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Journal of Prime Research in Mathematics, 2026, 41–52

Journal of Prime Research in Mathematics

Mathematical Modelling in Petroleum Exploration and Prospect Generation: An Integrated Review of Quantitative and Computational Methods

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Abstract

Petroleum exploration is becoming more difficult and more capital-intensive as conventional basins mature and the remaining targets grow structurally and stratigraphically subtler. Persistently low exploration success rates have made formal quantitative methods central to reducing pre-drill uncertainty. This paper reviews the principal mathematical and computational modelling approaches applied across the exploration and prospect generation workflow. Although individual techniques are well documented in the literature, they have rarely been assessed together as a coherent, integrated framework spanning the full workflow, and this review addresses that gap. The methods are organized around the petroleum systems concept and grouped into three areas. The first covers mathematical and statistical modelling, including basin modelling and thermal maturity assessment through kinetic models such as EASY%Ro, probabilistic volumetric estimation based on Monte Carlo simulation, and Bayesian risk analysis, together with geostatistical techniques spanning variogram analysis, kriging, and sequential Gaussian simulation. The second examines GIS-based prospectivity mapping through play fairway analysis (PFA) and common risk segment (CRS) methods, alongside the expanding role of machine learning (ML) and deep learning in seismic interpretation, facies classification, and spatial risk prediction. The third evaluates the limitations shared across these methods, including data sparsity, model non-uniqueness, validation constraints, and the limited transferability of data-driven models between geological settings. The review finds that the integration of physics-based process modelling with data-driven analytics, increasingly enabled by digital twin and hybrid modelling concepts, offers the most defensible path toward more reliable and auditable exploration decisions.

Keywords: Petroleum exploration, Prospect generation, Petroleum systems modelling, Geostatistics, GIS prospectivity, Machine learning, Exploration risk assessment.

2010 Mathematics Subject Classification: 62P10, 62H11, 68T05, 86A15

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Received : 25 May 2026*; Accepted:* 18 June 2026*; Published Online:* 05 August 2026

1. Introduction

Petroleum exploration has always meant deciding under uncertainty. What's changed is the scale of that uncertainty over the past two decades. The remaining inventory of conventional prospects is structurally more complex, stratigraphically subtler, and operationally more expensive to test than it has ever been. Easy oil, the kind sitting in large anticlinal closures with a strong seismic expression, has largely been found. What's left tends to be deeper, smaller, or harder to image.

Exploration success rates have stayed stubbornly low. Ren et al. (2023) report that PetroChina, drilling thousands of new exploratory wells every year since 1980, has averaged a technical success rate of just 42.6% [33]. Milkov [27] documents a broader pattern: explorers consistently overestimate their pre-drill probability of success. Empirical success-versus-failure analyses by Peel and Brooks [30] echo the same finding. The conclusion is hard to avoid. Geological intuition, however experienced, isn't enough to consistently guide high-cost exploration decisions. It has to be supported, constrained, and tested by formal quantitative methods [27, 30].

The mathematical modelling reviewed in this paper isn't a single technique. It's a multi-disciplinary framework that draws on deterministic basin physics, stochastic simulation, spatial statistics, probabilistic inference, and machine intelligence. What connects these methods is the petroleum system, the concept, formalized by Magoon and Dow (1994) and applied across all the studies reviewed here [11, 2, 10], that requires source rock, reservoir, seal, trap, and correct timing to be present before any commercial accumulation can form. Every modelling approach considered here is, ultimately, an effort to quantify the probability that one or more of those elements is present, effective, and correctly positioned in space and time. The standard language for expressing that probability, the P10/P50/P90 framework used in Monte Carlo volumetrics and prospect risking [21, 41, 29], provides the common output currency that links subsurface analysis to management decisions.

This review covers the methods most directly relevant to exploration and prospect generation. That's the analytical work done before any development decision gets made. Our focus sits on basin modelling and thermal maturity assessment through kinetic models like EASY%Ro and TTI [37, 19], probabilistic and Bayesian approaches to prospect risk and sequential drilling optimization [27, 26], geostatistical property estimation through variogram analysis, kriging, and sequential Gaussian simulation [14, 9], GIS-based play fairway and spatial prospectivity analysis [5], and machine learning and deep learning for seismic fault detection, facies classification, and risk prediction [6, 38, 36].

We deliberately leave out reservoir simulation, production forecasting, history matching, and field development optimization. Each is a substantial field on its own, with a different decision context. The emerging concept of the digital twin gets attention too, as a possible integration platform that couples physics-based and data-driven models inside a single operational framework [34].

This review addresses a gap that's been quietly widening in the exploration literature. Individual modelling techniques have been well documented in isolation. But there's been comparatively little effort to evaluate them as a coherent, integrated framework applicable across the full prospect generation workflow. We argue here that the real value of quantitative modelling in exploration isn't in any single method but in how these tools connect, basin physics informing charge, geostatistics characterizing reservoir uncertainty, probabilistic analysis carrying risk through to a drillable prospect, and machine learning accelerating interpretation where data volumes exceed human capacity. The aim throughout is not to survey techniques for their own sake, but to show how, when applied together within a petroleum systems context, they form a genuinely practical and intellectually defensible approach to one of the most consequential decisions in the energy industry: where to drill.

2. Fundamentals of Petroleum Prospect Generation

Every exploration programme is organized around the petroleum system. That's the framework linking the geological processes needed to create a commercial hydrocarbon accumulation [17]. In its classical formulation, the system depends on five essential elements:

1. A source rock with enough organic richness to generate and expel hydrocarbons.
2. A reservoir with adequate porosity and permeability to store them.
3. A seal with sufficient integrity to retain the trapped fluids.
4. A trap geometry that physically focuses and holds the charge.
5. A migration pathway connecting the source to the reservoir.

None of these elements can compensate for another missing one. Source rock quality gets characterized by total organic carbon (TOC) and thermal maturity, which is expressed as vitrinite reflectance (Ro%). Oil generation typically happens within a maturation window of about 0.6 to 1.3% Ro. Expulsion temperatures run between roughly 120 and 150°C in most basins [24].

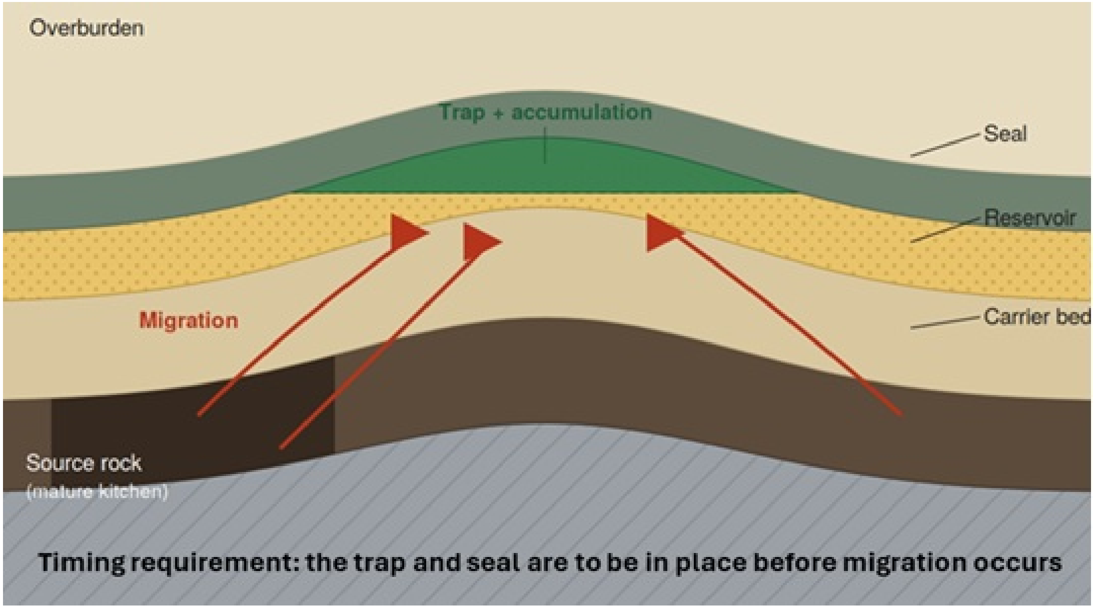

Figure 1: Schematic of the petroleum system showing the required essential elements for a commercial accumulation.

Timing is the critical sixth dimension. The trap has to be in place and sealed right when migration happens. If it isn't, the charge disperses and no accumulation forms. This is more than a theoretical concern. Fluid inclusion evidence from the Bight Basin, Australia, identified multiple discrete palaeo-hydrocarbon migration phases spanning from the Late Cretaceous through to the Miocene, demonstrating that timing constraints are real, resolvable, and consequential even in frontier settings [4]. Migration itself introduces further complexity: losses along the pathway, phase fractionation during upward fluid movement, and lag effects from continued cracking of retained source-rock fluids all modify the volume and composition of hydrocarbons reaching the trap, sometimes well after the source kitchen has left its main generation window [12]. These realities explain why timing is typically embedded within the migration and trap probability assessments as a conditional modifier rather than treated as a standalone multiplicative risk factor.

Trap style also dictates which mathematical tools you reach for downstream. Structural traps, anticlines, fault blocks, and salt-cored domes can be mapped straight from seismic data. From there, the volumes can be deterministically estimated using closure geometry and the spill point. Stratigraphic traps are a different matter. They're defined by depositional or diagenetic processes, which means they carry spatial uncertainties that seismic data can't resolve directly. To evaluate them, you need probabilistic facies modelling and stochastic simulation [27]. That distinction really matters if the wrong analytical approach was picked for the trap type, as this will introduce avoidable errors in both resource estimation and risk assessment.

The geological chance of success (COS), sometimes called the probability of geological success (PGS), is the probability that all five elements are present and effective at the same spot. Standard practice treats the total COS as a serial product, assessing independent probabilities for source, reservoir, seal, and trap or migration, and multiplying them [27, 29]. The count of factors isn't fixed; published frameworks run from four to nineteen, depending on how finely you break the system down [27]. The governing logic doesn't change, and the product can't exceed its smallest input, which directs analytical attention straight at the weakest link.

COS assessment works at two related scales. Play level comes first, where geoscientists evaluate petroleum system viability across a regionally defined play fairway. That's a spatially bounded risk envelope inside a basin where a coherent set of geological conditions is expected to prevail. Regional evaluation sets prior element probabilities before any specific drilling target gets committed [30]. Then comes the prospect level, where everything narrows to a specific drillable location and the probabilities are sharpened using local well control, seismic attributes, and geochemical observations [29]. A low play-level probability for any element imposes a hard ceiling that no amount of favorable local evidence can lift.

That hierarchy is precisely why mathematical tools are not supplementary but necessary. Each new dataset, whether a seismic survey, a geochemical programme, or a well result, should update one or more element probabilities and move the COS toward a more defensible and polarized estimate. Without a structured quantitative framework, exploration decisions revert to intuition, which has been shown to be inconsistent even among experienced geoscientists working from identical data [27]. The objective is not to eliminate uncertainty, which remains irreducible at the predrill stage, but to make it explicit, auditable, and communicable across every discipline that must together commit capital to the well.

3. Mathematical and Statistical Modelling in Petroleum Exploration

The shift from qualitative geological interpretation to rigorous quantitative analysis is one of the defining developments in modern petroleum geoscience. Mathematical and statistical methods are now central to every phase of the exploration workflow, from reconstructing a basin's thermal history to constraining porosity distribution between wells.

3.1. Basin Modelling and Thermal Maturity Assessment

A one-dimensional basin model reconstructs the burial history of a sedimentary sequence, along with how heat flow and temperature evolved over time. That's the thermal framework all source rock maturity assessments rest on. Without it, predicting whether hydrocarbons were ever generated is just guesswork.

The math at the heart of maturity analysis is the time-temperature index, or TTI. Lopatin introduced the concept, and Waples later calibrated it [37]. The idea is straightforward. Reaction rates in organic matter roughly double for every 10°C rise in temperature. It's essentially an Arrhenius-type relationship. The TTI integrates this over geological time:

$$\mathrm{TTI} = \sum \left(\Delta t_n \times 2^{\frac{T_n - 105}{10}} \right) \tag{3.1}$$

where Δt_n is the duration in million years for interval n, and T_n is that interval's mean temperature in °C. The reference point of 105°C is the midpoint of the 100–110°C base interval ($n = 0$).

Waples [37] calibrated threshold values that are still in routine use: oil generation starts at TTI ≈ 15, peaks at TTI ≈ 75, and ends at TTI ≈ 160. Higher values mark gas preservation windows. These thresholds correlate with vitrinite reflectance ($Ro\%$), kerogen H/C ratios, and thermal alteration indices across a range of geological settings [37]. The method has real limitations. Its fixed doubling-rate assumption oversimplifies the Arrhenius relationship. Predictions can diverge from measured $Ro\%$ at high maturity, or in basins with multiperiodic thermal histories [19, 28].

The Easy%Ro model of Sweeney and Burnham [35] tackles this problem. It treats vitrinite maturation as parallel first-order Arrhenius reactions, each with distinct activation energies, and integrates the full temperature history continuously. Kang et al. [19] showed its advantage in rifting basins, where TTI can't resolve the varying sensitivity of Ro to heating time versus geothermal gradient. Nielsen et al. [28] found that even Easy%Ro can overestimate Ro% by up to 0.35% in the 0.5–1.7% range, which makes borehole calibration essential.

When 1D models extend to 2D and 3D, hydrocarbon migration is governed by Darcy's law:

$$q = -\frac{k}{\mu}\nabla P \tag{3.2}$$

where q is the Darcy flux (m/s), k is permeability (m^2), μ is fluid viscosity ($\mathrm{Pa}\cdot\mathrm{s}$), and ∇P is the pressure gradient (Pa/m) driving flow from high to low pressure. This principle is applied to modern coupled wellbore-reservoir frameworks to combine wellbore physics with reservoir flow [32].

Badejo et al. [2] applied 3D petroleum systems modelling in the Central North Sea. The team combined multiphase Darcy flow with invasion percolation to trace migration from the Kimmeridge Clay into Tertiary Tay sandstones. Overpressure, faulting geometry, and salt diapirs were all shown to modify migration pathways, and the model identified two previously unrecognized prospects. Commercial platforms like PetroMod automate this workflow, integrating burial history, heat flow, source rock kinetics, and fluid migration into a calibrated model [2].

3.2. Probabilistic and Statistical Methods

Basin modelling gives a pretty clear, deterministic picture of the charge and thermal history. However, the volumetric unknowns that follow are governed by uncertainty, not physics, which is where probabilistic methods take over. The inputs to volumetric calculations all carry irreducible predrill uncertainty, including gross rock volume, net-to-gross, porosity, water saturation, and fluid expansion factors. Treating any of them as fixed creates false precision. Monte Carlo simulation propagates this uncertainty by assigning probability distributions to each input and sampling thousands of times. The result is a full distribution of hydrocarbon volume [41]. This operates on the standard volumetric equations:

$$\mathrm{STOIIP} = \mathrm{GRV} \times \mathrm{NG} \times \phi \times \frac{1 - S_w}{B_{oi}} \tag{3.3}$$

$$\mathrm{GIIP} = \mathrm{GRV} \times \mathrm{NG} \times \phi \times \frac{1 - S_w}{B_{gi}} \tag{3.4}$$

where GRV is the gross rock volume, NG is net-to-gross (fraction), ϕ is porosity (fraction), and S_w is water saturation (fraction). B_{oi} is the oil formation volume factor (reservoir bbl/stock tank bbl), and B_{gi} is the gas formation volume factor.

All parameters are treated as stochastic. Zhao et al. [41] applied this to the S oilfield in offshore Malaysia. Monte Carlo delivered credible estimates from sparse predrill data. Sensitivity analysis found net-to-gross accounted for 39.6% of STOIIP variance, pointing to where data acquisition effort matters most [41]. A Justine et al. [18] study of the Rio Del Rey basin in Cameroon used Monte Carlo to refine STOIIP and GIIP estimates across nine wells. The probabilistic results were more defensible than single deterministic calculations.

Results are reported using the P10/P50/P90 convention. P90 is the volume exceeded with 90% probability, the low case. P50 is the median. P10 is the high case (10% probability). Al-Mudhafar et al. [1] drew these boundaries from ensemble geostatistical realizations. They used them for development planning and carbon storage assessment at the Luhais oil field, Iraq.

Bayesian inference provides a complementary framework for prospect risk, formally updating prior probability estimates as new evidence arrives:

$$P(H|E) = \frac{P(E|H) \times P(H)}{P(E)} \tag{3.5}$$

where H is the geological hypothesis (e.g., a commercial accumulation exists), and E is observed evidence. $P(H)$ is the prior probability, $P(E|H)$ is the likelihood of E given H, and $P(E)$ is the marginal probability of the evidence.

Guo et al. [10] applied a Bayesian network classifier to the Sangonghe Formation, Junggar Basin. They integrated source rock quality, reservoir depth, trap geometry, and sedimentary facies to predict hydrocarbon occurrence across 12,951 grid units. The model achieved 85.2% accuracy on 203 exploratory wells. Ren et al. [33] extended this with a k-dependence Bayesian network classifier (SKDB). SKDB captures richer dependency structures between geological variables, improving accuracy by 3.55–7.63%.

Regression analysis builds empirical subsurface relationships from well data. Li et al. [23] evaluated eight models for porosity prediction from well logs. Kernel ridge regression and piecewise ridge regression consistently outperformed standard linear approaches in datasets affected by multicollinearity. At the Volve offshore field, Ilyushin and Nosova [15] compared Random Forest to Lasso regression. Random Forest performed better for production rate forecasting. Lawal et al. [22] reviewed the broader shift from multiple linear regression to machine learning-based methods for porosity and permeability prediction from well logs, reflecting the growing role of data-driven approaches in exploration-stage characterization.

3.3. Geostatistical Methods in Subsurface Characterization

Porosity, permeability, and net sand thickness all vary continuously in three-dimensional space, yet they can be sampled only at well locations. Getting from those point measurements to a spatially continuous reservoir description is the central challenge of subsurface characterization, and geostatistics is how it's done.

The variogram quantifies spatial autocorrelation by measuring how dissimilarity between sample pairs changes with separation distance:

$$\gamma(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} \left[Z(x_i) - Z(x_i + h)\right]^2 \tag{3.6}$$

where h is the lag distance, $N(h)$ is the number of pairs at that separation, and $Z(x_i)$ is the property value at location x_i. Three parameters define the fitted model: the range, beyond which values are no longer spatially correlated, reflecting the geological heterogeneity scale; the sill, capturing the total variance; and the nugget effect, which picks up measurement noise below the sampling resolution [9].

Variography of the Shurijeh-B reservoir identified N75W as the principal continuity direction and N15E as the minor direction for both porosity and permeability, directly shaping flow pathway representation [14]. Variograms were similarly applied across 24 sand layers of the Ss reservoir in China before property modelling began [39].

Ordinary kriging uses the variogram to produce the best linear unbiased estimator (BLUE) at any unsampled location:

$$Z^*(x_0) = \sum \lambda_i Z(x_i), \quad \text{subject to } \sum \lambda_i = 1 \tag{3.7}$$

where $Z^*(x_0)$ is the estimate at x_0, $Z(x_i)$ are neighboring measured values, and λ_i are kriging weights from the variogram system. The unbiasedness constraint prevents systematic bias, and the simultaneously produced kriging variance map quantifies estimation uncertainty, identifying where new data would most help [9, 1].

Kriged outputs are smoothed, though, suppressing between-point variability and making them unsuitable as the sole input to flow simulation. Sequential Gaussian Simulation (SGS) resolves this by generating multiple equiprobable stochastic realizations, each honouring the conditioning data and reproducing the variogram's spatial structure. Al-Mudhafar et al. [1] generated 50 realizations of lithofacies, porosity, and permeability for the Luhais oil field, Iraq, running dynamic history matching on all 50 to identify the optimal model for production forecasting. The ensemble captures spatial uncertainty and feeds directly into P10/P50/P90 volumetric calculations.

Falade et al. [8] applied SGS and indicator simulation to the Falad field, Niger Delta, where stochastic property distributions combined with structural maps identified prospective intervals in data-sparse areas. Where seismic data are available, cokriging and collocated cosimulation workflows use seismic impedance or amplitude to constrain geostatistical interpolation between wells at a resolution far exceeding well spacing.

Collocated co-kriging approximates a target property, such as porosity from the dense coverage of a secondary variable, making full use of both data sources [1]. These outputs feed into volumetric estimation, flow simulation, and risk-adjusted prospect ranking.

4. GIS, Spatial Prospectivity Modelling, and Machine Learning

4.1. GIS-Based Hydrocarbon Prospectivity Mapping

Geographic Information Systems (GIS) are the standard spatial integration platform in petroleum exploration. Geological, geophysical, geochemical, and remote sensing data layers can be brought together, weighted, and queried across a basin or play fairway at the same time. What you get is a composite prospectivity map that is inherently multi-evidential, capable of ranking and prioritizing acreage in ways no single dataset manages alone [11, 5].

Play fairway analysis puts a structured, repeatable workflow around this. Each critical petroleum system element gets mapped as a discrete evidence layer: source rock presence and maturity, reservoir facies distribution, seal integrity, and trap geometry. Every evidence layer comes paired with a confidence layer reflecting how reliable and spatially complete the underlying data really is. DeAngelo et al. [5] describe a well-developed GIS-based PFA framework where evidence and confidence layers are multiplied to produce risk layers for individual system components. Those are then aggregated, using a weighted sum, into Common Risk Segment (CRS) maps. These component maps are combined into a Composite CRS map that quantifies the joint favorability of conditions across the study area. The generalized weighted overlay prospectivity index is:

$$\mathrm{PI} = \sum_{i=1}^{n} w_i \times E_i \times C_i \tag{4.1}$$

where PI is the prospectivity index at each spatial pixel, w_i is the normalized criterion weight, E_i is the normalized evidence score, and C_i is the spatial confidence of that evidence.

Criterion weights get assigned through Multi-Criteria Decision Analysis (MCDA) frameworks, using expert elicitation or data-driven optimization. Hamzeh and Karimipour [11] demonstrate a sophisticated MCDA application in the Red River petroleum system of the Canadian Williston Basin using an optimized fuzzy PROMETHEE outranking approach. Eight petroleum system criteria are integrated: TOC, T-max, hydrogen index, source, reservoir, and cap rock thicknesses. Each is encoded as a triangular fuzzy number to accommodate the imprecision built into expert-assigned weights. Criterion weights are then refined using the cuckoo search (CS) metaheuristic algorithm to maximize spatial correspondence with known oil pool locations. The optimized model substantially outperformed non-optimized expert weights in predicting pool distribution, confirming the predictive value of GIS-MCDA workflows and the practical importance of rigorous weight calibration [11].

In frontier settings where seismic coverage is limited, gravity and magnetic data take on a bigger role, supporting basin delineation, basement depth estimation, and structural high identification [5]. Remote sensing provides low-cost reconnaissance inputs. Satellite synthetic aperture radar (SAR) imagery can detect surface hydrocarbon seeps through spectral anomalies. Multispectral analysis identifies near-surface clay mineralogy changes and geochemical alteration halos linked to vertical migration pathways [2]. Both data types work as useful first-order GIS inputs in frontier and deepwater environments where conventional subsurface data are sparse.

GIS prospectivity maps carry a clear limitation: their quality is entirely bound by the quality of the input layers and the validity of the assumptions embedded in the weighting scheme. A poorly constrained weight for a critical criterion can distort the resulting prospectivity surface in ways that don't announce themselves in the final map [11]. These outputs are relative ranking and prioritization tools for allocating exploration effort; they are not absolute probability of discovery assessments and do not substitute for geological judgement at the prospect scale [27].

4.2. Machine Learning and AI in Petroleum Exploration

Machine learning, a branch of artificial intelligence (AI), is a pattern-recognition approach, not a process-simulation approach. It does not model the physical processes that generated a petroleum system; it learns the statistical relationships from labeled training examples and applies those relationships to new data. In petroleum exploration, its strongest contribution is processing large, high-dimensional datasets where human interpretation becomes intractable at scale, particularly 3D seismic volumes [6, 40]. The consistent message across the literature is that ML performs best alongside physics-based models and domain expertise, not in place of them.

It helps to separate the three learning settings that recur across these applications:

- **Supervised learning** trains on labelled examples where each input (a log interval or a seismic patch) is paired with a known output class. Most of the facies and lithology classifiers operate this way.
- **Semi-supervised learning** trains on a small set of labelled data plus a vast amount of unlabeled data, which suits exploration settings where labels are scarce but raw seismic is abundant.
- **Transfer learning** takes a model already trained in a data-rich setting and adapts it to a new, data-poor target with limited relabeling [6].

The distinction matters in frontier exploration, where labelled well control is usually the binding constraint.

Artificial Neural Networks (ANNs) with feed-forward architectures are widely used for petrofacies classification and seismic facies interpretation. In a supervised training workflow, labelled wireline log intervals combining gamma ray, resistivity, bulk density (RHOB), and neutron porosity (NPHI) serve as training examples, and the network learns the multivariate log signature of each facies class. The trained model is then applied to predict facies along uncored wells or spatially across seismic attribute grids. ANN-based models have demonstrated consistently strong predictive performance for water saturation, porosity, and lithology across carbonate and clastic reservoir settings [3]. The practical constraint in frontier exploration is training data scarcity: with only a small number of wells penetrating the prospective section, the network's ability to generalize to unseen geological variability is inherently limited.

Support Vector Machines (SVMs) and Random Forest (RF) classifiers tackle similar problems, including lithology prediction and reservoir quality characterization from wireline log suites. SVMs find optimal class boundaries in high-dimensional seismic attribute space and have been applied to fault detection. Correlation and cluster analysis help select the most discriminatory attribute inputs [20]. RF's practical edge comes from its ensemble structure. It aggregates predictions across hundreds of decision trees, each trained on a random data subset, returning a class label plus an inherent uncertainty estimate from the variance of tree outputs [6, 3]. That built-in uncertainty matters in prospect evaluation, as it quantifies the epistemic component of prediction uncertainty—the part reducible with more data—which is central to responsible risk assessment [31].

The application of Convolutional Neural Networks (CNNs) to 3D seismic volumes is the most significant ML development in seismic interpretation. CNNs learn hierarchical spatial features straight from raw seismic amplitude or attribute cubes through their convolutional filter layers, with no manually preselected attributes required. This opens up automated horizon picking, fault and fracture delineation, and salt body detection at the basin scale [40, 20].

Wu et al. [38] provide a clear published benchmark for fault segmentation. They trained a simplified U-Net architecture on 200 automatically generated synthetic seismic fault volume pairs. Folding, faulting geometry, wavelet peak frequencies, and noise level were all randomly parameterized. Training stayed entirely synthetic; despite that, the model transferred accurately to real field datasets from several independent surveys. It also outperformed every conventional coherence and attribute-based method on precision, recall, and receiver operating characteristic metrics. The computational advantage is striking: the trained CNN processed a $450 \times 1,950 \times 1,200$ sample volume in under three minutes on a single GPU. Conventional fault likelihood computation took roughly 1.5 hours on a 32-core CPU cluster [38]. For salt body delineation, CNN-based pixel-wise segmentation from raw seismic amplitude outperforms multi-attribute SVM approaches, especially in zones of weak reflectivity and structurally complex geometry [20].

The most persistent challenge for ML in exploration, unlike production settings, is the scarcity of labelled training data. Producing fields offer years of well histories, 4D seismic, and dense petrophysical logs, whereas frontier settings have almost none of this. Dramsch [6] flags two active directions targeting this gap: transfer learning and semi-supervised approaches. Wu et al. [38]'s synthetic data strategy provides a practical workaround for structural interpretation tasks, where geologically realistic volumes can be generated automatically.

The clearest path forward for ML in petroleum exploration is integration within probabilistic and geostatistical workflows, not standalone deployment. Take CNN-derived facies classifications: these can serve as soft conditioning inputs in sequential indicator co-simulation, constraining spatial facies geometries beyond well control while preserving formal uncertainty distributions [38]. This hybrid modelling approach combines data-driven pattern recognition with physics-informed modelling and probabilistic uncertainty quantification, representing the current best practice for ML-assisted prospect generation [40, 3].

5. Challenges, Limitations, and Future Directions

No mathematical model, however sophisticated, fully escapes the data problem that runs through all subsurface work. Seismic data is inherently bandwidth-limited, with low signal-to-noise ratios that demand heavy processing before any geological interpretation can begin [7]. Borehole sampling covers only a tiny fraction of any basin, and extrapolating from well observations introduces assumptions that are rarely made explicit. Underpinning all of this is the non-uniqueness of geophysical inverse problems: distinct subsurface configurations can produce observationally indistinguishable results, making the path from data to model inherently ill-posed [13]. These uncertainties don't sit in isolation. Errors in seismic interpretation propagate into structural models, which shape facies distributions, which constrain volumetric estimates. No single technique in the current toolkit fully resolves this cascade, and practitioners who treat any one model output as authoritative do so at their own risk.

Computational complexity makes all this tougher in practice. Generating the ensemble of realizations needed for meaningful uncertainty quantification is expensive, and the cost grows fast with model resolution and areal extent. Simulating flow in geologically realistic subsurface models often means discretized grids with hundreds of millions to over a billion cells [16]. Even with modern high-performance computing and multiscale solvers, there's a real tension between resolution that honors geological detail, spatial coverage that captures basin-scale controls, and a run time the exploration project schedule can realistically accommodate. The SAIGUP study made this concrete: building and simulating over 35,000 full-field reservoir models to characterize geological uncertainty consumed more than 23 CPU years of computation, and that was on relatively simple synthetic geometries [25]. In most operational settings, that level of ensemble coverage simply isn't feasible.

Model validation is a structural challenge unique to exploration, and it's one the discipline hasn't solved. In reservoir engineering, production history gives an iterative calibration loop, so a model that doesn't reproduce observed pressures or flow rates gets corrected. Exploration models don't have that feedback. The subsurface stays inaccessible until a well is drilled, meaning validation happens at the drill bit—often years after the model was finalized. Hoffimann et al. [13] document a real exploration case where a conceptual geological model built from 2D seismic and regional analogues turned out to be fundamentally wrong. Production wells drilled in 2015 penetrated far less reservoir thickness than expected, requiring reserves to be revised significantly down. The probabilistic framework they propose helps shorten this feedback loop by updating scenario probabilities as new data arrive, but the core problem doesn't go away: in exploration, ground truth arrives late and at real cost [13].

Geological heterogeneity adds another layer that no current modelling framework fully handles. Sedimentary and structural systems operate across scales, from lamination to basin architecture. Manzocchi et al. [25] showed that heterogeneity at all levels—lamina-scale permeability, fault density, and diagenetic cementation—influences recovery in ways that resist simple ranking or isolation. The choice of model resolution is always a defensible compromise, never an objectively correct answer [25].

Looking ahead, several directions stand out as genuinely consequential. The first is big data integration. Major operators are already combining seismic, well, satellite, and production streams at cloud scale using digital twin frameworks. Real-time model updating during drilling is also gaining traction, utilizing measurement-while-drilling (MWD) and logging-while-drilling (LWD) data. Digital twin technology can now compare downhole measurements against pre-drill simulations and flag discrepancies in near-real time [34].

Hybrid, physics-informed AI is the direction that most directly targets these architectural limits. Conventional ML learns statistical associations from data alone, so it can predict well inside its training distribution and fail without warning outside it. Physics-informed models constrain the learning so that predictions respect known physical relationships—the governing flow equations, mass balance, or rock-physics behavior—rather than fitting data in isolation. The payoff for exploration is twofold: the model needs fewer labelled examples to generalize, and its outputs stay physically plausible where data is sparse. That is exactly the frontier condition. Complex-valued neural networks are one concrete example, since they preserve the phase information in seismic data more efficiently than standard real-valued networks [7]. Coupled with the broader move toward embedding ML inside physics-based process models rather than replacing them [40, 3], this hybrid approach is the most credible route to exploration models that are both data-efficient and physically grounded.

6. Conclusion

The mathematical and computational approaches in petroleum exploration work best as parts of a single quantitative framework, not a collection of standalone tools. Each method answers a different question. Basin modelling and thermal maturity assessment, through indices such as TTI and kinetic models such as EASY%Ro, reconstruct whether and when a source rock generated and expelled hydrocarbons. Probabilistic volumetrics, built on Monte Carlo simulation paired with Bayesian risk analysis, change the game by taking uncertain inputs and turning them into defensible estimates (P10, P50, P90). As new evidence rolls in, they keep updating prospect risk. Geostatistical methods, from variogram analysis and kriging to sequential Gaussian simulation, describe how reservoir properties vary in space where well control is thin. GIS-based play fairway and prospectivity mapping combine geological, geochemical, and geophysical layers into ranked, mappable targets. Machine learning and deep learning scale all this up to seismic volumes and log datasets that are simply too large for manual interpretation. Convolutional networks now match or beat conventional methods for fault and salt detection.

However, none of these methods is sufficient on its own. Each has real limits: data is sparse and noisy, geological heterogeneity spans multiple structural scales, and you cannot validate an exploration model until you actually drill a well. Recognizing those limits is part of using the methods well. Built around the petroleum systems concept, the methods together cover the uncertainty that exploration teams actually face. They do not remove that uncertainty; what they do is make it explicit, auditable, and open to revision when the drill bit tests the prediction. Looking ahead, the integration of physics-based process modelling with data-driven AI, increasingly delivered through hybrid and digital twin frameworks, is the most promising path toward exploration models that are both flexible and grounded in physical reality.

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