzkowitz & Leydesdorff, 2000), while research on the historical development of national systems, competitive advantage, and innovation processes shows that national performance depends on coordinated institutions rather than isolated investments (Kline & Rosenberg, 1986; Mowery, 1992; Porter, 1990; Rothwell, 1994). Open innovation and technology-transfer research further demonstrate that knowledge moves through networks, intermediaries, and organizational boundaries (Bozeman, 2000; Chesbrough, 2003).

These systemic perspectives have direct implications for resource allocation. Additional funding does not automatically produce proportional outcomes because actors differ in their ability to recognize, assimilate, transform, and exploit knowledge. The concept of absorptive capacity explains why identical resource allocations can generate different results across organizations (Cohen & Levinthal, 1990; Zahra & George, 2002). Weak coordination and insufficient investment in intermediate stages may also create a "valley of death" between research and commercialization (Beard et al., 2009). Consequently, a national policy model should account for endogenous implementation capacity, complementarity among programs, and the gap between nominal allocation and effective use. It should also distinguish universities and research institutions, technology firms, laboratories and pilot facilities, and regulatory or market intermediaries, because each class of actor converts resources into outcomes through a different technological and institutional process.

Iran's nanotechnology system provides a relevant setting for examining these issues. Iran has developed substantial scientific capacity and has achieved a prominent position in nanotechnology publication output (Guan & Ma, 2007; Statnano, 2025). Domestic research has evaluated national nanotechnology policies through outcome and impact indicators and has examined the alignment of long-term programs with socioeconomic and mission-oriented objectives (Sahebinejad & Ali, 2024; Soltani et al., 2020). Other studies have proposed national planning models based on evolving governmental roles, simulated the Iranian nanotechnology innovation network using agent-based methods and absorptive-capacity concepts, and designed innovation-survey frameworks suited to the field (Alizade & Tabatabaiean, 2015; Ghazinoory et al., 2009; Mahmoudzadeh & Alborzi, 2017). Recent analysis has also addressed market-shaping policies and the institutional measures needed to create and expand demand for nanotechnology products (Fartash et al., 2025). Together, these studies provide rich diagnostic and policy knowledge, but they do not offer a unified optimization framework that links national allocations to heterogeneous actor responses, implementation capacity, uncertainty, and downside risk.

The literature therefore reveals a fragmented pattern of progress. Bilevel optimization provides rigorous leader–follower formulations and increasingly sophisticated algorithms; robust and stochastic optimization provide tools for uncertainty; CVaR provides explicit control of severe losses; multifollower models represent heterogeneous responses; and innovation-system research explains institutional interaction and absorptive capacity. Yet these elements are seldom integrated within one national science and technology policy model. Existing application studies commonly emphasize a single follower, nominal allocation, one source of uncertainty, or a specific industrial setting. They rarely model the implementation gap as an endogenous outcome, and even more rarely combine heterogeneous followers with CVaR-based downside risk control. A systematic synthesis is therefore needed to compare solution approaches across their mathematical assumptions, clarify the circumstances in which KKT/MPCC, exact, regularization, stochastic, robust, or metaheuristic methods are appropriate, and connect these methods to the substantive requirements of national resource allocation.

Accordingly, this study aims to systematically review and meta-synthesize the literature on bilevel optimization in order to classify its algorithms and computational characteristics, compare approaches to uncertainty and risk, identify gaps in resource-allocation applications, and develop an integrated conceptual framework for robust national science and technology resource allocation with heterogeneous multiple followers, endogenous absorptive capacity, an explicit implementation gap, and CVaR-based downside risk control.

2. Methods and Materials

In terms of its purpose, this research is a systematic review adopting a meta-synthesis approach. Meta-synthesis goes beyond merely summarizing the findings of previous studies to analyze, synthesize, and interpret them in an integrated manner, fundamentally distinguishing it from traditional narrative reviews. This section describes the research design, review questions, search strategy, inclusion and exclusion criteria, source selection process, and coding and analytical framework.

2.1. Research Design

The meta-synthesis approach in this study is based on four main steps: (1) defining the review questions, (2) systematically searching for and screening sources, (3) coding and classifying findings into the main streams, and (4) critically synthesizing the findings and identifying research gaps. This design follows the common approach in systematic reviews of bilevel optimization, in which previous studies are compared and synthesized according to methodological criteria, the type of uncertainty modeling, and the leader–follower structure (Beck et al., 2023; Caselli et al., 2026; Kleinert et al., 2021).

2.2. Systematic Review Questions

This meta-synthesis seeks to answer three main questions:

How can bilevel optimization algorithms and solution methods be classified, and what advantages and limitations does each category exhibit in addressing computational complexity? (Ben-Ayed & Blair, 1990; Camacho-Vallejo et al., 2023; Colson et al., 2005).

How do approaches to uncertainty in bilevel optimization—stochastic, robust, and CVaR-based—compare, and which is more suitable for resource allocation problems involving discrete scenarios? (Beck et al., 2023; Rockafellar & Uryasev, 2000, 2002; Shapiro et al., 2009).

What research gaps exist in simultaneously integrating heterogeneous multifollower structures, downside risk control, and applications in science and technology policymaking? (Beck et al., 2023; Khorramfar et al., 2024; Nurkanović et al., 2024).

2.3. Search Strategy

The sources for this meta-synthesis were identified through targeted searches in three citation databases: Scopus, Web of Science, and Google Scholar. Combinations of search terms included “bilevel optimization,” “hierarchical programming,” “robust optimization,” “conditional value-at-risk,” “national innovation system,” and “nanotechnology policymaking,” along with their Persian equivalents. The search period primarily covered the past decade, although foundational classical works, such as von Stackelberg’s original formulation (von Stackelberg, 2011) and foundational papers on KKT and MPCC (Fortuny-Amat & McCarl, 1981; Luo et al., 1996), were also included in the analysis when necessary. In addition to academic sources, official and statistical reports on Iran’s nanotechnology innovation system, including STATNANO reports and official media coverage, were considered as the study’s application context (Statnano, 2025).

- **Inclusion and Exclusion Criteria**

The identified sources were screened using two main criteria:

Inclusion criterion: Direct relevance to the leader–follower structure or the resource allocation problem; publication in reputable, peer-reviewed journals or publications.

Exclusion criterion: Studies lacking an explicit mathematical formulation; purely descriptive articles unrelated to bilevel optimization; and nonacademic sources or sources lacking publisher credibility.

2.4. Source Selection Process

Source selection proceeded in several stages. First, the initial search identified a broad range of studies. Titles and abstracts were then screened against the inclusion and exclusion criteria. Next, the full texts of selected sources were examined, and those without direct relevance were excluded. Ultimately, 64 sources were selected for the final analysis.

2.5. Coding and Analytical Framework

The selected sources were classified into four main streams forming the basis of the meta-synthesis:

Theory and solution algorithms for bilevel optimization: Mathematical formulation, computational complexity, KKT conditions and MPCC reformulation, regularization and smoothing methods, and exact and metaheuristic solution methods (Bard, 1991; Ben-Ayed & Blair, 1990; Camacho-Vallejo et al., 2023; Colson et al., 2005, 2007; Dempe & Dutta, 2012; Fortuny-Amat & McCarl, 1981; Hansen et al., 1992; Kleinert et al., 2021; Luo

et al., 1996; Nurkanović et al., 2024; Scholtes, 2001; Sinha et al., 2018).

Uncertainty, robustness, and risk: Stochastic and robust optimization, the CVaR measure, and its applications in bilevel optimization (Beck et al., 2023; Ben-Tal et al., 2009; Bertsimas et al., 2011; Bertsimas & Sim, 2004; Rockafellar & Uryasev, 2000, 2002; Shapiro et al., 2009).

Policy, energy, and environmental applications: Resource allocation in energy, supply chains, and water allocation (Almutairi & Elhedhli, 2014; Bao & Zhang, 2018; Calvete et al., 2023; Caselli et al., 2026; Martelli et al., 2020).

Multifollower structures and security games: Multifollower models in resource allocation and Stackelberg security games (Aussel & Svensson, 2020; Bucarey et al., 2021; Casorrán et al., 2019; Khorramfar et al., 2024; Nurkanović et al., 2024).

The comparison criteria within each stream include variable type (continuous/integer), number of followers (single follower/multiple followers), uncertainty structure (deterministic/stochastic/robust), risk measure (CVaR/no risk measure), and type of mathematical reformulation (KKT/MPCC or other).

3. Findings and Results

This section presents the findings from the analysis of 69 selected sources in five subsections: (3.1) quantitative analysis of trends; (3.2) a novel four-dimensional classification; (3.3) systematic review of the four main streams; (3.4) a decision tree for selecting a solution method; (3.5) critical synthesis and interpretive contradictions; (3.6) research gaps; and (3.7) an integrated conceptual framework.

3.1. Quantitative Analysis of Literature Trends

The quantitative analysis of 64 selected sources provides a clear picture of the literature's evolution. In terms of temporal distribution, more than 60% of the sources belong to the past decade (2015–2025). In terms of thematic distribution, 22 sources (32%) address theory and algorithms, 12 sources (18%) address uncertainty and robustness, 18 sources (26%) address policy and energy applications, and 17 sources (24%) address multifollower structures and security games.

Regarding coverage of key features, 26 sources (38%) address uncertainty (stochastic or robust), 15 sources (22%) model a multifollower structure, 10 sources (14%) use the CVaR risk measure, and 6 sources (8%) simultaneously incorporate multiple followers and CVaR. No source simultaneously models all four features: heterogeneous multiple followers, CVaR, endogenous absorptive capacity, and the implementation gap.

This quantitative analysis numerically confirms the principal gap: the simultaneous intersection of heterogeneous multiple followers and downside risk control in science and technology policymaking remains an unaddressed area in the literature.

3.2. A Novel Four-Dimensional Classification of Bilevel Methods

Based on the analysis of 64 sources, a four-dimensional classification is proposed that goes beyond existing two-dimensional classifications (Beck et al., 2023; Kleinert et al., 2021). This classification combines four independent mathematical dimensions:

Dimension 1: Lower-level convexity. Lower-level convexity is a necessary condition for the validity of the KKT reformulation (Dempe & Dutta, 2012). In the literature, 55% of problems are convex and 45% are nonconvex.

Dimension 2: Decision variable type. The presence of integer variables increases computational complexity (Kleinert et al., 2021). In the literature, 48% of problems are continuous and 52% involve integer or mixed variables.

Dimension 3: Uncertainty structure. Problems are divided into four categories: deterministic, stochastic, robust, and CVaR-based. In the literature, 62% are deterministic, 18% stochastic, 12% robust, and 8% CVaR-based.

Dimension 4: Number and heterogeneity of followers. In the literature, 68% of problems involve a single follower, 20% involve homogeneous multiple followers, and only 12% involve heterogeneous multiple followers (Aussel & Svensson, 2020; Khorramfar et al., 2024).

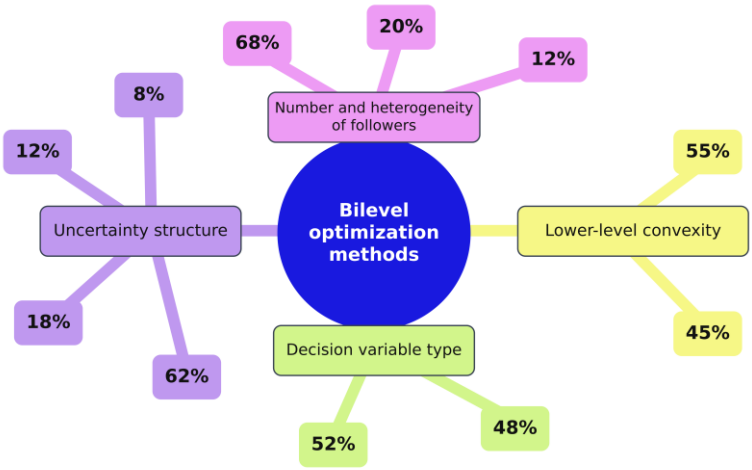
Table 1

Four-Dimensional Classification of Bilevel Methods

Dimension	Categories	Frequency in the literature	Key source
Lower-level convexity	Convex / nonconvex	55% / 45%	(Dempe & Dutta, 2012)
Variable type	Continuous / integer / mixed	48% / 52%	(Kleinert et al., 2021)
Uncertainty structure	Deterministic / stochastic / robust / CVaR	62% / 18% / 12% / 8%	(Beck et al., 2023; Rockafellar & Uryasev, 2000)
Number of followers	Single follower / homogeneous multiple followers / heterogeneous multiple followers	68% / 20% / 12%	(Aussel & Svensson, 2020; Khorramfar et al., 2024)

Figure 1

Four-Dimensional Classification of Bilevel Optimization Methods



3.3. Systematic Review of the Four Main Streams

3.3.1. Stream 1: Theory and Solution Algorithms for Bilevel Optimization

Mathematical formulation and computational complexity. The conceptual origins date back to Stackelberg duopoly competition (von Stackelberg, 2011). Its modern formulation emerged in the 1970s (Colson et al., 2005, 2007). Colson, Marcotte, and Savard define the problem as minimizing an objective function over the graph of the solution-set mapping of a parametric problem (Colson et al., 2005). Dempe and Zemkoho present the general formulation with an upper-level variable (x) and a lower-level variable (y) (Dempe & Zemkoho, 2020). Sinha, Malo, and Deb show that the principal complexity arises from the implicit dependence of the upper-level feasible region on the lower-level optimal solution set (Sinha et al., 2018). Ben-Ayed and Blair demonstrated that even linear bilevel problems are computationally difficult (Ben-Ayed & Blair, 1990). Bard showed that an optimal solution, if one exists, lies at a vertex of the polyhedral upper-level feasible region (Bard, 1991).

KKT conditions and MPCC reformulation. Fortuny-Amat and McCarl linearized the complementarity constraints arising from KKT using binary variables and a large constant M (Fortuny-Amat & McCarl, 1981). Dempe and Dutta showed that the validity of this substitution depends on the convexity of the follower's problem and the satisfaction of a constraint qualification (Dempe & Dutta, 2012). The principal challenge is the irregularity of the MPCC feasible region at points where several complementarity constraints are simultaneously active (Dempe & Dutta, 2012). Luo, Pang, and Ralph also presented a comprehensive framework for mathematical programs with equilibrium constraints (Luo et al., 1996).

Regularization and smoothing methods. Scholtes introduced a global regularization scheme in which an exact complementarity constraint is replaced by an approximate inequality and a threshold parameter (Scholtes, 2001). Nurkanović et al. divided this family into three branches—

regularization, smoothing, and penalty methods—and showed that regularization methods offer better numerical accuracy and stability (Nurkanović et al., 2024).

Exact solution methods. Kleinert et al. classified exact methods into three subgroups: branch-and-bound, branch-and-cut, and Benders decomposition (Kleinert et al., 2021). Hansen et al. developed specialized branch-and-bound rules for linear bilevel programming (Hansen et al., 1992).

Metaheuristic methods. Camacho-Vallejo et al. identified three dominant frameworks: nested, single-level reformulation, and coevolutionary approaches (Camacho-Vallejo et al., 2023). Their study warns that many studies have shortcomings in reproducibility (Camacho-Vallejo et al., 2023).

3.3.2. Stream 2: Uncertainty, Robustness, and Risk

Uncertainty in bilevel optimization. Beck, Ljubić, and Schmidt show that sources of uncertainty in bilevel problems are more diverse than in single-level problems (Beck et al., 2023). Shapiro et al. presented the foundations of stochastic programming (Shapiro et al., 2009). Ben-Tal, El Ghaoui, and Nemirovski established the foundations of robust optimization (Ben-Tal et al., 2009). Ben-Tal and Nemirovski had previously formulated robust convex optimization (Ben-Tal & Nemirovski, 1998). Bertsimas and Sim introduced the concept of the "price of robustness" (Bertsimas & Sim, 2004). Bertsimas, Brown, and Caramanis provided a comprehensive review (Bertsimas et al., 2011). Gorissen et al. developed a practical guide (Gorissen et al., 2015).

The CVaR measure. Rockafellar and Uryasev defined CVaR as the average loss in the worst-case tail (Rockafellar & Uryasev, 2000) and extended it to general distributions (Rockafellar & Uryasev, 2002). In bilevel optimization, incorporating CVaR enables the simultaneous control of expected value and tail risk (Beck et al., 2023).

3.3.3. Stream 3: Policy, Energy, and Environmental Applications

Martelli et al. designed a bilevel model of subsidies and carbon taxation (Martelli et al., 2020). Almutairi and Elhedhli formulated a carbon tax based on the emission factor (Almutairi & Elhedhli, 2014). Bao and Zhang developed a multiperiod Stackelberg game for green procurement (Bao & Zhang, 2018). Caselli et al. provided a comprehensive review of sustainability applications (Caselli et al., 2026). Calvete et al. developed a decision-support tool for water allocation (Calvete et al., 2023). Chen et al. presented a Stackelberg game analysis of government subsidy policy in the green product market (Chen et al., 2024), and Long and Zheng examined the dynamic complexity of a Stackelberg–Bertrand game with one-way R&D spillovers and government subsidies (Long & Zheng, 2025).

In R&D portfolio management, Salehi et al. presented a multifollower bilevel model for the R&D portfolio of a pharmaceutical holding company (Salehi et al., 2023). Solak et al. (Solak et al., 2010), Stummer and Heidenberger (Stummer & Heidenberger, 2003), Hassanzadeh et al. (Hassanzadeh et al., 2014), and Perez and Gomez (Perez & Gomez, 2016) addressed various dimensions of uncertainty and multiple objectives in public and organizational R&D portfolio management. Cooper, Edgett, and Kleinschmidt also presented the classical framework for new product development portfolio management (Cooper et al., 2001).

3.3.4. Stream 4: Multifollower Structures and Security Games

Khorramfar et al. presented a multifollower bilevel model for resource allocation in a semiconductor firm (Khorramfar et al., 2024). Aussel and Svensson developed the theoretical framework for multileader–multifollower games (Aussel & Svensson, 2020). Bucarey et al. (Bucarey et al., 2021) and Casorrán et al. (Casorrán et al., 2019) examined Stackelberg security games.

3.3.5. Links to National Innovation System Theory and Absorptive Capacity

From a theoretical perspective, the national innovation system is an analytical framework that views innovation as the outcome of interactions among firms, universities, government institutions, and supporting infrastructure within an economic and institutional system, rather than as a linear product of research (Edquist, 1997; Etzkowitz & Leydesdorff, 2000; Freeman, 1995; Lundvall, 1992; Metcalfe, 1995; Nelson, 1993). Mowery (Mowery, 1992), Porter (Porter, 1990), Kline and Rosenberg (Kline & Rosenberg, 1986), Chesbrough (Chesbrough, 2003), Rothwell (Rothwell, 1994), and Bozeman (Bozeman, 2000) also examined various dimensions of innovation, technology transfer, and public policy. Fagerberg, Mowery, and Nelson provided a comprehensive reference in this field (Fagerberg et al., 2005).

At the firm or organizational level, Cohen and Levinthal introduced absorptive capacity as an organization's ability to

recognize, assimilate, and commercially apply external knowledge and resources (Cohen & Levinthal, 1990), and Zahra and George distinguished between potential and realized absorptive capacity (Zahra & George, 2002). Beard et al. also showed that the commercialization "valley of death" mainly results from an imbalance in investment between the early and intermediate stages of innovation (Beard et al., 2009). Guan and Ma examined China's emerging position in nanoscience and nanotechnology through a bibliometric study (Guan & Ma, 2007).

3.3.6. *Review of Domestic Studies on Nanotechnology Policymaking in Iran*

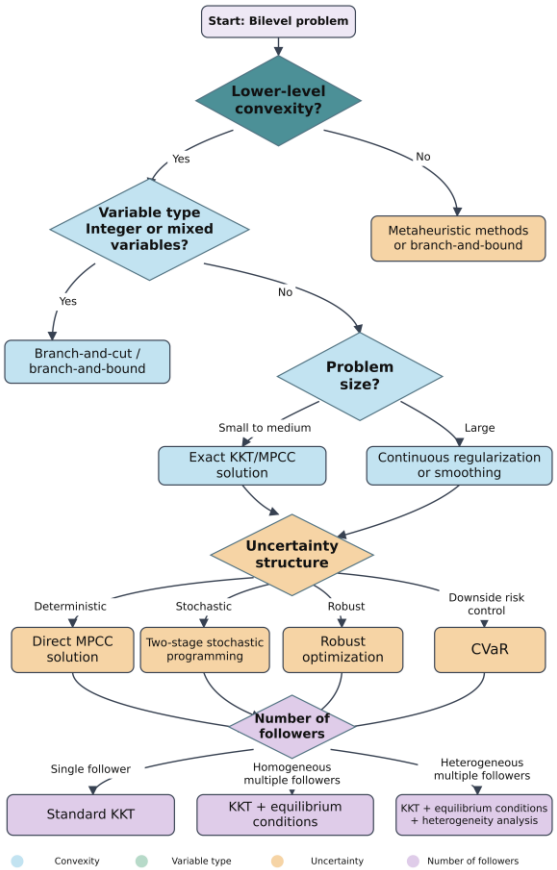
In nanotechnology policymaking, domestic studies have mainly focused on indicator development, program evaluation, and national strategy design. Soltani, Tabatabaeian, Hanafizadeh, and Bamdadsoofi proposed a framework for evaluating Iran's national nanotechnology program based on 46 outcome and impact indicators (Soltani et al., 2020). Sahebinejad and Ali examined Iran's third ten-year national nanotechnology development program in relation to mission-oriented policymaking (Sahebinejad & Ali, 2024). Ghazinoory, Mirzaei, and Ghazinoori proposed a national planning model based on the government's new roles (Ghazinoory et al., 2009). Mahmoudzadeh and Alborzi modeled Iran's nanotechnology innovation network using the SKIN agent-based simulation framework and the concept of absorptive capacity (Mahmoudzadeh & Alborzi, 2017). Alizade and Tabatabaiean presented a framework for an innovation survey of nanotechnology in Iran (Alizade & Tabatabaiean, 2015), and Fartash, Navab Irani, and Ghorshidi examined market-shaping policies for nanotechnology in Iran (Fartash et al., 2025). However, these studies lack an explicit optimization model that simultaneously links the policymaker's resource allocation decision to the strategic and heterogeneous responses of implementing actors.

3.4. *Decision Tree for Selecting a Solution Method*

Based on the four-dimensional classification, a decision tree is presented for selecting a solution method:

Figure 2

Research Decision Tree



Step 1: Is the lower level convex?

Yes: The KKT/MPCC reformulation is valid (Dempe & Dutta, 2012). Proceed to Step 2.

No: Use metaheuristic methods (Camacho-Vallejo et al., 2023) or branch-and-bound (Kleinert et al., 2021).

Step 2: Are there integer or mixed variables?

Yes: Use branch-and-cut or branch-and-bound (Kleinert et al., 2021).

No: Proceed to Step 3.

Step 3: What is the problem size?

Small to medium: Use an exact KKT/MPCC solution (Fortuny-Amat & McCarl, 1981).

Large: Use continuous regularization (Scholtes, 2001) or smoothing (Nurkanović et al., 2024).

Step 4: What is the uncertainty structure?

Deterministic: Solve the MPCC directly.

Scenario-based stochastic: Two-stage stochastic programming (Shapiro et al., 2009).

Set-based robust: Robust optimization (Ben-Tal et al., 2009; Bertsimas & Sim, 2004).

Downside risk control: CVaR (Rockafellar & Uryasev, 2000, 2002).

Step 5: How many followers?

Single follower: Standard KKT.

Homogeneous multiple followers: KKT for each follower + equilibrium conditions (Aussel & Svensson, 2020).

Heterogeneous multiple followers: KKT for each follower + equilibrium conditions + heterogeneity analysis (Aussel & Svensson, 2020; Khorramfar et al., 2024).

3.5. Critical Synthesis and Interpretive Contradictions

The synthesis of the four streams reveals three trends and two key contradictions:

Trend 1: A shift from deterministic single-follower to stochastic/robust multifollower models. The early literature focused on deterministic problems with a single follower (Ben-Ayed & Blair, 1990; Colson et al., 2005, 2007). Stochastic and robust models (Beck et al., 2023; Ben-Tal et al., 2009; Bertsimas et al., 2011; Bertsimas & Sim, 2004; Shapiro et al., 2009) and multifollower models (Aussel & Svensson, 2020; Khorramfar et al., 2024) gradually emerged. However, these two paths have been pursued separately.

Trend 2: Expansion from technical to policy domains. Early applications involved network design and pricing (Colson et al., 2005, 2007) and gradually expanded to energy, supply chains, and water allocation (Almutairi & Elhedhli, 2014; Bao & Zhang, 2018; Calvete et al., 2023; Caselli et al., 2026; Martelli et al., 2020). Applications in science and technology governance remain emergent (Caselli et al., 2026; Chen et al., 2024; Long & Zheng, 2025).

Trend 3: Diversification of approaches to uncertainty. Classical robust optimization focuses on the absolute worst case (Ben-Tal et al., 2009), whereas CVaR emphasizes the average of the tail of the worst plausible scenarios (Rockafellar & Uryasev, 2000, 2002).

Contradiction 1: The interpretation of robustness. The fundamental difference between the Ben-Tal–Nemirovski approach (Ben-Tal et al., 2009) and CVaR (Rockafellar & Uryasev, 2000) lies in their interpretation of robustness (Beck et al., 2023).

Contradiction 2: The validity of KKT in nonconvex problems. While some studies (Fortuny-Amat & McCarl, 1981) use KKT reformulation even in nonconvex problems, Dempe and Dutta (Dempe & Dutta, 2012) show that this is valid only under specific conditions.

3.6. Identified Research Gaps

Based on the above analysis, five specific research gaps are identified:

Methodological and application gap: The absence of a bilevel model that simultaneously integrates national resource allocation, heterogeneous responses, and uncertainty (Caselli et al., 2026; Khorramfar et al., 2024).

Follower heterogeneity gap: Most policy applications are based on a single follower or a homogeneous group (Aussel & Svensson, 2020; Khorramfar et al., 2024).

Downside risk control gap: No integration of CVaR with multifollower bilevel optimization in science and technology policymaking was found (Beck et al., 2023; Rockafellar & Uryasev, 2000).

Implementation gap: The literature focuses on the efficiency of nominal allocation rather than effective implementation (Beard et al., 2009; Khorramfar et al., 2024; Martelli et al., 2020).

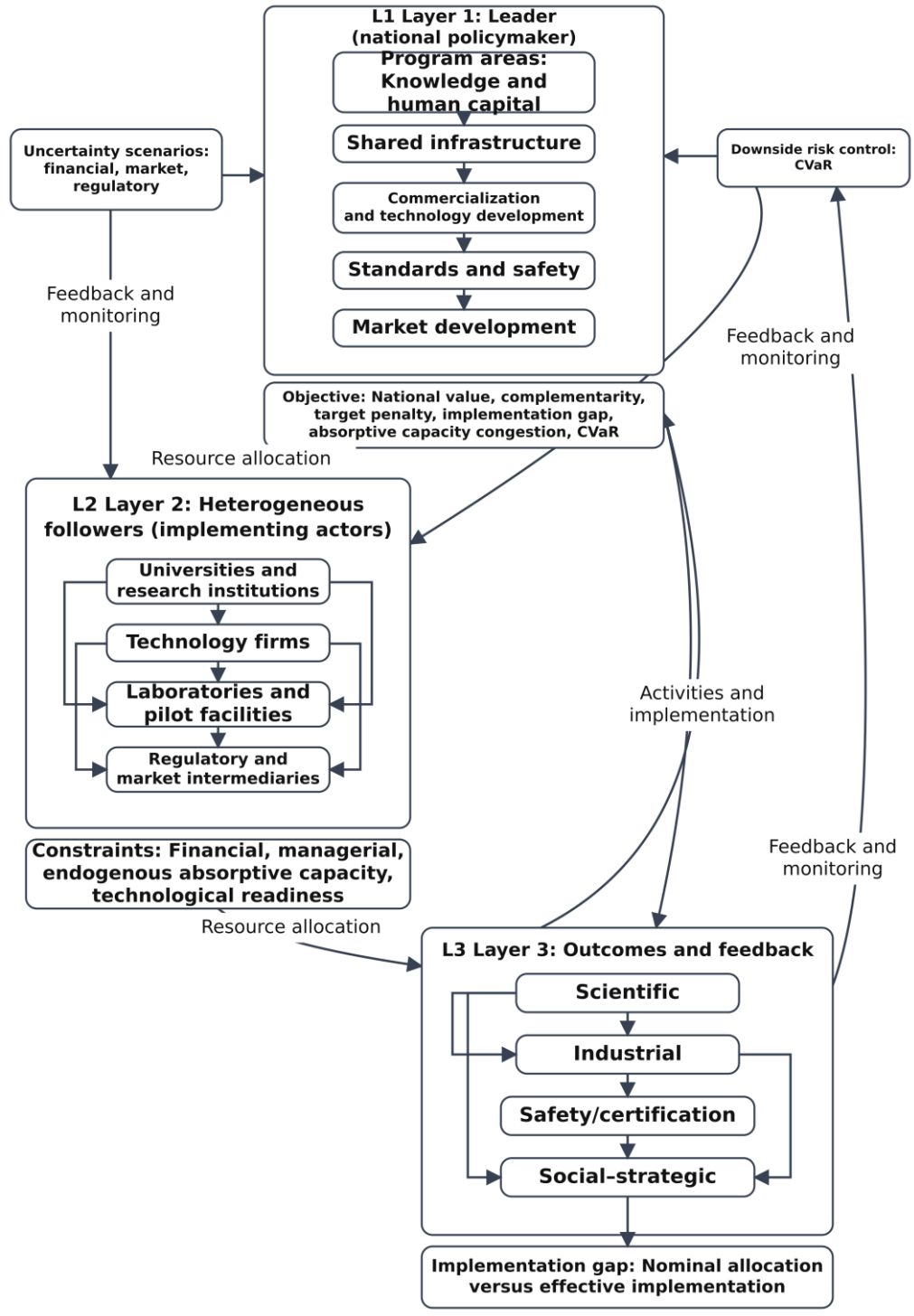
Contextual and geographical gap: Applications in developing-country contexts have not been examined (Caselli et al., 2026; Guan & Ma, 2007; Soltani et al., 2020).

3.7. Integrated Conceptual Framework: The Final Output of the Meta-Synthesis

The final output of this meta-synthesis is an integrated conceptual framework that connects the four main streams of the literature within a coherent structure and simultaneously addresses the five identified gaps. This framework provides the theoretical foundation for the robust bilevel optimization model.

Figure 3

Integrated Conceptual Framework of the Study



Framework structure. The proposed framework consists of three interconnected layers:

Layer 1—Leader (national policymaker). Acting as the leader, the policymaker allocates limited national resources among five program areas: knowledge and human capital, shared infrastructure, commercialization and industrial development, standards and safety, and market development. The leader's objective function combines direct national value, interprogram complementarity, a target shortfall penalty, the implementation gap, absorptive capacity congestion, and CVaR-based downside risk. The leader's allocation is an ex ante decision that remains common across all uncertainty scenarios (Beck et al., 2023; Ben-Tal et al., 2009).

Layer 2—Heterogeneous followers (implementing actors). Four classes of actors—universities and research institutions, technology firms, laboratories and pilot facilities, and regulatory and market intermediaries—act as heterogeneous followers. Each actor chooses its optimal activity level subject to its financial and managerial constraints, endogenous absorptive capacity (Cohen & Levinthal, 1990; Zahra & George, 2002), and technological readiness. Differences in these actors' benefits, costs, and capacities justify modeling heterogeneous multiple followers (Aussel & Svensson, 2020; Khorramfar et al., 2024).

Layer 3—Outcomes and feedback. The activities of follower actors are translated through outcome production equations into national outcomes in five dimensions: scientific, industrial, safety/certification, market, and social–strategic. The gap between nominal allocation and effective implementation is modeled as an explicit variable and feeds back to the first layer through a feedback mechanism (Beard et al., 2009; Khorramfar et al., 2024; Martelli et al., 2020).

Links to the literature streams. The proposed framework simultaneously integrates the four reviewed streams:

From Stream 1 (theory and algorithms): The leader–follower structure, KKT/MPCC reformulation, and the continuous regularization algorithm (Dempe & Dutta, 2012; Fortuny-Amat & McCarl, 1981; Nurkanović et al., 2024; Scholtes, 2001).

From Stream 2 (uncertainty and risk): Discrete scenarios, robust optimization, and the CVaR measure (Beck et al., 2023; Ben-Tal et al., 2009; Rockafellar & Uryasev, 2000, 2002).

From Stream 3 (policy applications): The allocation of limited resources among complementary programs and implementation bottlenecks (Caselli et al., 2026; Chen et al., 2024; Long & Zheng, 2025; Martelli et al., 2020).

From Stream 4 (multiple followers): A heterogeneous multifollower structure with limited shared resources (Aussel & Svensson, 2020; Khorramfar et al., 2024).

Coverage of the gaps. This framework simultaneously addresses all five identified gaps:

Table 2

Framework for Addressing the Gaps

Gap	How the framework addresses the gap
Methodological and application	Integrates national resource allocation + heterogeneous responses + uncertainty within a single model
Follower heterogeneity	Explicitly represents four classes of heterogeneous actors rather than one representative follower
Downside risk control	Adds CVaR to the upper-level objective function within a multifollower structure
Implementation gap	Defines explicit implementation-gap variables between nominal allocation and effective implementation
Contextual and geographical	Applies the model in the institutional context of a developing country with resource constraints

Unlike Beck et al. (Beck et al., 2023), who review uncertainty alone, this framework simultaneously integrates heterogeneous multiple followers + CVaR + absorptive capacity + the implementation gap. Unlike Caselli et al. (Caselli et al., 2026), who focus on sustainability, this framework introduces national science and technology resource allocation as its application context. Unlike the domestic reviews (Sahebinejad & Ali, 2024; Soltani et al., 2020), which are qualitative, this framework provides an explicit mathematical formulation for resource allocation.

4. Discussion and Conclusion

The present systematic review and meta-synthesis consolidated 64 sources into four interconnected streams: the theory and algorithms of bilevel optimization; uncertainty, robustness, and risk; policy, energy, and environmental applications; and multifollower structures and security games. The findings show that the field has progressed from relatively simple deterministic single-follower formulations toward models that include

uncertainty, discrete decisions, multiple followers, and policy-oriented objectives. More than 60% of the reviewed sources were published between 2015 and 2025, indicating that bilevel optimization has recently attracted growing attention as a framework for complex hierarchical decisions. Nevertheless, the distribution of studies remained uneven. Theory and algorithms constituted the largest stream, whereas fewer studies combined multiple followers, uncertainty, and explicit downside-risk measures. This pattern is consistent with major reviews showing that advances in formulation and computation have outpaced the development of integrated models for institutionally complex policy settings (Colson et al., 2005, 2007; Dempe & Zemkoho, 2020; Kleinert et al., 2021; Sinha et al., 2018).

The four-dimensional classification developed in this review demonstrates that lower-level convexity, decision-variable type, uncertainty structure, and follower multiplicity must be considered jointly when selecting a solution method. The results indicated that 55% of the reviewed problems were convex and 45% were nonconvex, while 52% included integer or mixed variables. These proportions explain why no single algorithm dominates the literature. KKT-based reformulation is attractive for continuous convex follower problems because it can transform a bilevel model into a single-level MPCC. However, the validity of this transformation depends on convexity and appropriate constraint qualifications, supporting the warning that bilevel programming cannot always be treated as a conventional complementarity-constrained problem (Dempe & Dutta, 2012). The continued use of binary linearizations reflects the practical influence of the Fortuny-Amat formulation (Fortuny-Amat & McCarl, 1981), whereas the importance of branch-and-bound and mixed-integer techniques agrees with research demonstrating their value for structured linear and discrete bilevel problems (Hansen et al., 1992; Kleinert et al., 2021).

The findings also support the increasing importance of regularization, smoothing, and metaheuristic methods. Exact KKT/MPCC methods were most defensible for small or medium-sized convex problems, but their performance and validity became less reliable as nonconvexity, discontinuity, dimensionality, or discrete follower decisions increased. Regularization offers a principled way to approximate difficult complementarity conditions and improve numerical stability (Scholtes, 2001). Recent analyses of MPCC algorithms similarly show that regularization, smoothing, and penalty approaches can provide useful alternatives when direct treatment of complementarity is numerically problematic (Nurkanović et al., 2024). For nonconvex or black-box models, metaheuristics may be more flexible, although their solutions require careful verification and transparent reporting. This interpretation aligns with the review of metaheuristic bilevel optimization, which identified nested, single-level, and coevolutionary frameworks while emphasizing weaknesses in reproducibility and lower-level solution accuracy (Camacho-Vallejo et al., 2023). Thus, algorithm choice should follow the mathematical structure of the problem rather than familiarity with a particular solver.

The review found that uncertainty has become a substantial but still incompletely integrated component of bilevel research. Thirty-eight percent of the sources addressed stochastic or robust uncertainty, yet only 14% employed CVaR and only 8% combined CVaR with a multifollower structure. This result confirms that uncertainty in bilevel models is more complex than uncertainty in single-level optimization because uncertain parameters may influence the leader, follower, information structure, and reaction mapping simultaneously (Beck et al., 2023). Scenario-based stochastic programming is suitable when probability distributions or credible discrete scenarios can be specified (Shapiro et al., 2009). Robust optimization is more appropriate when distributions are unreliable but defensible uncertainty sets can be constructed (Ben-Tal et al., 2009; Ben-Tal & Nemirovski, 1998). The reviewed evidence also supports budgeted robustness as a way to regulate the trade-off between protection and excessive conservatism (Bertsimas et al., 2011; Bertsimas & Sim, 2004; Gorissen et al., 2015).

The results further show that CVaR occupies a distinctive position between expected-value optimization and strict worst-case protection. CVaR focuses on the mean loss within the adverse tail of a distribution and therefore allows the policymaker to penalize severe but plausible outcomes directly (Rockafellar & Uryasev, 2000, 2002). This feature is especially relevant to national resource allocation, where extreme implementation failures, market contractions, or regulatory disruptions may have substantial social costs. The synthesis suggests that scenario-based CVaR can be less conservative and more policy-informative than an absolute worst-case robust criterion when a discrete scenario set is available. At the same time, the limited number of studies integrating CVaR with heterogeneous followers indicates that risk modeling and actor modeling have largely evolved as separate research paths. Their integration is therefore a

substantive contribution rather than a minor technical adjustment.

The application stream demonstrates that bilevel optimization is already capable of representing realistic regulatory and resource-allocation relationships. Models of renewable-energy subsidies and carbon taxation show how a public authority can anticipate the reactions of producers and energy systems (Almutairi & Elhedhli, 2014; Martelli et al., 2020). Applications to green procurement and product markets similarly capture the interaction between regulation, subsidies, supply-chain behavior, and market decisions (Bao & Zhang, 2018; Chen et al., 2024). Water-allocation research demonstrates the value of hierarchical optimization where a central authority and local users have related but nonidentical objectives (Calvete et al., 2023). Dynamic Stackelberg–Bertrand models further show that government support, R&D spillovers, and information can generate complex long-term behavior (Long & Zheng, 2025). These findings align with the conclusion that sustainability applications are expanding, but also confirm that many existing models remain sector-specific and do not represent the full institutional diversity of national science and technology systems (Caselli et al., 2026).

The multifollower results are particularly important for interpreting national resource allocation. Twenty-two percent of the reviewed studies modeled multiple followers, but only 12% considered heterogeneous followers. This limited coverage indicates that many models continue to represent decentralized actors through a single follower or a homogeneous group. Such simplification may be unsuitable when universities, firms, laboratories, and regulatory intermediaries differ in their objectives, absorptive capacities, costs, and technological readiness. Research on industrial transitions shows that multifollower bilevel models can coordinate shared resources across distinct operational units (Khorramfar et al., 2024). The theory of multileader–multifollower games also confirms that equilibrium properties depend on the form of interaction among followers (Aussel & Svensson, 2020). Evidence from Stackelberg security games reinforces the practical value of anticipating several strategic responses to a limited central allocation (Bucarey et al., 2021; Casorrán et al., 2019). Accordingly, heterogeneous follower modeling improves both descriptive realism and the policy relevance of the resulting allocation.

The integrated conceptual framework also aligns with national innovation system theory. Innovation results from interactions among institutions rather than from a linear transfer of research inputs into commercial outputs (Edquist, 1997; Freeman, 1995; Lundvall, 1992; Nelson, 1993). Evolutionary and systemic studies likewise emphasize cumulative learning, institutional coordination, and the co-development of technology and policy (Fagerberg et al., 2005; Metcalfe, 1995). The importance assigned in the framework to universities, industry, and government is consistent with the triple-helix model (Etzkowitz & Leydesdorff, 2000), while the inclusion of market and regulatory intermediaries reflects research on open innovation and technology transfer (Bozeman, 2000; Chesbrough, 2003). The framework therefore interprets resource allocation as a system-level coordination problem rather than a simple budget-distribution exercise.

The explicit inclusion of absorptive capacity and an implementation gap is another important result. Absorptive-capacity theory explains why organizations differ in their ability to identify, assimilate, and exploit external knowledge and resources (Cohen & Levinthal, 1990; Zahra & George, 2002). Consequently, nominally equal allocations need not produce equal activity or outcomes. The implementation gap in the proposed framework represents the difference between assigned resources and effectively utilized resources, while absorptive-capacity congestion captures diminishing effectiveness when allocations exceed implementation capability. This interpretation is supported by research on the commercialization “valley of death,” which attributes weak translation partly to discontinuities and imbalances across stages of innovation (Beard et al., 2009). It also corresponds with the broader view that national competitiveness and innovation depend on linked capabilities, institutions, and feedback processes (Kline & Rosenberg, 1986; Porter, 1990; Rothwell, 1994).

The Iranian nanotechnology literature provides contextual support for applying the framework. Iran’s substantial scientific publication activity indicates the presence of an established knowledge base (Guan & Ma, 2007; Statnano, 2025). National studies have developed outcome and impact indicators, examined mission-oriented development programs, and analyzed the alignment of nanotechnology with socioeconomic goals (Sahebinejad & Ali, 2024; Soltani et al., 2020). Other research has modeled national planning, innovation networks, absorptive capacity, and innovation-survey processes (Alizade & Tabatabaiean, 2015; Ghazinoory et al., 2009; Mahmoudzadeh & Alborzi, 2017). Market-shaping research has additionally highlighted the need for coordinated demand creation and institutional support (Fartash et al., 2025). These studies establish the

relevance of the proposed program areas, but the present review shows that they have not yet been combined within an explicit optimization model linking national allocations, heterogeneous reactions, implementation capacity, and downside risk.

This review has several limitations. Its sources were identified through Scopus, Web of Science, and Google Scholar, so relevant studies indexed elsewhere or published in other languages may have been omitted. Because the four analytical streams overlap, classifying some studies required interpretive judgment. The reported frequencies describe the reviewed corpus rather than the entire global literature. Differences in terminology, notation, problem scale, computational platforms, and reporting quality also constrained comparisons among algorithms. Finally, the integrated framework remains conceptual and has not yet been validated using empirical data, calibrated scenarios, or comparative computational experiments.

Future studies should test the proposed robust multifollower model using national nanotechnology data and transparent scenario-generation procedures. KKT/MPCC, regularization, decomposition, branch-and-bound, and metaheuristic implementations should be compared using common benchmarks that report optimality gaps, runtime, scalability, and sensitivity. Research should also examine cooperative, competitive, and equilibrium-based follower interactions and estimate actor-specific absorptive-capacity and implementation-gap functions. Distributionally robust, data-driven, and multistage extensions could be evaluated alongside scenario-based CVaR. Longitudinal studies should test whether model-generated allocations improve national outcomes and whether the framework transfers to other technologies and developing-country settings.

Policymakers should use the framework to link national budgets to the implementation capacities and expected responses of distinct actor groups. Allocations should be accompanied by actor-specific capacity assessments, explicit implementation targets, and periodic monitoring of nominal funding versus effective use. Decision makers should construct credible financial, market, regulatory, and technological scenarios and set an acceptable downside-risk threshold before finalizing allocations. Investments across program areas should be coordinated because weaknesses in infrastructure, standards, commercialization, or market development can reduce the return on scientific funding. Allocation decisions should then be updated as implementation data and feedback from universities, firms, laboratories, and intermediaries become available.

Authors' Contributions

Authors contributed equally to this article.

Declaration

In order to correct and improve the academic writing of our paper, we have used the language model ChatGPT.

Transparency Statement

Data are available for research purposes upon reasonable request to the corresponding author.

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Ethics Considerations

In this research, ethical standards including obtaining informed consent, ensuring privacy and confidentiality were considered.

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