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Editorial

One hundred grand challenges in petroleum science

A B S T R A C T

Petroleum science stands at a historic turning point: exploration extends to ultra-deep and deepwater frontiers, unconventional resources become dominant, and the dual imperatives of carbon neutrality and artificial intelligence are reshaping the industrial landscape and disciplinary boundaries. Building upon the “100 Grand Challenges in Petroleum Science” initiative launched by *Petroleum Science* in 2021, this paper presents a curated list of 100 fundamental scientific problems through systematic literature synthesis, expert deliberation, and multi-criteria selection. The challenges span six domains: exploration and development, transport and pipelines, refining and petrochemicals, materials science, carbon capture, utilization and storage-geothermal-hydrogen, and energy economics and digital transformation. In-depth analysis reveals three archetypes: mechanism-oriented problems that seek unified theories of multi-scale coupling, technology-oriented problems that push engineering limits under extreme conditions, and system-level problems that address full-chain integration and energy transition. A key insight is that artificial intelligence has evolved from an enabler to a core driver, and together with the low-carbon transition it is redefining the very paradigm of petroleum science. This roadmap is intended to guide research planning, investment, and talent development over the coming decades and to foster interdisciplinary collaboration on a global scale.

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1. Introduction

The advancement of science often begins with the precise identification and clear articulation of key questions. In 1900, the German mathematician David Hilbert presented 23 mathematical problems (Hilbert, 1900) at the International Congress of Mathematicians in Paris, charting the course for 20th-century mathematics and profoundly influencing algebra, geometry, analysis, and many other branches. More than a century later, petroleum science—a discipline that underpins modern industrial civilization—faces a similar “problem-driven” moment. With the continued growth of global energy demand, the gradual depletion of conventional oil and gas resources, the extension of exploration toward deep, ultra-deep, and unconventional frontiers, and the binding constraints of climate change on the low-carbon transition, petroleum science stands at a historic turning point. On 27 October 2021, the journal *Petroleum Science* officially launched the “100 Grand Challenges in Petroleum Science” initiative (Petroleum Science Editorial Office, 2021). Its aim was to pool the wisdom of scientists, engineers, and researchers from interdisciplinary fields worldwide and to refine and publish a list of challenging, forward-looking scientific problems that represent the frontiers of petroleum science. This initiative is not merely an academic survey but a strategic move—it hopes to systematically define the “bottleneck” scientific problems, guide global research efforts toward focused tackling, and, through interdisciplinary exchange, catalyze disruptive theories and technologies, thereby reshaping the journal's academic appeal and enhancing the voice of petroleum science and technology on the international stage.

The history of petroleum science shows that almost every major breakthrough has originated from a new understanding of some fundamental scientific question—from the early formulation of trap theory, through the quantification of basin modelling and accumulation dynamics, to the shale revolution driven by horizontal wells and hydraulic fracturing (Jia, 2017; Zou et al., 2013). Yet the challenges facing petroleum science today are far broader and deeper than ever before. First, exploration targets have shifted toward ultra-deep (>8000 m), ultra-high-pressure (>140 MPa), and ultra-high-temperature (>200 °C) settings, where conventional accumulation theories and geophysical techniques frequently fail, urgently requiring new models of geomechanics, fluid phase behavior, and transport. Second, unconventional resources (shale oil/gas, tight oil/gas, coalbed methane) have become the mainstay of reserve and production growth, but the mechanisms of multiphase flow in nanopores (Blunt et al., 2013), the evolution of complex fracture networks, and the causes of rapid production decline remain poorly understood, leading to recovery factors far below expectations. Third, global climate governance is accelerating the low-carbon transition of energy systems, forcing petroleum science to deeply integrate with emerging fields such as carbon capture, utilization and storage (CCUS), hydrogen energy, geothermal energy, and large-scale energy storage, thus forming a new “oil-gas plus low-carbon” knowledge system

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(Celia et al., 2015; Middleton et al., 2015; Xiong et al., 2025; IEA, 2023). Fourth, the wave of digital transformation and artificial intelligence (AI) is penetrating the entire chain of exploration, development, transport, refining, and management at an unprecedented speed; data have risen from a supporting role to a core productive factor, and technologies such as AI, digital twins, and edge computing are demanding a fundamental reshaping of traditional research paradigms (Tao et al., 2019; Karniadakis et al., 2021; Raissi et al., 2019). (In this paper, "AI" is used in a broad sense to encompass machine learning, data analytics, digital twins, edge computing, and other data-driven technologies.)

Faced with these multiple transformations, piecemeal technological improvements are no longer sufficient. Petroleum science urgently needs a systematic "problem inventory"—from fundamental mechanisms to engineering limits, from individual links to full-chain integration, from resource-oriented to system-oriented thinking. This is precisely the starting point of the present work. Inspired by the *Petroleum Science* "100 Grand Challenges" initiative, the authors, after extensive literature review, expert consultation, and multiple rounds of deliberation, followed six main criteria (scientific originality, practical urgency, transformative potential, interdisciplinary nature, temporal impact, and disciplinary balance) to finally select and refine 100 of the most representative and forward-looking grand challenges in petroleum science. These problems span six major domains: exploration and development, transport and pipelines, refining and petrochemicals, materials science, CCUS-geothermal-hydrogen, and energy economics and digital transformation, covering a vast range from quantum-scale molecular simulations to global trade network evolution.

The purpose of this paper is not to provide definitive answers, but to offer a credible roadmap that may serve as a basis for discussion and a reference for action for academia, industry, and policy makers. We are fully aware that any list of scientific grand challenges is inherently open and dynamic. As theoretical breakthroughs and engineering practices advance, old challenges will be solved and new ones will emerge. Yet at this moment, clearly defining "what we do not know" is an essential step toward the future. As Hilbert famously said, the vitality of a discipline is measured by the number of profound questions it can raise. The next era of petroleum science will be written by those who dare to confront the truly difficult challenges.

2. Selection methodology and main criteria

The 100 grand challenges in petroleum science presented in this paper are not an arbitrary list but the result of a systematic, rigorous, and iterative process of selection and refinement. The following sections detail the sources of candidate challenges, the selection workflow, the core criteria, and the quality assurance measures, so as to ensure the scientific soundness, representativeness, and forward-looking nature of the list.

2.1. Sources of candidate challenges

The candidate pool was derived from three main sources.

(1) Original submissions to the *Petroleum Science* "100 Grand Challenges" initiative. The call launched in 2021 received several hundred suggestions from domestic and international scholars. These suggestions covered exploration, development, transport and storage, refining, materials, CCUS, geothermal, hydrogen, smart oil/gas fields, economics, and management, forming a rich "problem raw material warehouse". Some of the submissions addressed specific technical bottlenecks (e.g., "how to improve fracture conductivity of shale gas fracturing"), while others were more macro scientific questions (e.g., "multi-factor coupling theory of ultra-deep hydrocarbon accumulation"). The detailed descriptions of the 100 challenges in the Supplementary Information are a further expansion and refinement of those initial contributions.
(2) Systematic literature review of top journals and major projects in petroleum science over the last decade. We analyzed review and perspective articles published between 2015 and 2025 in journals such as *AAPG Bulletin*, *SPE Journal*, *Energy*, *Fuel*, *Energy & Fuels*, *Reviews of Geophysics*, and *Petroleum Science*, as well as the funding directions of the National Natural Science Foundation of China, National Key R&D Program, EU Horizon Program, and US Department of Energy Projects. Frequently mentioned and widely recognized unsolved scientific problems were extracted.
(3) White papers and strategic reports from industry. We also referred to future technology roadmaps and strategic research agendas issued by the International Energy Agency (IEA), American Association of Petroleum Geologists (AAPG), Society of Petroleum Engineers (SPE), China Petroleum Society, and other organizations, ensuring close alignment with the practical needs of industry.

Through these channels, an initial pool of approximately 200 candidate challenges was collected, spanning scales from molecular to global.

2.2. Selection workflow

The selection of the 100 grand challenges was not a mechanical "crowdsourcing" exercise but a highly expert-driven process grounded in deep, iterative discussions among leading researchers. The workflow consisted of four stages.

Stage 1: Candidate collection and initial consolidation. An initial pool of approximately 200 candidate problems was assembled from the three sources described above (open submissions, literature review, and industry white papers). The author then conducted a preliminary consolidation by merging near-duplicate entries and removing those that were clearly incremental engineering refinements rather than fundamental scientific questions. This resulted in a working set of about 160 distinct challenges.

Stage 2: In-depth expert workshops and iterative refinement. Over a period of several months, the author organized multiple rounds of one-on-one and small-group discussions with senior experts from diverse disciplines (geology, geophysics, reservoir engineering, drilling, transport and storage, refining, materials, CCUS, hydrogen, geothermal, economics, and management). These discussions were not anonymous surveys but intensive, critical dialogues. During these sessions, many candidate problems were re-framed, merged, split, or discarded. For example, several specific technical bottlenecks were elevated to more general scientific questions (e.g., "methods for evaluating shale oil mobility" became "multi-scale evaluation theory and methods for continental shale oil mobility"). This stage also identified major gaps (such as data value, digital twins, and algorithmic trading regulation) that were not well represented in the initial pool. The output of this stage was a consolidated list of approximately 110 challenges, each accompanied by a clear scientific justification.

Stage 3: Broad external review by the wider expert community. The consolidated list was then circulated to a larger group of highly regarded experts (including those who had not participated in the earlier workshops) for written review. Each expert was asked to provide individual feedback on each challenge: whether it should be kept, merged with another, revised, or deleted; and to suggest any missing challenges of comparable importance. The authors synthesized all feedback, eliminated or merged challenges that received consistent negative assessments, and made substantive revisions to the wording and scope of many others. After two rounds of this broad external review, the list was narrowed to 100 challenges.

Stage 4: Final polishing and consensus checking. The penultimate version of the 100 challenges was shared once more with a subset of the experts to verify that no critical scientific issue had been overlooked and that the phrasing was both precise and accessible. The final list achieved a high degree of expert approval. Nevertheless, it is emphasized that this is not a "voted" list; the final responsibility for selection and wording rests with the author, informed by the collective wisdom of the expert community.

2.3. Six main criteria

Every challenge in the final list had to satisfy the following six criteria. The design of the criteria was inspired by authoritative frameworks such as *Science* magazine's "125 Scientific Questions", the US National Academy of Sciences' "Grand Challenges in Geology", and the EU Horizon programme.

Scientific originality. The challenge must address a fundamental scientific mechanism that remains unsolved, rather than an incremental improvement of an already established technology. For example, "unified non-Darcy flow theory in ultra-low-permeability and nanoporous media" (Challenge 8) is an original scientific problem, whereas "optimizing numerical simulation methods for flow in nanopores" is an engineering refinement and was given lower priority. Original problems usually reveal contradictions in existing theories or phenomena that cannot be explained by current models.

Practical urgency. The challenge must be directly relevant to a major technological bottleneck faced by the petroleum industry. Problems that, if solved, would significantly reduce costs, enhance safety, or unlock otherwise inaccessible resources were prioritized.

Transformative potential. The solution of the challenge should have the potential to trigger a technological leap (e.g., increase oil recovery by more than 5 percentage points, reduce energy consumption by more than 30%), create new research directions, or change industrial operating models. Challenges with high transformative potential were given higher priority. For example, a breakthrough in proppant transport mechanisms of supercritical CO_2 water-less fracturing (Challenge 11) could completely eliminate water constraints—a dual technological and environmental transformation (Middleton et al., 2015).

Interdisciplinary nature. The challenge must require the integration of knowledge from two or more traditional disciplines (e.g., geology + physics + data science, chemical engineering + materials + AI). Purely single-discipline technical problems were not prioritized. Interdisciplinary challenges are often where innovation is most likely to emerge.

Disciplinary balance. To ensure the list fully reflects the breadth of petroleum science, each of the six domains must contain a sufficient number of representative challenges. No single domain was allowed to dominate simply because it is currently "hot", nor was any traditional domain neglected. The final distribution of challenges across domains is: exploration and development (30), transport and pipelines (15), refining and petrochemicals (15), materials science (10), CCUS-geothermal-hydrogen (15), energy economics and digital transformation (15), summing to 100.

2.4. Authors' deliberation and expert consultation

To ensure the rigour and credibility of the final list, the following measures were taken.

Cross-disciplinary expert consultation. The authors consulted senior experts from domestic and international universities, research institutes, and major energy companies, covering geology, geophysics, reservoir engineering, drilling, transport and storage, refining, materials, CCUS, hydrogen, geothermal, economics, and management. These consultations were conducted through in-depth interviews and structured discussions, rather than anonymous voting. The experts provided independent feedback on each candidate challenge—suggesting merges, revisions, or additions—and their inputs were used to refine the wording and justifications through multiple rounds of revision. The final 100 challenges reflect the authors' synthesis of expert insights and own judgment.

Traceable documentation. The original records of candidate challenges, merging decisions, expert comments, and revision history were archived for transparency and traceability.

External review. Before finalization, a draft of the 100 challenges was shared with renowned scholars who had not participated in the earlier consultations. Based on their individual feedback, the wording and priorities of about 10 challenges were fine-tuned.

Consensus not required. It is explicitly noted that this list is not the outcome of a democratic vote or a requirement for unanimous agreement. Rather, it represents the authors' deliberate judgment, informed by extensive literature synthesis, expert consultations, and a clear set of prioritization criteria. The value of the list lies in its forward-looking perspective and its ability to stimulate debate and guide research, not in achieving a statistical measure of inter-rater reliability.

3. 100 grand challenges in petroleum science

For brevity, the detailed descriptions are provided in **Supplementary Information**. The 100 challenges are as follows.

3.1. Petroleum Exploration and Development (Challenges 1–30)

1. Multi-factor coupling theory of hydrocarbon accumulation and preservation in ultra-deep formations (>8000 m)
2. Control mechanisms for the survival limit of liquid hydrocarbons and downward extension of the liquid window in ultra-deep formations
3. Pore evolution and preservation mechanisms in ultra-deep carbonate reservoirs
4. Limits of high-precision geophysical prediction for ultra-deep (>8000 m) reservoirs
5. Dynamic mechanisms of shale oil/gas "sweet spot" formation and mechanism-driven prediction models
6. Occurrence, phase behavior, and efficient recovery mechanisms of multi-component crude oil in nanopores of shale reservoirs
7. Multi-scale evaluation theory and methods for continental shale oil mobility
8. Unified non-Darcy flow theory in ultra-low-permeability and nanoporous media
9. Formation and dynamic evolution mechanisms of complex hydraulic fracture networks
10. Real-time fracture extension inversion and adaptive control in intelligent fracturing parameter optimization
11. Phase-transition control and proppant transport enhancement mechanisms of supercritical CO_2 water-free fracturing

12. Physics-data dual-driven production decline models for unconventional wells
13. Cross-scale coupling from microscopic displacement mechanisms to macroscopic recovery response
14. Dual conduit-seal role of deep fault systems in hydrocarbon accumulation and production
15. Dynamic evolution and quantitative evaluation of fault seal capacity in complex fault-block reservoirs
16. Fine 3D modeling of fracture-vug structures and remaining oil characterization in carbonate fractured-vuggy reservoirs
17. *In-situ* visualization and mobilization mechanisms of microscopic remaining oil in high-water-cut reservoirs
18. Mobility control and channeling suppression mechanisms of polymer flooding in highly heterogeneous conglomerate reservoirs
19. Multiphase flow and mass transfer mechanisms in deep-water reservoirs under high-pressure and low-temperature conditions
20. Thermo-hydro-mechanical-chemical coupled prediction of wellbore stability in deep drilling
21. Rheology control and high-temperature material design for drilling fluids under ultra-high temperature and pressure (>200 °C, >140 MPa)
22. Integrity failure mechanisms and life prediction of casing-cement-formation wellbore systems in deep wells and unconventional reservoirs
23. Physical limits and reliability of logging and downhole real-time sensing technologies under extreme environments
24. Real-time monitoring and dynamic imaging methods for hydrocarbon migration and accumulation processes
25. Surface/interface design of reservoir nano-tracers and inversion of their transport-adsorption-desorption behavior
26. Theory and technology of passive magnetic ranging for real-time inter-well steering during drilling
27. Inter-well dynamic connectivity inversion and development optimization for complex fault-block reservoirs
28. Multi-scale transport model (adsorption-desorption-diffusion-seepage) for deep coalbed methane and in-situ conversion potential
29. Genesis mechanisms and geophysical identification criteria for volcanic hydrocarbon reservoirs
30. Reservoir response and sand control during combined depressurization-heating-chemical production of gas hydrates in muddy-silty reservoirs

3.2. Petroleum storage, transportation, pipeline networks, and flow assurance (Challenges 31–45)

31. Unified theory of flow regime transition and flow stability in long-distance multiphase oil-gas transportation systems
32. Complex flow evolution during shutdown and restart of long-distance pipelines transporting easy-gelling high-viscosity crude oil
33. Mechanistic model and real-time monitoring of internal corrosion rates in multiphase pipelines
34. Formation, evolution, and control mechanisms of multi-component deposits (wax, asphaltenes, hydrates) in pipelines
35. Decompression wave propagation, fracture mechanics, and arrest toughness design for supercritical CO_2 pipelines
36. Hydrogen embrittlement and material compatibility assessment for hydrogen/hydrogen-blended pipeline transportation
37. Adaptability of compressors, valves, and seals to hydrogen blending in natural gas pipelines
38. Flow assurance and deposit control technologies for deep-sea oil/gas transportation
39. Fatigue life prediction of free-span subsea pipelines under vortex-induced vibration and active vibration suppression technologies
40. Dynamic mechanisms of thermal-mass coupling stratification and rollover in large-scale liquefied natural gas storage tanks
41. Full life-cycle degradation mechanisms and failure probability prediction theory for pipeline integrity
42. High-sensitivity real-time leak detection, localization, and quantification mechanisms in pipelines
43. Digital twin model of the mixed-oil interface and cut-point optimization in batch transportation of refined products
44. Adaptive operation control of long-distance oil/gas pipeline inspection tools and multi-modal data fusion intelligent analysis
45. System coordination, resilience assessment, and emergency control theory for multi-energy coupled pipeline networks (oil, gas, hydrogen, ammonia, methanol, CO_2)

3.3. Petroleum refining, chemical engineering, and low-carbon conversion (Challenges 46–60)

46. Molecular-level characterization of crude oil and reaction network construction for “molecular refining”
47. Molecular dynamics of asphaltene aggregation and coke formation in slurry-bed hydrocracking of heavy residue
48. Pore confinement effects of zeolites and reaction path control for light olefin production in fluid catalytic cracking (Corma, 1997)
49. Coke inhibition and selectivity control in direct crude-to-chemicals (CTC) catalytic cracking
50. Atomic-scale structure regulation of active phases (CoMoS/NiMoS) in hydrodesulfurization (HDS) catalysts
51. Unified theory of gas-liquid-solid interfacial transfer and reaction kinetics coupling in multiphase catalysis
52. Quantitative structure-performance relationships and multi-scale predictive models for industrial catalysts
53. Unified mechanisms of industrial catalyst deactivation, regeneration, and lifecycle prediction under complex operating conditions
54. Digital twin modeling, calibration, and real-time optimization for full-chain refining and petrochemical processes (Tao et al., 2019)
55. System reconfiguration and pathway optimization for low-carbon refining processes under carbon neutrality goals (IEA, 2023)
56. Degradation mechanisms and recycling of ionic liquids in clean alkylation processes
57. Novel catalyst design and reaction mechanisms for CO_2 hydrogenation to high-value chemicals (methanol, olefins, etc.)
58. Catalyst oxygen tolerance and selective isomerization mechanisms for hydroprocessed esters and fatty acids to sustainable aviation fuel (Huber et al., 2006)
59. Design of bimetallic catalysts and regeneration cycles for catalytic pyrolysis of waste plastics to aromatics and light olefins

60. Multiphase mixing, mass transfer, and scale-up rules for microreactor process intensification in petrochemical plants

3.4. Petroleum materials science (Challenges 61–70)

61. Multi-field coupling mechanisms of material corrosion under extreme oil/gas environments
62. Stress corrosion cracking mechanism and life prediction of ultra-high-strength casing/tubing steels in high-H_2S/CO_2 environments
63. Microstructural evolution and corrosion resistance degradation in the heat-affected zone of Ni-base alloy welds for high-sour gas field gathering lines
64. Accelerated coating failure mechanisms and long-life protection systems for steel structures in the splash zone of offshore platforms
65. Low-temperature toughness and microstructure matching of weld metal for 9% Ni steel used in liquefied natural gas storage tanks at -162 °C
66. Degradation rate control and mechanical property matching of dissolvable bridge plug/ball materials (Mg/Al-based alloys) for oil/gas field fracturing
67. Molecular design and performance limits of elastomer sealing materials for downhole service above 300 °C
68. Dual failure mechanisms (coarse-grained heat affected zone (HAZ) embrittlement and softened zone strength loss) in the HAZ of high-strength pipeline steel (X80 and above) welds
69. Interfacial regulation mechanisms of nanomaterials for enhanced oil recovery
70. Design theory and evaluation systems for hydrogen-embrittlement-resistant materials under high-pressure hydrogen environments (Robertson et al., 2015)

3.5. CCUS, geothermal, hydrogen, and underground energy systems (Challenges 71–85)

71. System efficiency and energy loss mechanisms along the full CCUS chain
72. High-efficiency, low-energy capture mechanisms and novel adsorbents for low-concentration CO_2 from industrial flue gas
73. Coupled mechanisms of multiphase flow, mass transfer, and geochemistry in CO_2-EOR and geological storage (Celia et al., 2015; Rutqvist, 2012)
74. Stochastic-deterministic coupled model for long-term integrity risk assessment of CO_2 geological storage
75. Synergistic regulation of reaction kinetics and rapid strength development in CO_2-mineralized concrete products
76. Dynamic interaction between artificial and natural fracture networks in enhanced geothermal systems (EGS) in hot dry rock (Zhou et al., 2024; Nath et al., 2024; Lu, 2018; Tester et al., 2006)
77. Source mechanisms and risk control methods for induced seismicity during EGS fracturing (Zhou et al., 2024)
78. Mechanisms of hydrogen geochemical and microbial consumption in depleted reservoir storage and their control (Xiong et al., 2025)
79. Caprock sealing assessment and cyclic-loading fatigue damage mechanisms for salt-cavern/depleted-reservoir hydrogen storage
80. Working-fluid selection and phase-change heat transfer limits in ultra-long gravity heat pipes for hot dry rock heat extraction
81. Competitive adsorption, diffusion hysteresis, and working gas volume prediction for hydrogen storage in underground reservoirs
82. Phase equilibrium and reservoir stability mechanisms for safe gas hydrate production
83. Fracture-filling type gas hydrate reservoir 3D distribution prediction and accumulation dynamics (Hu et al., 2023)
84. Multi-field coupling mechanisms for large-scale underground storage (hydrogen, compressed air, CO_2) in salt caverns and aquifers
85. Absorption/desorption kinetics and thermal management synergy of high-capacity solid-state hydrogen storage materials (e.g., MgH_2) (Züttel, 2004)

3.6. Energy economics, management, and digital transformation (Challenges 86–100)

86. Nonlinear prediction model and geopolitical risk quantification for global oil and gas supply-demand dynamics (Kilian, 2009; Hamilton, 2009)
87. Quantification of multi-scale driving mechanisms of oil price volatility and extreme risk early warning
88. Reconstructed valuation theory for oil/gas assets under energy transition and stranded asset risk assessment (IEA, 2023)
89. Simulation of impact pathways of carbon market mechanisms (e.g., carbon border adjustment mechanism (CBAM) on global petroleum trade patterns
90. Global oil and gas supply chain resilience and geopolitical landscape evolution
91. Techno-economic principles and dynamic investment decisions for low-carbon transformation of oil/gas enterprises under carbon neutrality goals
92. Game-theoretic model for optimal timing, scale, and market impact of strategic petroleum reserve releases
93. Dynamic game equilibrium of international petroleum contracts (e.g., production sharing agreement (PSA)) and optimal fiscal term design
94. Cross-scenario generalization, customized adaptation, and trustworthy decision mechanisms for industrial foundation models in the oil/gas industry (Karniadakis et al., 2021; Raissi et al., 2019; Reichstein et al., 2019)
95. Intelligent modeling methods for "small sample, multi-modal, cross-scale" oil/gas data with physics-constrained fusion (Reichstein et al., 2019)
96. Real-time monitoring of global tanker fleet capacity and freight rate forecasting based on multi-source data (automatic identification system, satellite remote sensing)
97. Disturbance mechanisms of algorithmic/high-frequency trading on oil futures prices and intelligent regulatory strategies
98. Value composition, ownership, and pricing mechanism of oil/gas data, especially subsurface data
99. Real-time construction and evolution theory of subsurface reservoir digital twins based on data-mechanism fusion (Tao et al., 2019)
100. Paradigm and knowledge system reconstruction from traditional petroleum science to "smart integrated energy science" under the dual drives of carbon neutrality and digitalization

4. Discussion

The 100 grand challenges in petroleum science presented in this paper are not a simple compilation of problems; rather, they constitute a structured map that reflects the internal logic, transitional directions, and knowledge gaps of the discipline. Through systematic analysis and classification of these challenges, several deep-seated characteristics and trends can be identified. The following discussion expands on five aspects: the structural features of the challenges, the dual drivers of disciplinary paradigm, the "meta-role" of AI, the integration of low-carbon transition with classical petroleum science, and the limitations of the list.

4.1. Structural features of the challenges: from "point-like bottlenecks" to "systematic map"

When the 100 challenges are categorized into "mechanisms and theories" (68 items), "technological features" (13 items), and "system-level issues" (19 items), a clear hierarchical structure emerges. Problems of mechanisms and theories form the "foundation" of the entire knowledge system; they answer the fundamental question "why does it happen?". For example, the multi-factor coupling theory of ultra-deep hydrocarbon accumulation (Challenge 1), the occurrence and phase behavior of multi-component crude oil in shale nanopores (Challenge 6), and the unified theory of gas-liquid-solid interfacial transfer in multiphase catalysis (Challenge 51) all attempt to establish new first principles under extreme conditions where classical theories fail. Breakthroughs in these foundational problems have a "multiplier effect"—progress in one basic theory may simultaneously solve several technological challenges.

Technological feature problems occupy the middle layer, focusing more on "how to achieve it given a mechanism". They typically represent engineering limits, such as the limits of high-precision geophysical prediction for ultra-deep reservoirs (Challenge 4), rheology control of drilling fluids under ultra-high temperature and pressure (Challenge 21), and scale-up rules for microreactors (Challenge 60). The solution of such problems heavily depends on advances in mechanisms and theories, but simultaneously poses new constraints and validation scenarios for the latter. For instance, only after the rock physics properties of ultra-deep formations are understood (mechanism) can seismic inversion algorithms be accurately designed (technology); in turn, discrepancies in inversion results feed back to refine the understanding of deep rock physics.

System-level problems reside at the top, dealing with "how to integrate and optimize under complex constraints". These problems often involve multiple agents, scales, and objectives, and cannot be solved by a single mechanism or a single technological breakthrough. For example, the full-chain efficiency of CCUS (Challenge 71), the evolution of global oil and gas supply chain resilience (Challenge 90), and the value and pricing mechanism of oil/gas data (Challenge 98) all require the integration of economic, policy, environmental, technological, and even behavioral factors. Solving system-level problems requires not only mechanistic understanding and technological tools, but also digital instruments and multi-disciplinary collaborative methodologies.

These three types of problems are not isolated; they form a closed loop of "mechanism driving technology, technology supporting systems, and systems feeding back constraints". Traditional petroleum science has often focused on one type (especially mechanism or technology), but in the face of sharply rising complexity, neglecting the feedback relationships among these levels has become a major reason why many studies struggle to achieve breakthroughs. For example, the failure of a digital twin reservoir (Challenge 99) is often not because the modelling algorithm is insufficiently advanced, but because of the lack of embedded micro-mechanisms (insufficient mechanism layer) and the lack of trustworthy data assimilation with real-time information (insufficient system layer). This structural feature suggests that future petroleum science research should pay greater attention to cross-level co-design.

4.2. Dual drivers of disciplinary paradigm: low-carbon transition and artificial intelligence

Through textual analysis and thematic clustering of the 100 challenges, two driving forces can be clearly identified that run through the entire list: low-carbon transition and AI. They are not external add-ons, but endogenous variables that are profoundly rewriting the core problems and research paradigms of petroleum science.

Low-carbon transition is reflected in more than 30 challenges, covering CCUS (Challenges 71–75), geothermal energy (Challenges 76–77), hydrogen energy (Challenges 78–85), biomass and waste plastic conversion (Challenges 58–59), and low-carbon refining (Challenge 55). A common feature of these challenges is that they no longer treat oil and gas resources as isolated extraction objects, but rather embed them in the larger context of the "carbon cycle" and the "energy system". For example, the coupling of CO_2-EOR and geological storage (Challenge 73) requires researchers to pursue both production enhancement and carbon storage (Celia et al., 2015; Rutqvist et al., 2012), fundamentally changing the traditional optimization logic that took economic recovery as the sole objective. Similarly, underground hydrogen storage (Challenges 78–81) redefines depleted reservoirs as energy storage infrastructure rather than abandoned assets (Xiong et al., 2025). This shift in perspective means that petroleum science is moving from "resource extraction science" toward "subsurface space utilization science".

AI penetrates even more widely. Among the 100 challenges, nearly 30 have data, algorithms, or intelligent systems as core keywords, and in many more challenges AI is implicitly relied upon as an enabling method. For instance, intelligent fracturing parameter optimization (Challenge 10) requires real-time data inversion and adaptive control; digital twin modeling of full-chain refining (Challenge 54) needs high-fidelity models and real-time data assimilation (Tao et al., 2019); real-time monitoring of tanker fleet capacity and freight rate forecasting (Challenge 96) needs multi-source data fusion and deep learning. More fundamentally, Challenge 98 (value and pricing mechanism of oil/gas data) and Challenge 99 (real-time construction of digital twins) directly challenge the knowledge production mode and asset form of petroleum science—data are no longer just research materials, but productive factors with independent economic value and legal attributes.

It is worth emphasizing that low-carbon transition and artificial intelligence are not parallel but deeply interactive. Digital tools reduce the cost and risk of implementing low-carbon technologies (e.g., optimizing CCUS storage schemes through digital twins, accelerating novel catalyst screening with AI); conversely, the low-carbon transition provides new application scenarios and data sources for AI (e.g., carbon monitoring data, hydrogen supply chain data). Together they form the "twin engines" of the paradigm transformation in petroleum science.

4.3. The "meta-role" of AI: from tool to epistemology

In traditional petroleum science, digital tools played mainly the role of an "auxiliary tool"—improving data processing efficiency, accelerating numerical simulations, and optimizing production parameters. However, through this systematic review of grand challenges, the role of artificial intelligence can be seen to be undergoing a qualitative change, gradually penetrating into the epistemological level (Karniadakis et al., 2021; Raissi et al., 2019; Reichstein et al., 2019).

First, data-driven approaches are challenging the sole authority of mechanism-driven reasoning. Traditional petroleum science emphasizes causal chains and explainable physical models. But under many extreme conditions (ultra-deep, nano-confinement), complete physical models are lacking or parameters cannot be calibrated. In such cases, machine learning methods can directly learn input-output mappings from data, providing useable predictions even when the intermediate mechanisms are unclear. This “predict first, understand later” mode has already demonstrated value in some challenges (e.g., production decline prediction, Challenge 12; real-time corrosion early warning, Challenge 33). It does not deny the importance of mechanistic studies, but it requires researchers to accept a “dual-track” cognitive style where mechanism and data proceed in parallel.

Second, digital twins are reshaping the ternary relationship of “theory – experiment – field”. The traditional research chain is: theoretical derivation → laboratory experiment → field test → industrial deployment. Digital twins allow high-fidelity simulation in virtual space, so that many “experiments” can be performed digitally, with only a small amount of field data needed to calibrate the models. This mode greatly shortens research and development cycles and reduces safety risks and costs of field tests. Challenge 99 (real-time construction and evolution theory of subsurface digital twins) is precisely a systematic call for this new paradigm.

Third, the explainability crisis of artificial intelligence is forcing the embedding of physical constraints. Black-box models are difficult to gain trust in petroleum engineering because engineers need to know “why the model predicts this way” to make high-risk operational decisions. Hence, the recent rise of physics-informed neural networks (PINNs), differentiable programming, and neural operators represents an attempt to embed physical knowledge (conservation laws, constitutive relations) into algorithmic structures (Karniadakis et al., 2021; Raissi et al., 2019). These “grey-box” models retain the flexibility of data-driven methods while providing partial explainability, representing an important direction for future computational petroleum science. Challenge 94 (cross-scenario generalization of industrial foundation models and trustworthy decision making) and Challenge 95 (intelligent modeling methods for small-sample, multi-modal, cross-scale data) directly address this challenge.

4.4. Integration of low-carbon transition with classical petroleum science: from “addition” to “reconstruction”

The impact of low-carbon transition on petroleum science is not simply adding a few new courses (such as CCUS, hydrogen energy) to the traditional curriculum, but a reconstruction of the discipline's core concepts, value standards, and knowledge system. This is clearly reflected in the 100 challenges (IEA, 2023).

Reconstruction of value standards. The traditional value core of petroleum science is “extract the most oil/gas at the lowest cost”. However, Challenge 88 (reconstructed valuation theory for oil/gas assets under energy transition) shows that the value of oil/gas assets must now account for carbon risk, stranding risk, and compliance cost. An oilfield with huge reserves but high carbon intensity may be worth far less than a smaller but low-carbon field. This shift in value standards will profoundly affect exploration investment decisions, development scheme design, and even capital flows across the industry.

Reconstruction of time scales. Traditional petroleum science focuses on production cycles of years to decades. CCUS and underground hydrogen storage extend the time scale to centuries or even millennia (Challenge 74: long-term safety of CO_2 geological storage). Such ultra-long-term prediction imposes unprecedented demands on model reliability and uncertainty quantification, requiring the gap between “geological time” and “engineering time” to be bridged.

Reconstruction of spatial scales. Traditional petroleum science deals mainly with the reservoir scale and wellbore scale. Low-carbon transition introduces the global scale of the carbon cycle (carbon emission allowance trading, CBAM, etc.) and the molecular scale of CO_2-mineral interfacial reactions. Challenge 89 (simulation of impact pathways of carbon market mechanisms) and Challenge 57 (catalyst design for CO_2 hydrogenation) represent these two extremes. Building traceable, coupled models across different scales becomes a new methodological challenge.

Reconstruction of disciplinary boundaries. The inclusion of CCUS, geothermal, hydrogen, biomass conversion, etc., forces petroleum science to engage with disciplines that were previously distant—geochemistry, thermodynamics, electrochemistry, plant science, and microbiology (Hu et al., 2023; Celia et al., 2015; Middleton et al., 2015; Rutqvist, 2012; Xiong et al., 2025; Zhou et al., 2024; Nath et al., 2024; Lu, 2018; Tester et al., 2006). This cross-disciplinary fusion is both an opportunity and a challenge—it may spawn major original breakthroughs, but it also demands a great deal from researchers' knowledge structures and research organization models.

5. Ten most disruptive grand challenges in petroleum science

Based on a comprehensive assessment across three dimensions—mechanistic and theoretical depth, technological breakthrough difficulty, and system-level impact breadth—the following ten challenges are identified as having the highest transformative potential to reshape the scientific foundation, engineering practice, and industrial landscape of petroleum science.

1). **Multi-factor coupling theory of hydrocarbon accumulation and preservation in ultra-deep formations (>8000 m) (Challenge 1)**

Domain: A. Petroleum Exploration and Development.

Mechanistic disruption: Challenges the applicability of classical trap and basin modeling at depths >8000 m. Requires a new dynamic theory integrating pressure-retarded cracking, mineral-catalyzed hydrocarbon generation, closed-system retention, and multi-field (T-P-fluid-rock) interactions—breaks the traditional “liquid window” concept.

Technological difficulty: Pressure-preserved coring below 10 km, ultra-high-T/P kinetic experiments, coupled diagenesis-accumulation simulations, and quantitative reconstruction of deep fluid-rock reaction networks—extremely high barriers in both measurement and modeling.

System-level impact: Extends effective exploration depth from 8000 m toward 10 000 m, dramatically expanding global hydrocarbon resources; transforms risk assessment for deep basins; gives rise to a new sub-discipline of “deep-Earth petroleum system dynamics”.

2). **Control mechanisms for the survival limit of liquid hydrocarbons and downward extension of the liquid window in ultra-deep formations (Challenge 2)**

Domain: A. Petroleum Exploration and Development.

Mechanistic disruption: Challenges the classic "death line" of the liquid window (150–200 °C). A new kinetic model incorporating ultra-high pressure, mineral catalysis, and closed-system retention is required, potentially rewriting organic geochemistry.

Technological difficulty: Pressure-preserved coring at 10 km depth, ultra-high-temperature high-pressure pyrolysis experiments, and in-situ geochemical analysis are required—extremely high barriers.

System-level impact: If the liquid window extends to 250 °C or deeper, global ultra-deep resource potential multiplies; dozens of "over-mature" basins regain exploration value; the petroleum industry's lifespan extends by 30–50 years, and a new "deep-Earth oil and gas" discipline emerges.

3). **Phase-transition control and proppant transport enhancement mechanisms of supercritical CO_2 water-free fracturing (Challenge 11)**

Domain: A. Petroleum Exploration and Development.

Mechanistic disruption: Reveals the multi-phase (supercritical → gas → liquid → solid) behavior of CO_2 in wellbore-fracture systems and the turbulence-settling coupling mechanism for low-viscosity fluid proppant transport.

Technological difficulty: CO_2-soluble polymeric thickeners, hydrophobically modified lightweight proppants, and adaptive injection schedules based on thermodynamic models are required—major material and engineering challenges.

System-level impact: Enables zero-freshwater fracturing, eliminating water constraints and environmental concerns; turns CCUS from a cost center into a profit center (capture → fracture → EOR → store); applicable to coalbed methane, geothermal, and hydrates.

4). **Surface/interface design of reservoir nano-tracers and inversion of their transport-adsorption-desorption behavior (Challenge 25)**

Domain: A. Petroleum Exploration and Development.

Mechanistic disruption: Reveals the multi-mechanism transport (Brownian diffusion, electrostatic, adsorption) of functionalized nanoparticles in nanoscale pore throats—establishes multiphase, multi-component nano-tracer transport models.

Technological difficulty: Synthesis of low-adsorption, high-stability "smart" nanoparticles (core-shell, temperature-responsive release) and solving high-dimensional ill-posed inversion problems (Bayesian/deep learning) are required.

System-level impact: Achieves "underground CT"—injection of nano-tracers followed by inversion gives pore-scale remaining oil distribution and connectivity, far exceeding geophysical methods; future generations can carry chemical payloads for autonomous treatment—a "smart patrol and therapy system" for reservoirs, revolutionizing characterization and EOR.

5). **Dynamic interaction between artificial and natural fracture networks in EGS (Challenge 76)**

Domain: E. CCUS, Geothermal, Hydrogen and Underground Energy Systems.

Mechanistic disruption: Reveals shear-slip conditions of natural fractures under high-pressure fluid, stress field perturbation, and dynamic network evolution—establishes a quantitative relationship between injection parameters and induced seismicity magnitude (Zhou et al., 2024; Nath et al., 2024; Lu, 2018; Tester et al., 2006).

Technological difficulty: True-triaxial large-scale fracturing experiments, microseismic moment-tensor inversion, and fully coupled 3D geomechanical simulations are required—multi-method cross-validation.

System-level impact: Removes the social-acceptance barrier of induced seismicity, enabling safe commercial EGS; the theory transfers to shale-gas fracturing, CO_2 storage, and deep waste injection—ushering in an era of scientifically controlled high-pressure fluid injection in underground engineering.

6). **Mechanisms of hydrogen geochemical and microbial consumption in depleted reservoir storage and their control (Challenge 78)**

Domain: E. CCUS, Geothermal, Hydrogen and Underground Energy Systems.

Mechanistic disruption: Elucidates the metabolic kinetics and ecological competition of hydrogen-utilizing microbes (methanogens, sulfate-reducing bacteria) under high-temperature, high-pressure, anoxic conditions, and their interaction with reservoir minerals and fluids.

Technological difficulty: Long-term (months) in-situ simulation experiments, metagenomic identification, and safe, economical inhibition strategies (biocides, bacteriophages, pH/salinity adjustment) are required.

System-level impact: Increases the working gas ratio of depleted-reservoir hydrogen storage from <50% to >80%; activates hundreds of thousands of abandoned wells for seasonal renewable energy storage—the decisive step for a commercial hydrogen economy.

7). **Working-fluid selection and phase-change heat transfer limits in ultra-long gravity heat pipes for hot dry rock heat extraction (Challenge 80)**

Domain: E. CCUS, Geothermal, Hydrogen and Underground Energy Systems.

Mechanistic disruption: Develops a unified heat-transfer model for ultra-long (3000–5000 m) two-phase closed heat pipes, covering entrainment, boiling, and capillary limits—pushing the theoretical boundaries of gravity heat pipes.

Technological difficulty: Kilometer-scale segmented test facilities, experiments with different working fluids (water, CO_2, mixtures) under various heat fluxes and inclinations, and solutions for long-term vacuum retention and corrosion are required.

System-level impact: Reduces the levelized cost of hot-dry-rock geothermal electricity to USD 0.05–0.08/kWh, competitive with coal; permits conversion of millions of abandoned wells into geothermal assets; elevates geothermal from a marginal source to a mainstay of clean baseload power.

8). **Real-time monitoring of global tanker fleet capacity and freight rate forecasting based on multi-source data (Challenge 96)**

Domain: F. Energy Economics, Management and Digital Transformation.

Mechanistic disruption: Establishes a quantitative physical-statistical inversion model from satellite imagery (SAR, hyperspectral, thermal) to tank levels and floating-storage draught—the first daily independent inventory monitoring system.

Technological difficulty: Multi-source satellite data fusion, geometric correction of tank shadows, identification of different crude grades, and detection of floating storage are required—major algorithmic and engineering hurdles.

System-level impact: Reduces oil price forecast errors by 30%–50%; exposes and deters market manipulation (e.g., squeezes, hoarding); provides independent intelligence for strategic petroleum reserve decisions—a “God's-eye view” of oil markets.

9). **Value composition, ownership and pricing mechanism of oil/gas data, especially subsurface data (Challenge 98)**

Domain: F. Energy Economics, Management and Digital Transformation.

Mechanistic disruption: Builds a data-valuation model based on information entropy, uncertainty reduction, decision utility, and real options—elevating data from “records” to a “factor of production”.

Technological difficulty: Integration of economics, information theory, blockchain for ownership verification, and secure multi-party computation; design of incentive-compatible trading and revenue-sharing mechanisms are required.

System-level impact: Allows data to be recognized as an independent asset on balance sheets, enabling trading and financing; breaks data silos, fostering “data exchanges” and “algorithm markets”; pressures revision of mining and data-security laws—a cornerstone of digital-era energy governance.

10). **Real-time construction and evolution theory of subsurface reservoir digital twins based on data-mechanism fusion (Challenge 99)**

Domain: F. Energy Economics, Management and Digital Transformation.

Mechanistic disruption: Moves beyond black-box history matching to a “grey-box” paradigm where reduced-order models (POD, neural networks) and ensemble Kalman filtering are combined with differentiable physics-constrained deep learning. Enables closed-loop “predict-assimilate-optimize- act” with real-time data.

Technological difficulty: High-dimensional, highly nonlinear reservoir models; convergence of differentiable PDE solvers; second-scale surrogate predictions; integration of asynchronous multi-source data (pressure, rates, tracers)—major algorithmic and computational challenges.

System-level impact: Transforms reservoir management from offline empirical operation to real-time adaptive optimization, substantially enhancing oil recovery; serves as a blueprint for digital twins in drilling, refining, and CCUS; fundamentally changes how subsurface decisions are made.

These ten challenges span exploration and development (4), geothermal (2), hydrogen (1), and digital transformation with data economy (3), reflecting the full spectrum of petroleum science's transformation toward smart integrated energy systems. Their resolution would fundamentally alter scientific paradigms, technological limits, and the industrial and economic architecture of the energy sector.

6. Limitations of the list and future directions

No list of scientific grand challenges can be fully objective or complete. The present list inevitably carries limitations stemming from both the selection process and the inherent breadth of the discipline. These limitations are openly acknowledged here, and a dynamic, community-driven updating mechanism is proposed to ensure the list remains a living reference.

Limitations of the selection process. Despite systematic literature synthesis, expert consultation, and multi-criteria qualitative assessment, the selection process is subject to inherent constraints. The expert team's knowledge backgrounds, while diverse, cannot cover every emerging frontier with equal depth. Consequently, some forward-looking problems that are currently less recognized—such as the application of quantum computing to petroleum exploration, the impact of novel energy storage materials on oil and gas assets, or the implications of space resources for energy systems—may have been insufficiently covered or inadvertently omitted. Moreover, the six criteria involve subjective judgments that cannot be fully standardized.

Content-based limitations. Beyond methodological boundaries, the list also exhibits content-based gaps.

Geopolitical and social dimensions. The list focuses primarily on natural science and engineering, with relatively less attention to sociological, political, and ethical issues. Yet the uneven global distribution of oil and gas resources, energy justice, community engagement, and employment transitions caused by “stranded assets” profoundly influence the direction of petroleum science. Public acceptance of carbon storage projects and cross-regional coordination of hydrogen infrastructure, for example, require perspectives beyond traditional engineering.

Data sharing and intellectual property. Although Challenge 98 touches on data assetization, the legal obstacles and security concerns in cross-border, cross-company data sharing are not deeply explored. In the context of commercial competition and national security, data silos may persist for a long time. Technologies such as federated learning and secure multi-party computation offer technical solutions, but their institutional implementation remains under-studied.

Talent and education transformation. Challenge 100 points out the paradigm shift of the discipline, but no explicit problem is dedicated to “how to cultivate interdisciplinary talent” or “how to reform the curriculum system”. The talent gap is widely recognized as one of the biggest bottlenecks to digital and low-carbon transformations. Future iterations could add problems such as “the competency composition and training pathways for interdisciplinary talent in petroleum engineering and data science”.

A living list and community updating mechanism. To address these limitations, the present list is offered not as a canonical document but as a living reference framework—open to critique, revision, and continuous improvement. The following updating mechanism is proposed:

Periodic global reassessment. Every five years, Petroleum Science may organize an international reassessment to add, revise, or retire challenges based on technological progress, societal needs, and community feedback.

Open submission and commentary. An online portal can be established, allowing researchers to submit new candidate challenges or comment on existing ones at any time. Submissions will be reviewed by the editorial board and, if suitable, placed on a “to-be-considered” list for the next update.

Challenge status tracking. A public “challenge status tracking” section could be created, labeling which challenges have seen significant progress, which have been partially solved, and which have been superseded or falsified.

7. Conclusions

Based on the “100 Grand Challenges in Petroleum Science” initiative launched by *Petroleum Science* in 2021, and through systematic literature review, expert consultation, and multiple rounds of selection, this paper has proposed a list of 100 fundamental scientific problems that are expected to shape the future of petroleum science. From the classification, analysis, and synthesis of these challenges, the following core conclusions can be drawn.

(1) Petroleum science is undergoing a profound paradigm shift. This shift manifests in three dimensions. Spatially, exploration and development extend from conventional shallow-intermediate depths to ultra-deep (>8000 m), deepwater, and unconventional settings. Temporally, research scales evolve from steady-state, short-term production to transient, long-term (centuries to millennia) processes. Structurally, the objects of study shift from single-phase, single-field systems to strongly coupled multi-phase, multi-field, multi-agent systems. Classical theories and methods face systematic failures under extreme conditions, urgently calling for new scientific frameworks (Jia, 2017; Zou et al., 2013; Blunt et al., 2013).

(2) The 100 grand challenges exhibit a clear hierarchical structure. According to their intrinsic nature, they can be classified into mechanisms and theories (68 items), technological features (13 items), and system-level issues (19 items). Mechanism-oriented problems form the “foundation” of the knowledge system; technology-oriented problems translate mechanisms into engineering practice; system-level problems deal with full-chain integration and multi-objective optimization. The three levels form a closed loop of “mechanism drives technology, technology supports systems, systems feed back constraints”. This structure reveals the intrinsic knowledge-production logic of petroleum science and provides a scientific basis for prioritizing future research efforts.

(3) AI has become a core driving force. More than 30% of the challenges rely on data, algorithms, or intelligent systems as key solution pathways. AI has evolved from an auxiliary tool into a “meta-role” at the methodological level, changing the cognitive style of petroleum science (convergence of data-driven and mechanism-driven approaches), the research chain (digital twins reshaping the “theory-experiment-field” ternary relationship), and value standards (data becoming an independent factor of production) (Tao et al., 2019; Karniadakis et al., 2021; Raissi et al., 2019; Reichstein et al., 2019). “Grey-box” methods such as physics-informed neural networks, differentiable programming, and neural operators represent important directions for future computational petroleum science.

(4) Low-carbon transition and artificial intelligence constitute the twin engines of the paradigm shift. The low-carbon transition (CCUS, hydrogen, geothermal, biomass, etc.) opens new problem domains for petroleum science and reconstructs its value standards, time scales, spatial scales, and disciplinary boundaries (Celia et al., 2015; Middleton et al., 2015; Rutqvist, 2012; Xiong et al., 2025; IEA, 2023). AI provides enabling tools for implementing low-carbon technologies, and a positive feedback loop exists between them: digitalization reduces the cost and risk of low-carbon technologies, while low-carbon demand creates new scenarios for AI. This twin-engine pattern is fully reflected in the grand challenges list.

(5) Petroleum science is moving from “resource extraction science” toward “smart integrated energy science”. Challenge 100 clearly states that, under the dual drives of carbon neutrality and digitalization, the identity and mission of the discipline are undergoing a fundamental change. Future petroleum science will no longer be confined to the exploration, development, transport, refining, and utilization of hydrocarbon resources, but will expand into a comprehensive system encompassing subsurface space utilization (energy storage, waste disposal, carbon sequestration), multi-energy coupling (oil-gas-hydrogen-electricity-heat), carbon cycle management, and intelligent decision-making. This transformation demands a systemic reconstruction of knowledge systems, educational models, and research organization.

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Appendix A. Supplementary data

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